Activity Report 2018

Section Software

<p style="text-align:center">**ABS Project-Team**</p>

4. New Software and Platforms

4.1. SBL

Structural Bioinformatics Library

KEYWORDS: Structural Biology - Biophysics - Software architecture

FUNCTIONAL DESCRIPTION: The SBL is a generic C++/python cross-platform software library targeting complex problems in structural bioinformatics. Its tenet is based on a modular design offering a rich and versatile framework allowing the development of novel applications requiring well specified complex operations, without compromising robustness and performances.

More specifically, the SBL involves four software components (1-4 thereafter). For end-users, the SBL provides ready to use, state-of-the-art (1) applications to handle molecular models defined by unions of balls, to deal with molecular flexibility, to model macro-molecular assemblies. These applications can also be combined to tackle integrated analysis problems. For developers, the SBL provides a broad C++ toolbox with modular design, involving core (2) algorithms, (3) biophysical models, and (4) modules, the latter being especially suited to develop novel applications. The SBL comes with a thorough documentation consisting of user and reference manuals, and a bugzilla platform to handle community feedback.

RELEASE FUNCTIONAL DESCRIPTION: In 2018, major efforts targeted two points. First, the simplification of installation procedures – now possible with conda/python. Second, the development of packages revolving on molecular flexibility at large: representations in internal and Cartesian coordinates, generic representation of molecular mechanics force fields (and computation of gradients), exploration algorithms for conformational spaces.

- Contact: Frédéric Cazals
- Publication: The Structural Bioinformatics Library: modeling in biomolecular science and beyond
- URL: https://sbl.inria.fr/

BEAGLE Project-Team

6. New Software and Platforms

6.1. aevol

Artificial Evolution

KEYWORDS: Bioinformatics - Genomics - Evolution

FUNCTIONAL DESCRIPTION: Aevol is a digital genetics model: populations of digital organisms are subjected to a process of selection and variation, which creates a Darwinian dynamics. By modifying the characteristics of selection (e.g. population size, type of environment, environmental variations) or variation (e.g. mutation rates, chromosomal rearrangement rates, types of rearrangements, horizontal transfer), one can study experimentally the impact of these parameters on the structure of the evolved organisms. In particular, since Aevol integrates a precise and realistic model of the genome, it allows for the study of structural variations of the genome (e.g. number of genes, synteny, proportion of coding sequences).

The simulation platform comes along with a set of tools for analysing phylogenies and measuring many characteristics of the organisms and populations along evolution.

An extension of the model (R-Aevol), integrates an explicit model of the regulation of gene expression, thus allowing for the study of the evolution of gene regulation networks.

RELEASE FUNCTIONAL DESCRIPTION: Fix compilation error on Mac (tr1 included in std). The new mac compiler includes the tr1 directly in std which caused a compilation error. This issue was specific to aevol-4.4.1

- Participants: Antoine Frénoy, Bérénice Batut, Carole Knibbe, David Parsons, Dusan Misevic, Guillaume Beslon, Jonathan Rouzaud-Cornabas and Vincent Liard
- Partners: UCBL Lyon 1 - INSERM - Université Paris-Descartes - Insa de Lyon
- Contact: Guillaume Beslon
- URL: http://www.aevol.fr/

6.2. DeCoSTAR

KEYWORDS: Bioinformatics - Evolution

FUNCTIONAL DESCRIPTION: DeCoSTAR reconstructs ancestral genomes and improves the assembly of extant genomes. It takes as input a set of gene trees, a species tree and adjacency relations between extant genes. It outputs ancestral genes, adjacencies between extant and ancestral genes, and a statistical support associated to each inferred adjacency.

NEWS OF THE YEAR: Publication of the software with several test sets in Genome Biology and Evolution

- Participants: Eric Tannier and Wandrille Duchemin
- Contact: Eric Tannier
- Publication: hal-01503766
- URL: http://pbil.univ-lyon1.fr/software/DeCoSTAR/

6.3. Evo2Sim

Evolution of Evolution Simulator

KEYWORDS: Bioinformatics - Biology - Evolution

FUNCTIONAL DESCRIPTION: In the context of the EvoEvo european project we developed an integrated model of microorganisms evolution. This model extends the evolutionary models developed in the team (Aevol and R-Aevol) by adding a metabolic level and an ecosystem level. It includes the genomic, genetic and metabolic levels.

- Participants: Carole Knibbe, Charles Rocabert and Guillaume Beslon
- Contact: Guillaume Beslon
- URL: http://www.evoevo.eu/

6.4. evowave

KEYWORDS: Data stream - Clustering - Evolution - Wireless network

FUNCTIONAL DESCRIPTION: This package is a toolbox to analyse signal strength in wifi activity logfiles. It includes three main modules. The first is a preprocessing module to agregate logfile contents. The second one is a subspace clustering module, based on an evolutionary algorithm, to identify similar wifi activity contexts. This similarity is defined on signal strength of wifi devices and the clusters can change over time. The third module is a visualisation tool to display the cluster modifications over time.

- Participants: Anthony Rossi, Christophe Rigotti, Guillaume Beslon, Jonas Abernot, Leo Lefebvre and Sergio Peignier
- Contact: Christophe Rigotti
- URL: http://evoevo.liris.cnrs.fr/download/4_-_deliverables/wp5/Deliverable_D5.1_software_archive.zip

6.5. FluoBacTracker

KEYWORDS: Bioinformatics - Biology - Biomedical imaging

SCIENTIFIC DESCRIPTION: FluoBacTracker is an ImageJ plugin allowing the segementation and tracking of growing bacterial cells from time-lapse microscopy movies. The segmentation and tracking algorithms used by FluoBacTracker have been developed by Lionel Moisan and colleagues at Université Paris Descartes.

FUNCTIONAL DESCRIPTION: FluoBacTracker has the following functionalities: 1) Select regions of interest in images of microcolonies 2) Denoise and renormalize the images 3) Identify each cells in each image (segmentation) 4) Follow cells through the whole movie (tracking), including the detection of cells washed out from a microfluidics channel 5) Detect divisions and construct cell lineage of the population

NEWS OF THE YEAR: Version 2 of FluoBacTracker also allows the analysis of microscopy of bacteria growing in a microfluidics device called "mother machine".

- Participants: Hugues Berry, Cyril Dutrieux, Hidde De Jong, Charles Kervrann, David Parsons and Magali Vangkeosay
- Partners: Université Descartes - UGA
- Contact: Hugues Berry
- URL: http://fluobactracker.inrialpes.fr

6.6. Tewep

Simulator of the dynamics of Transposable Elements Within Expanding Populations

KEYWORDS: Simulator - Transposable elements - Population genetics - Geographic expansion

FUNCTIONAL DESCRIPTION: Transposable elements, found in the genomes of most living organisms (including humans), are pieces of DNA able to replicate themselves and to proliferate. Their presence is a source of mutations which are, most of the time, detrimental to their host. As a consequence, natural selection usually limits their spread. There are, however, some conditions where natural selection cannot be efficient enough to remove them, for example when the population size is small. It is also hypothesized that when a population geographically expands, the efficiency of natural selection could be reduced at the expansion front. TEWEP is an individual-based simulator designed to test whether transposable elements could proliferate in large expanding populations. It combines several population genetics models to simulate the evolution of the number of transposable elements in each individual of an expanding population.

- Partner: Laboratoire de Biométrie et Biologie Evolutive (LBBE) - UMR CNRS 5558
- Contact: Carole Knibbe
- URL: https://gforge.inria.fr/projects/tewep/

6.7. Treerecs

KEYWORDS: Bioinformatics - Biology - Computational biology

SCIENTIFIC DESCRIPTION: The reconciliation between gene trees and species trees is a modern method of molecular phylogeny, which does not yet have its standard software, as for example phylogeny from DNA or amino acid sequences. Treerecs has this ambition, incorporating the classic functionalities of reconciliation: annotating the vertices of a gene tree with the tops of a species tree, rooting and correcting the gene tree. Rooting and correction are calculated to minimize the number of duplications and losses in reconciliation. Medium-sized solutions are randomly sampled according to a uniform law. A likelihood can then be calculated using probabilistic methods. In addition, Treerecs is integrated into a standard software ecosystem of phylogeny, bio ++, ALE, Seaview, and has a graphical interface. Some original features are implemented, such as the possibility of combining two types of likelihoods, the one calculated from the sequences and the one calculated from the reconciliations, the possibility of estimating the costs of the evolutionary events, the possibility of exploring the space of trees according to a joined likelihood.

FUNCTIONAL DESCRIPTION: Treerecs takes as minimum input a gene tree and a species tree. It "reconciles" them, that is, it annotates gene tree nodes with events and assign them to species tree nodes. Biologically, it is a reconstruction of the gene history, given the species history, in terms of duplications, speciations, losses.

With the appropriate options Treerecs can root and correct the gene tree.

NEWS OF THE YEAR: Release of a 0.1 stable version

- Participants: Nicolas Comte, David Parsons, Eric Tannier and Benoît Morel
- Partner: Laboratoire de Biométrie et Biologie Evolutive (LBBE) - UMR CNRS 5558
- Contact: Eric Tannier

6.8. EvoMove

KEYWORDS: Music - Improvisation - Clustering - Evolution - Evolutionary Algorithms

FUNCTIONAL DESCRIPTION: EvoMove uses data from Inertial Measurement Units carried by dancers. It classifies these data in a non-supervised way to recognise "moves" and from these triggers music samples that accompany the dancers.

- Contact: Guillaume Beslon

BIGS Project-Team (section vide)

BONSAI Project-Team

5. New Software and Platforms

5.1. BCALM 2

KEYWORDS: Bioinformatics - NGS - Genomics - Metagenomics - De Bruijn graphs

SCIENTIFIC DESCRIPTION: BCALM 2 is a bioinformatics tool for constructing the compacted de Bruijn graph from sequencing data. It is a parallel algorithm that distributes the input based on a minimizer hashing technique, allowing for good balance of memory usage throughout its execution. It is able to compact very large datasets, such as spruce or pine genome raw reads in less than 2 days and 40 GB of memory on a single machine.

FUNCTIONAL DESCRIPTION: BCALM 2 is an open-source tool for dealing with DNA sequencing data. It constructs a compacted representation of the de Bruijn graph. Such a graph is useful for many types of analyses, i.e. de novo assembly, de novo variant detection, transcriptomics, etc. The software is written in C++ and makes extensive use of the GATB library.

- Participants: Antoine Limasset, Paul Medvedev and Rayan Chikhi
- Contact: Rayan Chikhi
- Publication: Compacting de Bruijn graphs from sequencing data quickly and in low memory
- URL: https://github.com/GATB/bcalm

5.2. NORINE

Nonribosomal peptides resource

KEYWORDS: Drug development - Knowledge database - Chemistry - Graph algorithmics - Genomics - Biology - Biotechnology - Bioinformatics - Computational biology

SCIENTIFIC DESCRIPTION: Since its creation in 2006, Norine remains the unique knowledgebase dedicated to non-ribosomal peptides (NRPs). These secondary metabolites, produced by bacteria and fungi, harbor diverse interesting biological activities (such as antibiotic, antitumor, siderophore or surfactant) directly related to the diversity of their structures. The Norine team goal is to collect the NRPs and provide tools to analyze them efficiently. We have developed a user-friendly interface and dedicated tools to provide a complete bioinformatics platform. The knowledgebase gathers abundant and valuable annotations on more than 1100 NRPs. To increase the quantity of described NRPs and improve the quality of associated annotations, we are now opening Norine to crowdsourcing. We believe that contributors from the scientific community are the best experts to annotate the NRPs they work on. We have developed MyNorine to facilitate the submission of new NRPs or modifications of stored ones.

FUNCTIONAL DESCRIPTION: Norine is a public computational resource with a web interface and REST access to a knowledge-base of nonribosomal peptides. It also contains dedicated tools : 2D graph viewer and editor, comparison of NRPs, MyNorine, a tool allowing anybody to easily submit new nonribosomal peptides, Smiles2monomers (s2m), a tool that deciphers the monomeric structure of polymers from their chemical structure.

- Participants: Areski Flissi, Juraj Michalik, Laurent Noé, Maude Pupin, Stéphane Janot, Valerie Leclère and Yoann Dufresne
- Partners: CNRS - Université Lille 1 - Institut Charles Viollette
- Contact: Maude Pupin
- Publications: Norine, the knowledgebase dedicated to non-ribosomal peptides, is now open to crowdsourcing - Smiles2Monomers: a link between chemical and biological structures for polymers - Norine: a powerful resource for novel nonribosomal peptide discovery - NORINE: a database of nonribosomal peptides. - Bioinformatics Tools for the Discovery of New Nonribosomal Peptides
- URL: http://bioinfo.lille.inria.fr/NRP

5.3. Vidjil

High-Throughput Analysis of V(D)J Immune Repertoire

KEYWORDS: Cancer - Indexation - NGS - Bioinformatics - Drug development

SCIENTIFIC DESCRIPTION: Vidjil is made of three components: an algorithm, a visualization browser and a server that allow an analysis of lymphocyte populations containing V(D)J recombinations.

Vidjil high-throughput algorithm extracts V(D)J junctions and gathers them into clones. This analysis is based on a spaced seed heuristics and is fast and scalable, as, in the first phase, no alignment is performed with database germline sequences. Each sequence is put in a cluster depending on its V(D)J junction. Then a representative sequence of each cluster is computed in time linear in the size of the cluster. Finally, we perform a full alignment using dynamic programming of that representative sequence against the germline sequences.

Vidjil also contains a dynamic browser (with D3JS) for visualization and analysis of clones and their tracking along the time in a MRD setup or in an immunological study.

FUNCTIONAL DESCRIPTION: Vidjil is an open-source platform for the analysis of high-throughput sequencing data from lymphocytes. V(D)J recombinations in lymphocytes are essential for immunological diversity. They are also useful markers of pathologies, and in leukemia, are used to quantify the minimal residual disease during patient follow-up. High-throughput sequencing (NGS/HTS) now enables the deep sequencing of a lymphoid population with dedicated Rep-Seq methods and software.

- Participants: Florian Thonier, Marc Duez, Mathieu Giraud, Mikaël Salson, Ryan Herbert and Tatiana Rocher

- Partners: CNRS - Inria - Université de Lille - CHRU Lille

- Contact: Mathieu Giraud

- Publications: High-Throughput Immunogenetics for Clinical and Research Applications in Immunohematology: Potential and Challenges. - High-throughput sequencing in acute lymphoblastic leukemia: Follow-up of minimal residual disease and emergence of new clones - Diagnostic et suivi des leucémies aiguës lymphoblastiques (LAL) par séquençage haut-débit (HTS) - Multiclonal Diagnosis and MRD Follow-up in ALL with HTS Coupled with a Bioinformatic Analysis - A dataset of sequences with manually curated V(D)J designations - Vidjil: A Web Platform for Analysis of High-Throughput Repertoire Sequencing - Multi-loci diagnosis of acute lymphoblastic leukaemia with high-throughput sequencing and bioinformatics analysis - Fast multiclonal clusterization of V(D)J recombinations from high-throughput sequencing - The predictive strength of next-generation sequencing MRD detection for relapse compared with current methods in childhood ALL.

- URL: http://www.vidjil.org

5.4. MATAM

Mapping-Assisted Targeted-Assembly for Metagenomics

KEYWORDS: Metagenomics - Genome assembling - Graph algorithmics

SCIENTIFIC DESCRIPTION: MATAM relies on the construction of a read overlap graph. Overlaps are computed using SortMeRNA. The overlap graph is simplified into relevant components related to specific and conserved regions. Components are assembled into contigs using SGA and contigs are finally assembled into scaffolds. The process yields nearly full length marker sequences with a very low error rate compared to the state of the art approaches. Taxonomic assignation of the obtained scaffolds is performed using the RDP classifier and is represented using Krona.

FUNCTIONAL DESCRIPTION: MATAM provides targeted genes assembly from the short metagenomic reads issued from environmental samples sequencing. Its default application focuses on the gold standard for species identification, 16S / 18S ribosomal RNA SSU genes. The produced gene scaffolds are highly accurate and suitable for precise taxonomic assignation. The software also provides a RDP classification for the reconstructed scaffolds as well as an estimation of the relative population sizes.

- Participants: Hélène Touzet, Pierre Pericard, Yoann Dufresne, Samuel Blanquart and Loïc Couderc
- Contact: Hélène Touzet
- Publication: MATAM: reconstruction of phylogenetic marker genes from short sequencing reads in metagenomes
- URL: https://github.com/bonsai-team/matam

CAPSID Project-Team

6. New Software and Platforms

6.1. Hex

KEYWORDS: 3D rendering - Bioinformatics - 3D interaction - Structural Biology

SCIENTIFIC DESCRIPTION: Hex is an interactive protein docking and molecular superposition program for Linux Mac-OS and Windows-XP. Hex understands protein and DNA structures in PDB format, and it can also read small-molecule SDF files. The recent versions now include CUDA support for Nvidia GPUs. On a modern workstation, docking times range from a few minutes or less when the search is constrained to known binding sites, to about half an hour for a blind global search (or just a few seconds with CUDA).

FUNCTIONAL DESCRIPTION: The underlying algorithm uses a novel polar Fourier correlation technique to accelerate the search for close-fitting orientations of the two molecules.

- Participant: David Ritchie
- Contact: David Ritchie
- URL: http://hex.loria.fr

6.2. Kbdock

KEYWORD: 3D interaction

SCIENTIFIC DESCRIPTION: Kbdock is a database of 3D protein domain-domain interactions with a web interface.

FUNCTIONAL DESCRIPTION: The Kbdock database is built from a snapshot of the Protein Databank (PDB) in which all 3D structures are cut into domains according to the Pfam domain description. A web interface allows 3D domain-domain interactions to be compared by Pfam family.

- Authors: Anisah Ghoorah, David Ritchie and Marie-Dominique Devignes
- Contact: David Ritchie
- URL: http://kbdock.loria.fr

6.3. Kpax

KEYWORDS: Bioinformatics - Structural Biology

SCIENTIFIC DESCRIPTION: Kpax is a program for aligning and superposing the 3D structures of protein molecules.

FUNCTIONAL DESCRIPTION: The algorithm uses a Gaussian representation of the protein backbone in order to construct a similarity score based on the 3D overlap of the Gaussians of the proteins to be superposed. Multiple proteins may be aligned together (multiple structural alignment) and databases of protein structures may be searched rapidly.

- Participant: David Ritchie
- Contact: David Ritchie

6.4. Sam

Protein Symmetry Assembler

KEYWORDS: Proteins - Structural Biology

SCIENTIFIC DESCRIPTION: Sam is a program for making symmetrical protein complexes, starting from a single monomer.

FUNCTIONAL DESCRIPTION: The algorithm searches for good docking solutions between protein monomers using a spherical polar Fast Fourier transform correlation in which symmetry restraints are built into the calculation. Thus every candidate solution is guaranteed to have the desired symmetry.

- Authors: David Ritchie and Sergey Grudinin
- Partner: CNRS
- Contact: David Ritchie
- URL: http://sam.loria.fr

6.5. gEMfitter

KEYWORDS: 3D reconstruction - Cryo-electron microscopy - Fitting
SCIENTIFIC DESCRIPTION: A program for fitting high resolution 3D protein structures into low resolution cryo-EM density maps.
FUNCTIONAL DESCRIPTION: A highly parallel fast Fourier transform (FFT) EM density fitting program which can exploit the special hardware properties of modern graphics processor units (GPUs) to accelerate both the translational and rotational parts of the correlation search.

- Authors: Van-Thai Hoang and David Ritchie
- Contact: David Ritchie
- URL: http://gem.loria.fr/gEMfitter/

6.6. ECDM

ECDomainMiner
KEYWORD: Functional annotation
SCIENTIFIC DESCRIPTION: EC-DomainMiner uses a recommender-based approach for associating EC (Enzyme Commission) numbers with protein Pfam domains from EC-sequence relationships that have been annotated previously in the SIFTS and Uniprot databases.
FUNCTIONAL DESCRIPTION: A program to associate protein Enzyme Commission numbers with Pfam domains

- Contact: David Ritchie
- URL: http://ecdm.loria.fr

6.7. GODM

GO-DomainMiner
KEYWORD: Functional annotation
FUNCTIONAL DESCRIPTION: GO-DomainMiner is is a graph-based approach for associating GO (gene ontology) terms with protein Pfam domains.

- Contact: David Ritchie
- URL: http://godm.loria.fr

6.8. BLADYG

A Block-centric graph processing framework for LArge Dynamic Graphs
KEYWORDS: Distributed computing - Dynamic graph processing

FUNCTIONAL DESCRIPTION: BLADYG is a block-centric framework that addresses the issue of dynamism in large-scale graphs. BLADYG starts its computation by collecting the graph data from various data sources. After collecting the graph data, BLADYG partitions the input graph into multiple partitions. Each BLADYG worker loads its block/partition and performs both local and remote computations, after which the status of the blocks is updated. The BLADYG coordinator orchestrates the execution of the considered graph operation in order to deal with graph updates.

- Partner: University of Trento
- Contact: Sabeur Aridhi

6.9. CGC

Clebsch-Gordan Coefficients
KEYWORDS: Clebsch-Gordan coupling coefficient - 3j symbol
FUNCTIONAL DESCRIPTION: Clebsch-Gordan coupling coefficients appear in many areas of physics and chemistry. CGC is a small library of functions and a demo driver program for calculating Clebsch-Gordan coupling coefficients up to very high principal quantum numbers.

- Contact: David Ritchie
- URL: http://cgc.loria.fr

6.10. GrAPFI

GrAPFI: Graph-based Automatic Protein Function Inference
KEYWORD: Proteins
FUNCTIONAL DESCRIPTION: GrAPFI is a Graph-based Automatic Protein Function Inference tool that aims to annotate protein sequences with EC numbers. The underlying philosophy of GrAPFI assumes that proteins can be linked through the domains, families, and superfamilies that they share. Several domain databases exist such as e.g. Pfam, SMART, CDD, Gene3D, and Prosite. Furthermore, InterPro aims to integrate information from all such databases by assigning them unique InterPro signatures. GrAPFI tool also shares Interpro signatures, as it includes information from several major family and domain databases. Our computational analysis and cross-validation show that GrAPFI achieves state-of-the-art performance in EC number prediction.

- Contact: Sabeur Aridhi
- URL: http://grapfi.loria.fr/

6.11. Platforms

6.11.1. The MBI Platform

The MBI (Modeling Biomolecular Interactions) platform (http://bioinfo.loria.fr) was established to support collaborations between Inria Nancy – Grand Est and other research teams associated with the University of Lorraine. The platform is a research node of the Institut Français de Bioinformatique (IFB), which is the French national network of bioinformatics platforms (http://www.france-bioinformatique.fr). **In 2018, funding for an engineer was awarded to Marie-Dominique Devignes for a project on bioinformatics service integration.**

- Contact: Marie-Dominique Devignes

DYLISS Project-Team

6. New Software and Platforms

6.1. AskOmics

Convert tabulated data into RDF and create SPARQL queries intuitively and "on the fly".

KEYWORDS: RDF - SPARQL - Querying - Graph - LOD - Linked open data

FUNCTIONAL DESCRIPTION: AskOmics aims at bridging the gap between end user data and the Linked (Open) Data cloud. It allows heterogeneous bioinformatics data (formatted as tabular files) to be loaded in a RDF triplestore and then be transparently and interactively queried. AskOmics is made of three software blocks: (1) a web interface for data import, allowing the creation of a local triplestore from user's datasheets and standard data, (2) an interactive web interface allowing "à la carte" query-building, (3) a server performing interactions with local and distant triplestores (queries execution, management of users parameters).

NEWS OF THE YEAR: (1) Improvements: Bugfixes and ui improvements in response to user feedback. (2) Versionning: Regular development cycle: a new version of AskOmics will be available every 3 months (currently 18.10, next 19.01) (3) Deployment: Deployment has been improved with docker and docker-compose. Virtual machine images are available on genostack to easy deploy AskOmics and Virtuoso (4) Federation: AskOmics can perform federated queries on mutliple triplestores, including other AskOmics endpoints, but also external endpoints like uniprot or dbpedia. (still in development)

- Authors: Charles Bettembourg, Xavier Garnier, Anthony Bretaudeau, Fabrice Legeai, Olivier Dameron, Olivier Filangi and Yvanne Chaussin
- Partners: Université de Rennes 1 - CNRS - INRA
- Contact: Olivier Dameron
- URL: https://github.com/askomics/askomics

6.2. CADBIOM

Computer Aided Design of Biological Models

KEYWORDS: Health - Biology - Biotechnology - Bioinformatics - Systems Biology

FUNCTIONAL DESCRIPTION: The Cadbiom software provides a formal framework to help the modeling of biological systems such as cell signaling network with Guarder Transition Semantics. It allows synchronization events to be investigated in biological networks among large-scale network in order to extract signature of controllers of a phenotype. Three modules are composing Cadbiom. 1) The Cadbiom graphical interface is useful to build and study moderate size models. It provides exploration, simulation and checking. For large-scale models, Cadbiom also allows to focus on specific nodes of interest. 2) The Cadbiom API allows a model to be loaded, performing static analysis and checking temporal properties on a finite horizon in the future or in the past. 3) Exploring large-scale knowledge repositories, since the translations of the large-scale PID repository (about 10,000 curated interactions) have been translated into the Cadbiom formalism.

NEWS OF THE YEAR: - Comprehensive command line to run the calculations and analyze the generated results. - Module designed to produce models through the interpretation of various databases or ontologies, formalized according to the BioPAX standard. - Update of the site and the documentation.

- Participants: Geoffroy Andrieux, Michel Le Borgne, Nathalie Theret, Nolwenn Le Meur, Pierre Vignet and Anne Siegel
- Contact: Anne Siegel
- URL: http://cadbiom.genouest.org

6.3. MiSCoTo

Microbiota Screening and COmmunity Selection with TOpology

KEYWORDS: Metabolic networks - ASP - Answer Set Programming - Logic programming

SCIENTIFIC DESCRIPTION: MiSCoTo solves combinatorial problems using Answer Set Programming. It aims at minimizing either the number of selected species or both the number of selected species and the cost of the interaction between them, characterized by the number of metabolic exchanges. In the first case, the level of modeling is called lumped or mixed-bag, in the latter, it is compartmentalized.

FUNCTIONAL DESCRIPTION: Metabolic networks are composed of biochemical reactions and gather the expected metabolic capabilities of species. For organisms that live in interaction altogether (microbiotas), complementarity between these networks can be exploited to predict cooperation events. This software takes as inputs metabolic networks for various species (host, symbionts of the microbiota), components of the growth medium and a metabolic objective (metabolites to be produced), and aims at selecting a minimal set of symbionts to ensure the metabolic objective can be achieved. The software can use two types of modelings: a simplified one and another that takes into account the cost of metabolic exchanges and aims at minimizing it.

NEWS OF THE YEAR: Release of the first version of the software

- Participants: Clémence Frioux, Anne Siegel, Enora Fremy and Camille Trottier
- Contact: Anne Siegel
- Publication: Scalable and exhaustive screening of metabolic functions carried out by microbial consortia
- URL: https://github.com/cfrioux/miscoto

6.4. Pathmodel

KEYWORDS: ASP - Answer Set Programming - Metabolic networks - Metabolic Pathway Drift - Bioinformatics - Systems Biology - Metabolomics

SCIENTIFIC DESCRIPTION: This tool is a prototype of the Metabolic Pathway Drift concept. This concept states that metabolic pathways undergo substantial turnover. The reactions involved in a pathway can change between species (change in reaction order or replacement of an enzyme by another one). Another goal of this tool is to linked genomics and metabolomics data. To implement this concept, Pathmodel uses the Answer Set Programming language. The input are the reactants and products involved in the pathway, known reactions occurring between these molecules, known m/z ratio, known domains shard by these molecules, an initial molecule and a goal molecule. Using these data, Pathmodel will infer reactions between molecules to reach the goal molecule using the known reactions. The result consist of potential alternative pathways for the studied organism.

FUNCTIONAL DESCRIPTION: A metabolic pathway is a series of biochemical reactions. These reactions modify metabolites in order to synthesize a new metabolite or to produce energy. One difficulties when dealing with pathways in non-model organism is their incomplete conservation during evolution. To deal with this problem, we developed a prototype inferring new biochemical reactions using reactions and metabolites from known metabolic pathways and metabolomics data. This method produce alternative pathway that could occurred in the species of interest.

RELEASE FUNCTIONAL DESCRIPTION: First version.

NEWS OF THE YEAR: Development of the tool. First release.

- Participants: Arnaud Belcour, Jacques Nicolas, Gabriel Markov and Anne Siegel
- Partner: Station Biologique de Roscoff
- Contact: Anne Siegel
- Publication: Inferring biochemical reactions and metabolite structures to cope with metabolic pathway drift
- URL: https://gitlab.inria.fr/DYLISS/PathModel

6.5. AuReMe

Automatic Reconstruction of Metabolic networks

KEYWORDS: Workflow - Bioinformatics - Metabolic networks - Omic data - Toolbox - Data management

FUNCTIONAL DESCRIPTION: AuReMe enables the reconstruction of metabolic networks from different sources based on sequence annotation, orthology, gap-filling and manual curation. The metabolic network is exported as a local wiki allowing to trace back all the steps and sources of the reconstruction. It is highly relevant for the study of non-model organisms, or the comparison of metabolic networks for different strains or a single organism.

Five modules are composing AuReMe: 1) The Model-management PADmet module allows manipulating and traceing all metabolic data via a local database. 2) The meneco python package allows the gaps of a metabolic network to be filled by using a topological approach that implements a logical programming approach to solve a combinatorial problem 3) The shogen python package allows genome and metabolic network to be aligned in order to identify genome units which contain a large density of genes coding for enzymes, it also implements a logical programming approach. 4) The manual curation assistance PADmet module allows the reported metabolic networks and their metadata to be curated. 5) The Wiki-export PADmet module enables the export of the metabolic network and its functional genomic unit as a local wiki platform allowing a user-friendly investigation.

NEWS OF THE YEAR: (1) Creation of a python package for the multiprocessing of Pathway-Tools. (2) Moving from Python 2 to Python 3. (3) Application of AuReMe to microbiome reconstructions and wikis.

- Participants: Marie Chevallier, Meziane Aite, Guillaume Collet, Nicolas Loira, Sylvain Prigent, Jeanne Got, Anne Siegel and Alejandro Maass
- Partner: University of Chile
- Contact: Meziane Aite
- Publication: Traceability, reproducibility and wiki-exploration for "à-la-carte" reconstructions of genome-scale metabolic models
- URL: http://aureme.genouest.org/

6.6. biseau

KEYWORDS: ASP - Answer Set Programming - Graph - Formal concept analysis

SCIENTIFIC DESCRIPTION: Use ASP as a Domain Specific Language to specify dot-based visualizations.

NEWS OF THE YEAR: First release.

- Contact: Lucas Bourneuf
- Publication: An Answer Set Programming Environment for High-Level Specification and Visualization of FCA
- URL: https://gitlab.inria.fr/lbourneu/biseau

ERABLE Project-Team

5. New Software and Platforms

5.1. C3Part/Isofun

KEYWORDS: Bioinformatics - Genomics

FUNCTIONAL DESCRIPTION: The C3PART / ISOFUN package implements a generic approach to the local alignment of two or more graphs representing biological data, such as genomes, metabolic pathways or protein-protein interactions, in order to infer a functional coupling between them.

- Participants: Alain Viari, Anne Morgat, Frédéric Boyer, Marie-France Sagot and Yves-Pol Deniélou
- Contact: Alain Viari
- URL: http://www.inrialpes.fr/helix/people/viari/lxgraph/index.html

5.2. Cassis

KEYWORDS: Bioinformatics - Genomics

FUNCTIONAL DESCRIPTION: Implements methods for the precise detection of genomic rearrangement breakpoints.

- Participants: Christian Baudet, Christian Gautier, Claire Lemaitre, Eric Tannier and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: http://pbil.univ-lyon1.fr/software/Cassis/

5.3. Coala

CO-evolution Assessment by a Likelihood-free Approach

KEYWORDS: Bioinformatics - Evolution

SCIENTIFIC DESCRIPTION: Despite an increasingly vaster literature on cophylogenetic reconstructions for studying host-parasite associations, understanding the common evolutionary history of such systems remains a problem that is far from being solved. Many of the most used algorithms do the host-parasite reconciliation analysis using an event-based model, where the events include in general (a subset of) cospeciation, duplication, loss, and host-switch. All known event-based methods then assign a cost to each type of event in order to nd a reconstruction of minimum cost. The main problem with this approach is that the cost of the events strongly inuence the reconciliation obtained.

To deal with this problem, we developed an algorithm, called Coala, for estimating the frequency of the events based on an approximate Bayesian computation approach.

FUNCTIONAL DESCRIPTION:COALA stands for "COevolution Assessment by a Likelihood-free Approach". It is thus a likelihood-free method for the co-phylogeny reconstruction problem which is based on an Approximate Bayesian Computation (ABC) approach.

- Participants: Beatrice Donati, Blerina Sinaimeri, Catherine Matias, Christian Baudet, Christian Gautier, Marie-France Sagot and Pierluigi Crescenzi
- Contact: Blerina Sinaimeri
- URL: http://coala.gforge.inria.fr/

5.4. CSC

KEYWORDS: Genomics - Algorithm

FUNCTIONAL DESCRIPTION: Given two sequences x and y, CSC (which stands for Circular Sequence Comparison) finds the cyclic rotation of x (or an approximation of it) that minimises the blockwise q-gram distance from y.

- Contact: Nadia Pisanti
- URL: https://github.com/solonas13/csc

5.5. Cycads

KEYWORDS: Systems Biology - Bioinformatics

FUNCTIONAL DESCRIPTION: Annotation database system to ease the development and update of enriched BIOCYC databases. CYCADS allows the integration of the latest sequence information and functional annotation data from various methods into a metabolic network reconstruction. Functionalities will be added in future to automate a bridge to metabolic network analysis tools, such as METEXPLORE. CYCADS was used to produce a collection of more than 22 arthropod metabolism databases, available at ACYPICYC (http://acypicyc.cycadsys.org) and ARTHROPODACYC (http://arthropodacyc.cycadsys.org). It will continue to be used to create other databases (newly sequenced organisms, Aphid biotypes and symbionts...).

- Participants: Augusto Vellozo, Hubert Charles, Marie-France Sagot and Stefano Colella
- Contact: Hubert Charles
- URL: http://www.cycadsys.org/

5.6. DBGWAS

KEYWORDS: Graph algorithmics - Genomics

FUNCTIONAL DESCRIPTION:DBGWAS is a tool for quick and efficient bacterial GWAS. It uses a compacted De Bruijn Graph (cDBG) structure to represent the variability within all bacterial genome assemblies given as input. Then cDBG nodes are tested for association with a phenotype of interest and the resulting associated nodes are then re-mapped on the cDBG. The output of DBGWAS consists of regions of the cDBG around statistically significant nodes with several informations related to the phenotypes, offering a representation helping in the interpretation. The output can be viewed with any modern web browser, and thus easily shared.

- Contact: Leandro Ishi Soares De Lima
- URL: https://gitlab.com/leoisl/dbgwas

5.7. Eucalypt

KEYWORDS: Bioinformatics - Evolution

FUNCTIONAL DESCRIPTION:EUCALYPT stands for "EnUmerator of Coevolutionary Associations in PoLYnomial-Time delay". It is an algorithm for enumerating all optimal (possibly time-unfeasible) mappings of a symbiont tree unto a host tree.

- Participants: Beatrice Donati, Blerina Sinaimeri, Christian Baudet, Marie-France Sagot and Pierluigi Crescenzi
- Contact: Blerina Sinaimeri
- URL: http://eucalypt.gforge.inria.fr/

5.8. Fast-SG

KEYWORDS: Genomics - Algorithm - NGS

FUNCTIONAL DESCRIPTION:FAST-SG enables the optimal hybrid assembly of large genomes by combining short and long read technologies.

- Contact: Alex Di Genova
- URL: https://github.com/adigenova/fast-sg

5.9. Gobbolino-Touché

KEYWORDS: Bioinformatics - Graph algorithmics - Systems Biology
FUNCTIONAL DESCRIPTION: Designed to solve the metabolic stories problem, which consists in finding all maximal directed acyclic subgraphs of a directed graph G whose sources and targets belong to a subset of the nodes of G, called the black nodes.

- Participants: Etienne Birmelé, Fabien Jourdan, Ludovic Cottret, Marie-France Sagot, Paulo Vieira Milreu, Pierluigi Crescenzi, Vicente Acuna Aguayo and Vincent Lacroix
- Contact: Marie-France Sagot
- URL: http://gforge.inria.fr/projects/gobbolino

5.10. HapCol

KEYWORDS: Bioinformatics - Genomics
FUNCTIONAL DESCRIPTION: A fast and memory-efficient DP approach for haplotype assembly from long reads that works until 25x coverage and solves a constrained minimum error correction problem exactly.

- Contact: Nadia Pisanti
- URL: http://hapcol.algolab.eu/

5.11. HgLib

HyperGraph Library
KEYWORDS: Graph algorithmics - Hypergraphs
FUNCTIONAL DESCRIPTION: The open-source library hglib is dedicated to model hypergraphs, which are a generalisation of graphs. In an *undirected* hypergraph, an hyperedge contains any number of vertices. A *directed* hypergraph has hyperarcs which connect several tail and head vertices. This library, which is written in C++, allows to associate user defined properties to vertices, to hyperedges/hyperarcs and to the hypergraph itself. It can thus be used for a wide range of problems arising in operations research, computer science, and computational biology.

RELEASE FUNCTIONAL DESCRIPTION: Initial version

- Participants: Martin Wannagat, David Parsons, Arnaud Mary and Irene Ziska
- Contact: Arnaud Mary
- URL: https://gitlab.inria.fr/kirikomics/hglib

5.12. KissDE

KEYWORDS: Bioinformatics - NGS
FUNCTIONAL DESCRIPTION: KISSDE is an R Package enabling to test if a variant (genomic variant or splice variant) is enriched in a condition. It takes as input a table of read counts obtained from an NGS data pre-processing and gives as output a list of condition-specific variants.

RELEASE FUNCTIONAL DESCRIPTION: This new version improved the recall and made more precise the size of the effect computation.

- Participants: Camille Marchet, Aurélie Siberchicot, Audric Cologne, Clara Benoît-Pilven, Janice Kielbassa, Lilia Brinza and Vincent Lacroix
- Contact: Vincent Lacroix
- URL: http://kissplice.prabi.fr/tools/kissDE/

5.13. KisSplice

KEYWORDS: Bioinformatics - Bioinfirmatics search sequence - Genomics - NGS

FUNCTIONAL DESCRIPTION: Enables to analyse RNA-seq data with or without a reference genome. It is an exact local transcriptome assembler, which can identify SNPs, indels and alternative splicing events. It can deal with an arbitrary number of biological conditions, and will quantify each variant in each condition.

RELEASE FUNCTIONAL DESCRIPTION: Improvements : KissReads module has been modified and sped up, with a significant impact on run times. Parameters : –timeout default now at 10000: in big datasets, recall can be increased while run time is a bit longer. Bugs fixed : Reads containing only 'N': the graph construction was stopped if the file contained a read composed only of 'N's. This is was a silence bug, no error message was produced. Problems compiling with new versions of MAC OSX (10.8+): KisSplice is now compiling with the new default C++ compiler of OSX 10.8+.

- Participants: Alice Julien-Laferrière, Leandro Ishi Soares De Lima, Vincent Miele, Rayan Chikhi, Pierre Peterlongo, Camille Marchet, Gustavo Akio Tominaga Sacomoto, Marie-France Sagot and Vincent Lacroix
- Contact: Vincent Lacroix
- URL: http://kissplice.prabi.fr/

5.14. KisSplice2RefGenome

KEYWORDS: Bioinformatics - NGS - Transcriptomics
FUNCTIONAL DESCRIPTION:KISSPLICE identifies variations in RNA-seq data, without a reference genome. In many applications however, a reference genome is available. KISSPLICE2REFGENOME enables to facilitate the interpretation of the results of KISSPLICE after mapping them to a reference genome.

- Participants: Audric Cologne, Camille Marchet, Camille Sessegolo, Alice Julien-Laferrière and Vincent Lacroix
- Contact: Vincent Lacroix
- URL: http://kissplice.prabi.fr/tools/kiss2refgenome/

5.15. KisSplice2RefTranscriptome

KEYWORDS: Bioinformatics - NGS - Transcriptomics
FUNCTIONAL DESCRIPTION:KISSPLICE2REFTRANSCRIPTOME enables to combine the output of KISSPLICE with the output of a full length transcriptome assembler, thus allowing to predict a functional impact for the positioned SNPs, and to intersect these results with condition-specific SNPs. Overall, starting from RNA-seq data only, we obtain a list of condition-specific SNPs stratified by functional impact.

- Participants: Helene Lopez Maestre, Mathilde Boutigny and Vincent Lacroix
- Contact: Vincent Lacroix
- URL: http://kissplice.prabi.fr/tools/kiss2rt/

5.16. MetExplore

KEYWORDS: Systems Biology - Bioinformatics
SCIENTIFIC DESCRIPTION: MetExplore stores metabolic networks of 160 organisms into a relational database. Information about metabolic networks mainly come from BioCyc-like databases. Two BioCyc-like databases contain information about several organisms: PlantCyc and MetaCyc. MetExplore contains also the information about metabolites stored in Metabolome.jp. Note that there is no information about reactions in this database and is only useful to identify compounds from masses. Several genome-scale models designed for Flux Balance Analysis have also been imported into MetExplore. The table below gives details about the sources of the metabolic networks present in MetExplore.

FUNCTIONAL DESCRIPTION: Web-server that allows to build, curate and analyse genome-scale metabolic networks. METEXPLORE is also able to deal with data from metabolomics experiments by mapping a list of masses or identifiers onto filtered metabolic networks. Finally, it proposes several functions to perform Flux Balance Analysis (FBA). The web-server is mature, it was developed in PHP, JAVA, Javascript and Mysql. METEXPLORE was started under another name during Ludovic Cottret's PhD in Bamboo, and is now maintained by the METEXPLORE group at the Inra of Toulouse.

- Participants: Fabien Jourdan, Hubert Charles, Ludovic Cottret and Marie-France Sagot
- Contact: Fabien Jourdan
- URL: https://metexplore.toulouse.inra.fr/index.html/

5.17. Mirinho

KEYWORDS: Bioinformatics - Computational biology - Genomics - Structural Biology
FUNCTIONAL DESCRIPTION: Predicts, at a genome-wide scale, microRNA candidates.

- Participants: Christian Gautier, Christine Gaspin, Cyril Fournier, Marie-France Sagot and Susan Higashi
- Contact: Marie-France Sagot
- URL: http://mirinho.gforge.inria.fr/

5.18. Momo

Multi-Objective Metabolic mixed integer Optimization
KEYWORDS: Metabolism - Metabolic networks - Multi-objective optimisation
FUNCTIONAL DESCRIPTION:MOMO is a multi-objective mixed integer optimisation approach for enumerating knockout reactions leading to the overproduction and/or inhibition of specific compounds in a metabolic network.

- Contact: Marie-France Sagot
- URL: http://momo-sysbio.gforge.inria.fr

5.19. MultiPus

KEYWORDS: Systems Biology - Algorithm - Graph algorithmics - Metabolic networks - Computational biology
SCIENTIFIC DESCRIPTION: Synthetic biology has boomed since the early 2000s when it started being shown that it was possible to efficiently synthetise compounds of interest in a much more rapid and effective way by using other organisms than those naturally producing them. However, to thus engineer a single organism, often a microbe, to optimise one or a collection of metabolic tasks may lead to difficulties when attempting to obtain a production system that is efficient, or to avoid toxic effects for the recruited microorganism. The idea of using instead a microbial consortium has thus started being developed in the last decade. This was motivated by the fact that such consortia may perform more complicated functions than could single populations and be more robust to environmental fluctuations. Success is however not always guaranteed. In particular, establishing which consortium is best for the production of a given compound or set thereof remains a great challenge. The algorithm MultiPus is based on an initial model that enables to propose a consortium to synthetically produce compounds that are either exogenous to it, or are endogenous but where interaction among the species in the consortium could improve the production line.

FUNCTIONAL DESCRIPTION:MULTIPUS (for "MULTIple species for the synthetic Production of Useful biochemical Substances") is an algorithm that, given a microbial consortium as input, identifies all optimal sub-consortia to synthetically produce compounds that are either exogenous to it, or are endogenous but where interaction among the species in the sub-consortia could improve the production line.

- Participants: Alberto Marchetti-Spaccamela, Alice Julien-Laferrière, Arnaud Mary, Delphine Parrot, Laurent Bulteau, Leen Stougie, Marie-France Sagot and Susana Vinga
- Contact: Marie-France Sagot
- URL: http://multipus.gforge.inria.fr/

5.20. Pitufolandia

KEYWORDS: Bioinformatics - Graph algorithmics - Systems Biology
FUNCTIONAL DESCRIPTION: The algorithms in PITUFOLANDIA (PITUFO / PITUFINA / PAPAPITUFO) are designed to solve the minimal precursor set problem, which consists in finding all minimal sets of precursors (usually, nutrients) in a metabolic network that are able to produce a set of target metabolites.

- Contact: Marie-France Sagot
- URL: http://gforge.inria.fr/projects/pitufo/

5.21. Sasita

KEYWORDS: Bioinformatics - Graph algorithmics - Systems Biology
FUNCTIONAL DESCRIPTION:SASITA is a software for the exhaustive enumeration of minimal precursor sets in metabolic networks.

- Contact: Marie-France Sagot
- URL: http://sasita.gforge.inria.fr/

5.22. Savage

KEYWORDS: Algorithm - Genomics
FUNCTIONAL DESCRIPTION: Reconstruction of viral quasi species without using a reference genome.

- Contact: Alexander Schonhuth
- URL: https://bitbucket.org/jbaaijens/savage

5.23. Smile

KEYWORDS: Bioinformatics - Genomic sequence
FUNCTIONAL DESCRIPTION: Motif inference algorithm taking as input a set of biological sequences.

- Participant: Marie-France Sagot
- Contact: Marie-France Sagot

5.24. Rime

KEYWORDS: Bioinformatics - Genomics - Sequence alignment
FUNCTIONAL DESCRIPTION: Detects long similar fragments occurring at least twice in a set of biological sequences.

- Contact: Nadia Pisanti

5.25. Totoro & Kotoura

KEYWORDS: Bioinformatics - Graph algorithmics - Systems Biology

FUNCTIONAL DESCRIPTION: Both TOTORO and KOTOURA decipher the reaction changes during a metabolic transient state, using measurements of metabolic concentrations. These are called metabolic hyperstories. TOTORO (for TOpological analysis of Transient metabOlic RespOnse) is based on a qualitative measurement of the concentrations in two steady-states to infer the reaction changes that lead to the observed differences in metabolite pools in both conditions. In the currently available release, a pre-processing and a post-processing steps are included. After the post-processing step, the solutions can be visualised using DINGHY (http://dinghy.gforge.inria.fr). KOTOURA (for Kantitative analysis Of Transient metabOlic and regUlatory Response And control) infers quantitative changes of the reactions using information on measurement of the metabolite concentrations in two steady-states.

- Contact: Marie-France Sagot
- URL: http://hyperstories.gforge.inria.fr/

5.26. WhatsHap

KEYWORDS: Bioinformatics - Genomics

FUNCTIONAL DESCRIPTION:WHATSHAP is a DP approach for haplotype assembly from long reads that works until 20x coverage and solves the minimum error correction problem exactly. PWHATSHAP is a parallelisation of the core dynamic programming algorithm of WHATSHAP.

- Contact: Nadia Pisanti
- URL: https://bitbucket.org/whatshap/whatshap

GENSCALE Project-Team

6. New Software and Platforms

6.1. GATB-Core

Genome Assembly and Analysis Tool Box

KEYWORDS: Bioinformatics - NGS - Genomics - Genome assembling

FUNCTIONAL DESCRIPTION: The GATB-Core library aims to lighten the design of NGS algorithms. It offers a panel of high-level optimized building blocks to speed-up the development of NGS tools related to genome assembly and/or genome analysis. The underlying data structure is the de Bruijn graph, and the general parallelism model is multithreading. The GATB library targets standard computing resources such as current multicore processor (laptop computer, small server) with a few GB of memory. From high-level API, NGS programming designers can rapidly elaborate their own software based on domain state-of-the-art algorithms and data structures. The GATB-Core library is written in C++.

- Participants: Charles Deltel, Rayan Chikhi, Erwan Drezen, Antoine Limasset, Gaëtan Benoit, Uricaru Raluca, Claire Lemaitre, Dominique Lavenier, Guillaume Rizk, Patrick Durand and Pierre Peterlongo
- Contact: Dominique Lavenier
- URL: http://gatb.inria.fr/

6.2. CARNAC-LR

Clustering coefficient-based Acquisition of RNA Communities in Long Reads

KEYWORDS: Transcriptomics - Clustering - Bioinformatics

FUNCTIONAL DESCRIPTION: Carnac-LR is a clustering method for third generation sequencing data. Used on RNA sequences it retrieves all sequences that relate to a same gene and put them in a cluster. CARNAC-LR is an efficient implementation of a novel clustering algorithm for detecting communities in a graph of reads from Third Generation Sequencing. It is a part of a pipeline that allows to retrieve expressed variants from each gene de novo (without reference genome/transcriptome), for transcriptomic sequencing data.

- Participants: Camille Marchet, Pierre Peterlongo and Jacques Nicolas
- Contact: Camille Marchet
- Publication: De Novo Clustering of Long Reads by Gene from Transcriptomics Data
- URL: https://github.com/kamimrcht/CARNAC

6.3. MindTheGap

KEYWORDS: Bioinformatics - NGS - Genome assembly

FUNCTIONAL DESCRIPTION: MindTheGap is a NGS software that performs local assembly of short reads. It is a structural variant detection tool as well as a genome assembly finishing tool. As a variant caller, it performs detection and assembly of DNA insertion variants in NGS read datasets with respect to a reference genome. It is designed to call insertions of any size, whether they are novel or duplicated, homozygous or heterozygous in the donor genome. Local assembly is performed to recover the inserted sequences from the whole read dataset. The local assembly module can also be used to fill the gaps between a set of input contigs without any a priori on their relative order and orientation, in order to improve a draft genome assembly.

RELEASE FUNCTIONAL DESCRIPTION: Since version 2.1.0, MindTheGap can also be used as a genome assembly finishing tool: it can fill the gaps between a set of input contigs without any a priori on their relative order and orientation. This new feature is available in the Fill module with option -contig.

- Participants: Claire Lemaitre, Guillaume Rizk, Pierre Marijon, Rayan Chikhi, Wesley Delage and Cervin Guyomar

- Contact: Claire Lemaitre

- Publication: MindTheGap: integrated detection and assembly of short and long insertions

- URL: https://gatb.inria.fr/software/mind-the-gap/

6.4. bcool

de Bruijn graph cOrrectiOn from graph aLignment

KEYWORDS: De Bruijn graphs - Reads correction - Short reads - Read mapping

FUNCTIONAL DESCRIPTION: BCool is a method to correct short reads using de Bruijn graphs. BCool includes two steps. As a first step, Bcool constructs a corrected compacted de Bruijn graph from the reads. This graph is then used as a reference and the reads are corrected according to their mapping on the graph.This approach yields a better correction than kmer-spectrum techniques, while being scalable, making it possible to apply it to human-size genomic datasets and beyond. The implementation is open source and available at github.com/Malfoy/BCOOL

- Participants: Antoine Limasset and Pierre Peterlongo

- Partner: Université libre de Bruxelles

- Contact: Pierre Peterlongo

- Publication: Toward perfect reads: self-correction of short reads via mapping on de Bruijn graphs

- URL: http://github.com/Malfoy/BCOOL

IBIS Project-Team

5. New Software and Platforms

5.1. WellFARE

KEYWORDS: Bioinformatics - Statistics - Data visualization - Data modeling

SCIENTIFIC DESCRIPTION: WellFARE is a Python library implementing linear inversion methods for the reconstruction of gene expression profiles from fluorescent or luminescent reporter gene data. WellFARE form the computational core of the WellInverter web application.

FUNCTIONAL DESCRIPTION: As input, WellFARE reads the primary data file produced by a 96-well microplate reader, containing time-series measurements of the absorbance (optical density) as well as the fluorescence and luminescence intensities in each well (if available). Various functions exist to analyze the data, in particular for detecting outliers, subtracting background, estimating growth rates, promoter activities and protein concentrations, visualizing expression profiles, synchronizing replicate profiles, etc. WellFARE is the computational core of the web application WellInverter.

NEWS OF THE YEAR: Submission of a journal publication describing the new version of WellInverter and WellFARE

- Participants: Delphine Ropers, Hans Geiselmann, Hidde De Jong, Michel Page, Valentin Zulkower and Yannick Martin
- Partner: UGA
- Contact: Hidde De Jong
- Publication: Robust reconstruction of gene expression profiles from reporter gene data using linear inversion
- URL: https://github.com/ibis-inria/wellfare

5.2. WellInverter

KEYWORDS: Bioinformatics - Statistics - Data visualization - Data modeling

SCIENTIFIC DESCRIPTION: WellInverter is a web application that implements linear inversion methods for the reconstruction of gene expression profiles from fluorescent or luminescent reporter gene data. WellInverter makes the methods available to a broad audience of biologists and bioinformaticians. In particular, we have put in place a parallel computing architecture with a load balancer to distribute the analysis queries over several back-end servers, redesigned the graphical user interface, and developed a plug-in system for defining high-level routines for parsing data files produced by microplate readers from different manufacturers.

FUNCTIONAL DESCRIPTION: As input, WellInverter reads the primary data file produced by a 96-well microplate reader, containing time-series measurements of the absorbance (optical density) as well as the fluorescence and luminescence intensities in each well (if available). Various modules exist to analyze the data, in particular for detecting outliers, subtracting background, estimating growth rates, promoter activities and protein concentrations, visualizing expression profiles, synchronizing replicate profiles, etc. The computational core of the web application consists of the Python library WellFARE.

NEWS OF THE YEAR: Deployment of WellInverter on an Inria server and on the new cloud of the French Institute for Bioinformatics (see the web page for details). Submission of a journal article describing the new version of the application.

- Participants: Delphine Ropers, Hans Geiselmann, Hidde De Jong, Johannes Geiselmann, Michel Page, Valentin Zulkower and Yannick Martin
- Partner: UGA
- Contact: Hidde De Jong
- Publication: Robust reconstruction of gene expression profiles from reporter gene data using linear inversion
- URL: https://team.inria.fr/ibis/wellinverter/

5.3. FluoBacTracker

KEYWORDS: Bioinformatics - Biology - Biomedical imaging

SCIENTIFIC DESCRIPTION: FluoBacTracker is an ImageJ plugin allowing the segementation and tracking of growing bacterial cells from time-lapse microscopy movies. The segmentation and tracking algorithms used by FluoBacTracker have been developed by Lionel Moisan and colleagues at Université Paris Descartes.

FUNCTIONAL DESCRIPTION: FluoBacTracker has the following functionalities: 1) Select regions of interest in images of microcolonies 2) Denoise and renormalize the images 3) Identify each cells in each image (segmentation) 4) Follow cells through the whole movie (tracking), including the detection of cells washed out from a microfluidics channel 5) Detect divisions and construct cell lineage of the population

NEWS OF THE YEAR: Version 2 of FluoBacTracker also allows the analysis of microscopy of bacteria growing in a microfluidics device called "mother machine".

- Participants: Hugues Berry, Cyril Dutrieux, Hidde De Jong, Charles Kervrann, David Parsons and Magali Vangkeosay
- Partners: Université Descartes - UGA
- Contact: Hugues Berry
- URL: http://fluobactracker.inrialpes.fr

5.4. GNA

Genetic Network Analyzer

KEYWORDS: Model Checking - Bioinformatics - Gene regulatory networks - Qualitative simulation

SCIENTIFIC DESCRIPTION: Genetic Network Analyzer (GNA) is the implementation of methods for the qualitative modeling and simulation of gene regulatory networks developed in the IBIS project-team.

FUNCTIONAL DESCRIPTION: The input of GNA consists of a model of the regulatory network in the form of a system of piecewise-linear differential equations (PLDEs), supplemented by inequality constraints on the parameters and initial conditions. From this information, GNA generates a state transition graph summarizing the qualitative dynamics of the system. In order to analyze large graphs, GNA allows the user to specify properties of the qualitative dynamics of a network in temporal logic, using high-level query templates, and to verify these properties on the state transition graph by means of standard model-checking tools, either locally installed or accessible through a remote web server.

RELEASE FUNCTIONAL DESCRIPTION: (1) it supports the editing and visualization of regulatory networks, in an SBGN-compatible format, (2) it semi-automatically generates a prototype model from the network structure, thus accelerating the modeling process, and (3) it allows models to be exported in the SBML Qual standard.

NEWS OF THE YEAR: New mode of distribution from the IBIS web site.

- Participants: Hidde De Jong, Michel Page and Delphine Ropers
- Partner: UGA
- Contact: Hidde De Jong
- Publications: Genetic Network Analyzer: A Tool for the Qualitative Modeling and Simulation of Bacterial Regulatory Networks - Piecewise linear approximations to model the dynamics of adaptation to osmotic stress by food-borne pathogens
- URL: http://www-helix.inrialpes.fr/gna

LIFEWARE Project-Team

6. New Software and Platforms

6.1. BIOCHAM

The Biochemical Abstract Machine

KEYWORDS: Systems Biology - Bioinformatics

FUNCTIONAL DESCRIPTION: The Biochemical Abstract Machine (BIOCHAM) is a software environment for modeling, analyzing and synthesizing biochemical reaction networks (CRNs) with respect to a formal specification of the observed or desired behavior of a biochemical system. BIOCHAM is compatible with the Systems Biology Markup Language (SBML) and contains some unique features about formal specifications in quantitative temporal logic, sensitivity and robustness analyses and parameter search in high dimension w.r.t. behavioral specifications, static analyses, and synthesis of CRNs.

RELEASE FUNCTIONAL DESCRIPTION: influence networks with forces – PAC learning of influence networks from time series data – synthesis of continuous reaction networks for mathematical functions defined by polynomial differential equations – complete modular rewriting of Biocham in SWI-Prolog

- Participants: François Fages, David Coudrin, Sylvain Soliman and Thierry Martinez
- Contact: François Fages
- URL: http://lifeware.inria.fr/biocham4/

6.2. Platforms

6.2.1. *Smart experimental platforms to automate microbiology experiments*

Models play a central role in our work, either to test our understanding or to guide the design of novel systems. Model development and parameter calibration necessitate informative experiments. We develop methods to assist with the optimal design of experiments. In consequence, we have to perform, in sequence or in parallel, experiments with possibly complex input profiles. This led us to develop experimental platforms that allow for flexible and automated stimulations and measurements. Three platforms are being developed, based on (i) a microplate photometer, (ii) a bioreactor platform coupled with a flow cytometer, and (iii) a microscope equipped with microfluidic systems, respectively. In all cases, the real-time measurement and actuation capabilities allow for making reactive experiments, notably including real-time control experiments.

MORPHEME Project-Team

5. New Software and Platforms

5.1. Obj.MPP

KEYWORDS: Object detection - Marked Point Process - Parametric model

FUNCTIONAL DESCRIPTION: Obj.MPP implements the detection of parametric objects using a Marked Point Process (MPP). A parametric object is an n-dimensional piece of signal defined by a finite set of parameters. Detecting an object in a signal amounts to finding a position at which the signal can be described well enough by a specific set of parameters (unknowns of the detection problem). The detection task amounts to finding all such objects. Typically, the signal is a 2-dimensional grayscale image and the parametric objects are bright disks on a dark background. In this case, each object is defined by a single parameter: the disk radius. Note however that the core function of Obj.MPP is not tied to a particular context (2-dimensional imaging is just an example).

- Author: Eric Debreuve

- Contact: Eric Debreuve

- Publications: Stochastic geometry for image analysis - Multiple objects detection in biological images using a marked point process framework - An efficient optimizer for simple point process models - Multiple Birth and Cut Algorithm for Multiple Object Detection

- URL: https://team.inria.fr/morpheme/obj-mpp-object-detection-using-a-marked-point-process/

5.2. ATOLS

Adaptative Threshold Operator based on Level Sets

KEYWORDS: Object detection - Level Set

FUNCTIONAL DESCRIPTION: Atols is a Python script allowing to detect features on images using a contrast scoring. Thus, it's possible to detect features at different levels of intensity unlike a simple threshold which would only keep features above its value.

- Authors: Kevin Giulietti and Guillaume Lavisse

- Contact: Xavier Descombes

- URL: https://team.inria.fr/morpheme/software/

5.3. Small particle detection

KEYWORDS: Image processing - Image segmentation - Object detection - Computational biology - Fluorescence microscopy - Biomedical imaging

FUNCTIONAL DESCRIPTION: An algorithm primarily design to detect objects whose sizes aren't larger a few pixels (particles) on fluorescence microscopy images.

It is an simplified version of marked point process.

- Contact: Nicolas Cedilnik

- Publications: SPADE: A Small Particle Detection Method Using A Dictionary Of Shapes Within The Marked Point Process Framework - SPADE: A Small Particle Detection Method Using A Dictionary Of Shapes Within The Marked Point Process Framework

- URL: https://gitlab.inria.fr/ncedilni/spade

MOSAIC Team

5. New Software and Platforms

5.1. treex

KEYWORDS: Graph algorithmics - Data structures - Combinatorics

SCIENTIFIC DESCRIPTION: Trees form an expanded family of combinatorial objects that offers a wide range of application fields, especially in biology, from plant modeling to blood vessels network analysis through study of lineages. Consequently, it is crucial for the team to develop numerical tools and algorithms for processing tree data, in particular to answer questions about the representation of biological organisms and their forms in silico.

treex is a Python 3 library dedicated to the manipulation of tree objects, whatever they are ordered or not, with or without quantitative or qualitative labels.

FUNCTIONAL DESCRIPTION: treex is a Python library for manipulating rooted trees. The trees can be ordered or not, with or without labels on their vertices.

The package provides a data structure for rooted trees as well as the following main functionalities: - Random generation algorithms - DAG compression for ordered or not, labeled or not, trees - Approximation algorithms for unordered trees - Edit distance for unordered labeled trees - Computation of coding processes (Harris path, Lukasiewicz walk and height process) - Visualization algorithms in Matplotlib or in LaTeX

Representations of trees. With treex, we aim to propose all the standard representations of trees as well as the one-to-one correspondences between them. Main coding processes (Harris path, Lukasiewicz walk, and height process), DAG representation, doubly-chained tree structures have been already coded. Standard exploration algorithms and editing methods have also been developed. Through these generic tools, treex enables the manipulation of trees from various application contexts.

Easy-to-use. We think that treex must be user-friendly to be adopted by collaborators from fields of biology. To this end, we develop high-level algorithms and provide an extensive documentation (with sphinx) as well as a simple installation method through conda.

Algorithms. The current version of treex provides edit distance algorithms, approximation algorithms (that can be used to control the complexity of the edit distance algorithms), and visualization algorithms (with an interface for TEX / LATEX and Matplotlib). A first statistical learning module is in progress.

RELEASE FUNCTIONAL DESCRIPTION: The first release of treex happened in the late 2018 after an intensive work to ease both installation and handling. A publication on treex is planned for the next early year. In addition, treex will be integrated in Gnomon in the following months.

NEWS OF THE YEAR: The first release of treex happened in the late 2018 after an intensive work to ease both installation and handling. A publication on treex is planned for the next early year. In addition, treex will be integrated in Gnomon in the following months.

- Participants: Romain Azais, Guillaume Cerutti, Didier Gemmerle and FLORIAN INGELS
- Contact: Romain Azais
- URL: https://gitlab.inria.fr/azais/treex

5.2. Gnomon

KEYWORDS: 4D - Modelization and numerical simulations - Finite element modelling - Computational biology - Data visualization

SCIENTIFIC DESCRIPTION: Gnomon is a user-friendly computer platform developed by the Mosaic team for seamless simulation of form development in silico. It is intended to be a major tool for the team members to develop, integrate and share their models, algorithms and tools. In Gnomon, a developing form is represented at any time by a central data-structure that contains topological, geometric, genetic and physiological information and that represents the state of the growing form. Flexible components (plugins) make it possible to up-load or to create such data-structures, to program their development, to analyze, visualize them and interact with them in 3D+time.

FUNCTIONAL DESCRIPTION: Gnomon is developed based on the past experience of the team with the OpenAlea platform, but moving towards a more scalable software engineering solution based on the dtk kernel developed by the group of software engineers (SED) from the Sophia-Antipolis Inria Center. Gnomon development uses extensively an agile methodology and emphasizes three main aspects:

Deployable and extensible software architecture. The Gnomon platform is intended to become a perennial common resource for the members of the team as well as a tool to easily diffuse our methods to collaborators. It is a plugin-based architecture, relying on the dtk meta-platform developed by the SED at Inria Sophia-Antipolis. dtk eases the conception of a high-level C++ environment inside which added-value components are injected autonomously by the team members as Python plugins wrapping our scientific libraries. A significant effort is put on the packaging and deployability of this software (using conda), adding up unit testing, continuous integration and cross-platform installation.

Exploration of forms. The environment will provide tools to create and visualize forms, and explore them in space and time. Building on the algorithmic resources developed by the team for image sequences of multicellular tissues, user-friendly interfaces are being designed for the exploration of such structures. This gives the user the possibility to reconstruct computational representations from experimental data in an intuitive way, and to explore these spatio-temporal data in an interactive and visual manner.

Integrated form simulation framework. Within a general framework for the modeling of dynamical systems that the team is developing, a core component is the mechanical simulation engine that will handle the resolution of physical equations controlling form development. We want the simulation framework to be integrated within the Gnomon platform in a nearly transparent way for the user. To achieve this, we develop a high-level interface for a generic differential equation solver based on the *fenics* FEM library. Mapping the general concepts of morphogenesis modeling to this engine will allow the user to specify behavior rules of the system at high-level and easily design simulation scenarios directly in the Gnomon application.

Gnomon project organization:

- Project leader: Christophe Godin
- Software development coordinator: Guillaume Cerutti
- DTK backend coordinator: Thibaud Kloczko
- Plugin coordinators: Jonathan Legrand (TimageTK), treex (Romain Azais), Olivier Ali (Mechanics), Frédéric Boudon (L-Systems).
- Diffusion to end-users: Teva Vernoux

This work is part of the *Gnomon* ADT project supported by the Inria centers of Grenoble Rhône-Alpes and Sophia-Antipolis Méditerranée.

RELEASE FUNCTIONAL DESCRIPTION: A first, fully functional, prototype of the Gnomon software platform, dedicated to the modeling and simulation of plant and animal morphogenesis, was developed during a series of intensive coding sessions in Lyon and Sophia-Antipolis. This new concept of platform dedicated to the study of morphogenesis was presented in November 2018 to a panel of modelers and biologists at the RDP lab, who will contribute next year to the further testing and refining the platform. This prototype is a clear milestone and results from a strong collaboration between the Inria software engineering group from Sophia-Antipolis (who provides the software architecture kernel - DTK)) and the Mosaic team and is supported by Inria (Action de Developpement Tecnologique, ADT).

NEWS OF THE YEAR: A first, fully functional, prototype of the Gnomon software platform, dedicated to the modeling and simulation of plant and animal morphogenesis, was developed during a series of intensive coding sessions in Lyon and Sophia-Antipolis. This new concept of platform dedicated to the study of morphogenesis was presented in November 2018 to a panel of modelers and biologists at the RDP lab, who will contribute next year to the further testing and refining the platform. This prototype is a clear milestone and results from a strong collaboration between the Inria software engineering group from Sophia-Antipolis (who provides the software architecture kernel - DTK)) and the Mosaic team and is supported by Inria (Action de Developpement Tecnologique, ADT).

- Participants: Olivier Ali, Frédéric Boudon, Guillaume Cerutti, FLORIAN GACON, Christophe Godin, Jonathan Legrand and Grégoire Malandain
- Contact: Christophe Godin

5.3. TimageTK: a Python package for image processing of multicellular architectures

Participants: Frédéric Boudon [External Collaborator], Guillaume Cerutti, Christophe Godin, Jonathan Legrand, Grégoire Malandain [External Collaborator].

- Related Research Works: **RA1** (*Representations of forms in silico*) & **RA2** (*Data-driven models*) & **RA3** (*Plasticity and robustness of forms*)
- Related Key Modeling Challenges: **KMC3** (*Realistic integrated digital models*)

Processing images of multicellular tissue architectures in plants and animals present difficult computational challenges, notably when dealing with heterogeneous data sources, temporal data. As for now, only limited computational tools exit to analyze these types of images efficiently. Based on our initial experience with the development of MARS-ALT, a pipeline for segmenting and tracking cell lineages, we have recently redesigned our software in order to develop a new high-level Python package named Tissue image ToolKit (TimageTK).

C/Python library. TimageTK is written in Python and is largely built on top of a C library (VT) developed by the Morpheme Inria team. Part of the C library was developed for MARS-ALT software by the Morpheme team. TimageTK provides high-level wrapping of these algorithms with additional functionalities directly written in Python, such as cell tracking.

Well documented, high-level image processing. TimageTK offer high-level methods, where few parameters are required to tune algotithms. They offer a safer use of function through well documented class methods. For experts in image processing, low-level functions and wrappings of C-functions are still accessible.

Easy deployment. TimageTK has simple and robust installation procedure based on conda (Conda is a package and environment management system that runs on Windows, macOS and Linux and allows to get rid of most installation issues, such as compilation or dependency errors). For now only macOSX and Linux version are packaged (x64 architecture) using Inria continuous integration tools.

Continuous integration. Using Inria continuous integration tools, TimageTK is regularly released through conda packaging mechanism. We also make use of these resources to regularly generate (sphinx) and publish updates in the documentation.

Compatibility with Gnomon. TimageTK is based on data structures representing images that are fully compatible with Gnomon. This makes it possible to use TimageTK as a plugin of the Gnomon software.

<p style="text-align: center; color: red;">**PLEIADE Team**</p>

6. New Software and Platforms

6.1. Magus

KEYWORDS: Bioinformatics - Genomic sequence - Knowledge database

SCIENTIFIC DESCRIPTION: MAGUS can be used on small installations with a web server and a relational database on a single machine, or scaled out in clusters or elastic clouds using Apache Cassandra for NoSQL data storage and Apache Hadoop for Map-Reduce.

FUNCTIONAL DESCRIPTION: The MAGUS genome annotation system integrates genome sequences and sequences features, in silico analyses, and views of external data resources into a familiar user interface requiring only a Web navigator. MAGUS implements annotation workflows and enforces curation standards to guarantee consistency and integrity. As a novel feature the system provides a workflow for simultaneous annotation of related genomes through the use of protein families identified by in silico analyses this has resulted in a three-fold increase in curation speed, compared to one-at-a-time curation of individual genes. This allows us to maintain standards of high-quality manual annotation while efficiently using the time of volunteer curators.

NEWS OF THE YEAR: Magus is now available as a Docker image, and can be integrated with other containerized services using Pleiade's Alcyone system.

- Participants: David Sherman, Florian Lajus, Natalia Golenetskaya, Pascal Durrens and Xavier Calcas
- Partners: Université de Bordeaux - CNRS - INRA
- Contact: David James Sherman
- Publication: High-performance comparative annotation
- URL: http://magus.gforge.inria.fr

6.2. Mimoza

KEYWORDS: Systems Biology - Bioinformatics - Biotechnology

FUNCTIONAL DESCRIPTION: Mimoza uses metabolic model generalization and cartographic paradigms to allow human experts to explore a metabolic model in a hierarchical manner. Mimoza generalizes genome-scale metabolic models, by factoring equivalent reactions and metabolites while preserving reaction consistency. The software creates an zoomable representation of a model submitted by the user in SBML format. The most general view represents the compartments of the model, the next view shows the visualization of generalized versions of reactions and metabolites in each compartment , and the most detailed view visualizes the initial model with the generalization-based layout (where similar metabolites and reactions are placed next to each other). The resulting map can be explored on-line, or downloaded in a COMBINE archive. The zoomable representation is implemented using the Leaflet JavaScript library for mobile-friendly interactive maps. Users can click on reactions and compounds to see the information about their annotations.

NEWS OF THE YEAR: Mimoza is now available as a Docker image, and can be integrated with other containerized services using Pleiade's Alcyone system.

- Participants: Anna Zhukova and David James Sherman
- Contact: David James Sherman
- Publications: Knowledge-based generalization of metabolic models - Knowledge-based zooming for metabolic models - Knowledge-based generalization of metabolic networks: a practical study
- URL: http://mimoza.bordeaux.inria.fr/

6.3. Declic

FUNCTIONAL DESCRIPTION: Declic is a Python library that provides several tools for data analysis in the domains of multivariate data analysis, machine learning, and graph based methods. It can be used to study in-depth the accuracy of the dictionary between molecular based and morphological based taxonomy.

Declic includes an interpreter for a Domain Specific Language (DSL) to make its Python library easy to use for scientists familiar with environments such as R.

- Partner: INRA
- Contact: Alain Franc

6.4. Diagno-Syst

diagno-syst: a tool for accurate inventories in metabarcoding
KEYWORDS: Biodiversity - Clustering - Ecology
FUNCTIONAL DESCRIPTION: Diagno-syst builds accurate inventories for biodiversity. It performs supervised clustering of reads obtained from a next-generation sequencing experiment, mapping onto an existing reference database, and assignment of taxonomic annotations.

- Participants: Alain Franc, Jean-Marc Frigerio, Philippe Chaumeil and Franck Salin
- Partner: INRA
- Contact: Alain Franc
- Publication: diagno-syst: a tool for accurate inventories in metabarcoding

6.5. Alcyone

Alcyone instantiates bioinformatics environments from specifications committed to a Git repository
KEYWORDS: Docker - Orchestration - Bioinformatics - Microservices - Versioning
SCIENTIFIC DESCRIPTION: Alcyone conceives the user's computing environment as a microservices architecture, where each bioinformatics tool in the specification is a separate containerized Docker service. Alcyone builds a master container for the specified environment that is responsible for building, updating, deploying and stopping these containers, as well as recording and sharing the environment in a Git repository. The master container can be manipulated using a command-line interface.
FUNCTIONAL DESCRIPTION: Alcyone defines a file structure for the specifying bioinformatics analysis environments, including tool choice, interoperability, and sources of raw data. These specifications are recorded in a Git repository. Alcyone compiles a specification into a master Docker container that deploys and orchestrates containers for each of the component tools. Alcyone can restore any version of an environment recorded in the Git repository.
NEWS OF THE YEAR: Alcyone was designed and implemented this year.

- Participants: Louise-Amelie Schmitt and David Sherman
- Contact: David Sherman
- URL: https://team.inria.fr/pleiade/alcyone/

6.6. family-3d

KEYWORDS: Biodiversity - Point cloud - 3D modeling
SCIENTIFIC DESCRIPTION: The method statistically selects a subset of pairwise distances between proteins in the family, constructs a weighted graph, and lays it out using an adaptation of the three-dimensional extension of the Kamada-Kawai force-directed layout.
FUNCTIONAL DESCRIPTION: Family-3D lays out high-dimension protein family point clouds in 3D space. The resulting lower-dimension forms can be printed, so that they can be explored and compared manually. They can also be explored interactively or stereographically.

Comparison of the 3D forms reveals classes of structurally similar families, whose characteristic shapes correspond to different evolutionary scenarios. Some of these scenarios are: neofunctionalization, subfunctionalization, founder gene effect, ancestral family.

To facilitate curator training, Family-3D includes an interactive terminal containing a microcontroller, an RFID reader, and an LED ring. A set of shapes that fall in predetermined classes is printed, with a unique RFID tag in each shape. Trainees classify family shapes by manual inspection and submit their classes to the terminal, which evaluates the proposed class and provides visual feedback.

- Participant: David Sherman
- Contact: David Sherman
- URL: https://gitlab.inria.fr/pleiade/family-3d

6.7. magecal

KEYWORD: Genomics
SCIENTIFIC DESCRIPTION: Magecal independently runs training and prediction steps for Augustus, Conrad, GeneID, GeneMark, and Snap. The results are cleaned and integrated into a common format. Jigsaw is trained and used for model reconciliation. Consistency constraints are applied to ensure that phase and intron structure are biologically plausible.
FUNCTIONAL DESCRIPTION: Magecal predicts a set of protein coding genes in fungal genomic sequences, using different de novo prediction algorithms, and reconciling the predictions with the aid of comparative data. Magecal applies consistency constraints to guarantee that the predicted genes are biologically valid.

RELEASE FUNCTIONAL DESCRIPTION: Dockerization and compatibility with Alcyone

- Participants: Pascal Durrens and David Sherman
- Contact: David Sherman
- URL: https://gitlab.inria.fr/magecal/magecal

6.8. AsebaHub

Turn-key bridging of Aseba mobile robots to wifi networks
KEYWORD: Robotics
SCIENTIFIC DESCRIPTION: Aseba is an open-source modular architecture for event-based control of multi-microcontroller robots, used in the Thymio-II educational robot, and integrated into development environments for teaching robotics programming to 8-18 year old children. Since 2014 Inria has contributed several modules to Aseba, including mDNS-sd support for discovering TCP/IP connections, an HTTP bridge that allows Aseba robots to be used with the Scratch programming environment, and photo-realistic 2D simulation.

Thymio-II robots only communicate through USB connections from a host computer, so until now it has been necessary to install Aseba software on that computer. This is not always possible in schools.

AsebaHub is a firmware image for wifi routers that takes responsibility for USB communication with Aseba robots. Each robot is exposed as a TCP/IP target, advertised using mDNS-sd. AsebaHub can group robots together in ad hoc Aseba networks. It provides HTTP access to robots so that they can be used with Scratch or Snap!. These services work out of the box, without any host configuration or software installation.

AsebaHub can operate as a wifi Access Point, or as a network Bridge to an existing local-area network. A slide switch on the side of the router seamlessly switches between these configurations.

AsebaHub is implemented by compiling Aseba software for the OpenWrt/LEDE open source router platform, adding interfacing code that automatically associates new robots, starts and stops the corresponding network services, and provides a web-based administrative interface.

FUNCTIONAL DESCRIPTION: AsebaHub is a small device with a USB port for connecting Aseba robots, single or with a USB hub. Every robot is made available as a network target on the wifi and wired local-area networks, where they can be discovered using mDNS-sd (Zeroconf/Bonjour). No network or user configuration is necessary.

AsebaHub works out of the box with the Aseba Studio and VPL programming environments. AsebaHub can be configured to also provide an HTTP service that is compatible with Scratch or other environments.

AsebaHub acts as either a wireless Access Point to which users may connect, or as a Bridge to an existing local-area network. Either configuration can be chosen seamlessly with the flick of a switch.

- Participants: David Sherman and Louise-Amelie Schmitt
- Contact: David Sherman

<h1 style="text-align:center; color:red">SERPICO Project-Team</h1>

6. New Software and Platforms

6.1. ATLAS

KEYWORDS: Image segmentation - Object detection - Photonic imaging - Image analysis - Fluorescence microscopy

FUNCTIONAL DESCRIPTION: The ATLAS software enables to detect spots in 2D fluorescence images. The spot size is automatically selected and the detection threshold adapts to the local image contrasts. ATLAS relies on the Laplacian of Gaussian (LoG) filter, which both reduces noise and enhances spots. A multiscale representation of the image is built to automatically select the optimal LoG variance. Local statistics of the LoG image are estimated in a Gaussian window, and the detection threshold is pointwise inferred from a probability of false alarm (PFA). The user only has to specify: i/ size of the Gaussian window, ii/ PFA value. The Gaussian window must be about the size of the background structures, increasing the PFA increases the number of detections.

- Participants: Antoine Basset, Patrick Bouthemy, Charles Kervrann, Jérôme Boulanger and Jean Salamero
- Partner: UMR 144 CNRS - Institut Curie
- Contact: Patrick Bouthemy
- Publication: Adaptive spot detection with optimal scale selection in fluorescence microscopy images
- URL: http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::ATLAS

6.2. C-CRAFT

KEYWORDS: Fluorescence microscopy - Photonic imaging - Image analysis - Detection - 3D - Health - Biology - Segmentation

FUNCTIONAL DESCRIPTION: The C-CRAFT software enables to jointly segment small particles and estimate background in 2D or 3D fluorescence microscopy image sequences. The vesicle segmentation and background estimation problem is formulated as a global energy minimization problem in the Conditional Random Field framework. A patch-based image representation is used to detect spatial irregularity in the image. An iterative scheme based on graph-cut algorithm is proposed for energy minimization.

- Participants: Thierry Pécot, Charles Kervrann, Patrick Bouthemy and Jean Salamero
- Partner: UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- Publication: Background Fluorescence Estimation and Vesicle Segmentation in Live Cell Imaging with Conditional Random Fields
- URL: http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::C-CRAFT

6.3. F2D-SAFIR

KEYWORDS: Biomedical imaging - Photonic imaging - Fluorescence microscopy - Image processing

FUNCTIONAL DESCRIPTION: The F2D-SAFIR software removes mixed Gaussian-Poisson noise in large 2D images, typically 10000 x 10000 pixels, in a few seconds. The method is unsupervised and is a simplified version of the method related to the ND-SAFIR software. The software is dedicated to microarrays image denoising for disease diagnosis and multiple applications (gene expression, genotyping, aCGH, ChIP-chip, microRNA, ...).

- Participant: Charles Kervrann
- Partner: INRA
- Contact: Charles Kervrann

6.4. GcoPS

KEYWORDS: Photonic imaging - Fluorescence microscopy - Image processing - Statistic analysis
FUNCTIONAL DESCRIPTION: The GCOPS (Geo-Co-Positioning System) software is dedicated to the co-localization of fluorescence image pairs for both conventional and super-resolution microscopy. The procedure is only controlled by a p-value and tests whether the Pearson correlation between two binary images is significantly positive. It amounts to quantifying the interaction strength by the area/volume of the intersection between the two binary images viewed as random distributions of geometrical objects. Under mild assumptions, it turns out that the appropriately normalized Pearson correlation follows a standard normal distribution under the null hypothesis if the number of image pixels is large. Unlike previous methods, GcoPS handles 2D and 3D images, variable SNRs and any kind of cell shapes. It is able to co-localize large regions with small dots, as it is the case in TIRF-PALM experiments and to detect negative co-localization. The typical processing time is two milliseconds per image pair in 2D and a few seconds in 3D, with no dependence on the number of objects per image. In addition, the method provides maps to geo-co-localize molecule interactions in specific image regions.

- Participants: Thierry Pécot, Frédéric Lavancier, Charles Kervrann and Liu Zengzhen
- Partners: Université de Nantes - UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- Publication: A Fast Automatic Colocalization Method for 3D Live Cell and Super-Resolution Microscopy
- URL: http://icy.bioimageanalysis.org/plugin/GcoPS

6.5. Hullkground

KEYWORDS: Biomedical imaging - Photonic imaging - Fluorescence microscopy - Image processing
FUNCTIONAL DESCRIPTION: The HullkGround software decomposes a fluorescence microscopy image sequence into two dynamic components: i) an image sequence showing mobile objects, ii) an image sequence showing the slightly moving background. Each temporal signal of the sequence is processed individually and analyzed with computational geometry tools. The convex hull is estimated automatically for each pixel and subtracted to the original signal. The method is unsupervised, requires no parameter tuning and is a simplified version of the shapes-based scale-space method.

- Participants: Anatole Chessel, Charles Kervrann and Jean Salamero
- Partner: UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- URL: http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::Hullkground

6.6. Motion2D

KEYWORDS: Image sequence - Motion model - 2D

FUNCTIONAL DESCRIPTION: The Motion2D software is a multi-platform object-oriented library to estimate 2D parametric motion models in an image sequence. It can handle several types of motion models, namely, constant (translation), affine, and quadratic models. Moreover, it includes the possibility of accounting for a global variation of illumination and more recently for temporal image intensity decay (e.g. due to photobleaching decay in fluorescence microscopy). The use of such motion models has been proved adequate and efficient for solving problems such as optic flow computation, motion segmentation, detection of independent moving objects, object tracking, or camera motion estimation, and in numerous application domains (video surveillance, visual servoing for robots, video coding, video indexing), including biological imaging (image stack registration, motion compensation in videomicroscopy). Motion2D is an extended and optimized implementation of the robust, multi-resolution and incremental estimation method (exploiting only the spatio-temporal derivatives of the image intensity function). Real-time processing is achievable for motion models involving up to six parameters. Motion2D can be applied to the entire image or to any pre-defined window or region in the image.

RELEASE FUNCTIONAL DESCRIPTION: Modifications and improvements in the PNG image file support. Support RAW and Mpeg2 video format as input (see CReader). The available video format which can be handled by the motion estimator are given by CReader::EReaderFormat. For the results, video sequences can be writen using the format specified by CWriter::EWriterFormat. Support Fedora 3 (g++ 3.4.2).

- Participants: Patrick Bouthemy, Jean Marc Odobez, Fabien Spindler, Thierry Pécot and Charles Kervrann
- Contact: Patrick Bouthemy
- URL: http://www.irisa.fr/vista/Motion2D/

6.7. ND-SAFIR

KEYWORDS: Fluorescence microscopy - Photonic imaging - Image analysis - Health - Biomedical imaging
SCIENTIFIC DESCRIPTION: ND-SAFIR is a software for denoising n-dimentionnal images especially dedicated to microscopy image sequence analysis. It is able to deal with 2D, 3D, 2D+time, 3D+time images have one or more color channel. It is adapted to Gaussian and Poisson-Gaussian noise which are usually encountered in photonic imaging. Several papers describe the detail of the method used in ndsafir to recover noise free images (see references).

- Participants: Jérôme Boulanger, Charles Kervrann, Patrick Bouthemy and Jean Salamero
- Partners: INRA - PiCT - UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- URL: http://serpico.rennes.inria.fr/doku.php?id=software:nd-safir:index

6.8. OWF

KEYWORDS: Image filter - Image processing - Statistics
FUNCTIONAL DESCRIPTION: The OWF software enables to denoise images corrupted by additive white Gaussian noise. In the line of work of the Non-Local means and ND-SAFIR algorithms, this adaptive estimator is based on the weighted average of observations taken in a neighborhood with weights depending on the similarity of local patches. The idea is to compute adaptive weights that best minimize an upper bound of the pointwise L2 risk. The spatially varying smoothing parameter is automatically adjusted to the image context. The proposed algorithm is fast and easy to control and is competitive when compared to the more sophisticated NL-means filters.

- Participants: Qiyu Jin, Ion Grama, Quansheng Liu and Charles Kervrann
- Partner: University of Bretagne-Sud
- Contact: Charles Kervrann
- Publication: Non-local means and optimal weights for noise removal
- URL: http://serpico.rennes.inria.fr/doku.php?id=software:owf

6.9. QuantEv

KEYWORDS: Photonic imaging - Fluorescence microscopy - Biomedical imaging - Image analysis - Image sequence - Statistic analysis

FUNCTIONAL DESCRIPTION: The QUANTEV software analyzes the spatial distribution of intracellular events represented by any static or dynamical descriptor, provided that the descriptors are associated with spatial coordinates. QUANTEV first computes 3D histograms of descriptors in a cylindrical coordinate system with computational cell shape normalization, enabling comparisons between cells of different shape. Densities are obtained via adaptive kernel density estimation, and we use the Circular Earth Mover's Distance to measure the dissimilarity between densities associated to different experimental conditions. A statistical analysis on these distances reliably takes into account the biological variability over replicated experiments.

- Participants: Thierry Pécot, Charles Kervrann, Jérôme Boulanger, Liu Zengzhen and Jean Salamero
- Partner: UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- Publication: QuantEv: quantifying the spatial distribution of intracellular events
- URL: http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::QuantEv-Densities

6.10. TMA-Lib

KEYWORDS: Photonic imaging - Fluorescence microscopy - Biomedical imaging - Image processing

FUNCTIONAL DESCRIPTION: The TMA-LIB enables to jointly detect suing adaptive wavelet transform, segment with parametric active contours and restore (i.e., artifact correction and deconvolution) TMA (Tissue MicroArrays) images.

- Participants: Hoai Nam Nguyen, Charles Kervrann, Cyril Cauchois and Vincent Paveau
- Partner: Innopsys
- Contact: Charles Kervrann
- Publications: A variational method for dejittering large fluorescence line scanner images - Generalized Sparse Variation Regularization for Large Fluorescence Image Deconvolution - ATMAD : robust image analysis for Automatic Tissue MicroArray De-arraying

6.11. TOTH

KEYWORDS: Photonic imaging - Fluorescence microscopy - Biomedical imaging - Classification - Statistical categorisation techniques - Statistics - Image sequence - Visual tracking

FUNCTIONAL DESCRIPTION: The TOTH software classifies trajectories of biomolecules computed with tracking algorithms. Trajectories in living cells are generally modelled with three types of diffusion processes: (i) free diffusion, (ii) subdiffusion or (iii) superdiffusion. We used a test approach with the Brownian motion as the null hypothesis, and developed a non-parametric three-decision test whose alternatives are subdiffusion and superdiffusion. First, we built a single test procedure for testing a single trajectory. Second, we proposed a multiple test procedure for testing a collection of trajectories. These procedures control respectively the type I error and the false discovery rate. Our approach can be considered as an alternative to the Mean Square Displacement (MSD) method commonly used to address this issue. It gives more reliable results as confirmed by our Monte Carlo simulations and evaluations on real sequences of images depicting protein dynamics acquired with TIRF or SPT-PALM microscopy.

- Participants: Vincent Briane, Charles Kervrann and Myriam Vimond
- Partner: ENSAI
- Contact: Charles Kervrann
- Publication: A Statistical Analysis of Particle Trajectories in Living Cells
- URL: http://serpico.rennes.inria.fr/doku.php?id=software:thot:index

6.12. SparseVolution

Sparse Variation for 2D Image Decovolution

KEYWORDS: 2D - Fluorescence microscopy - Image processing - Problem inverse - Deconvolution

FUNCTIONAL DESCRIPTION: In order to improve the resolution of acquired fluorescence images, we introduced a method of image deconvolution by considering a family of convex regularizers. The considered regularizers are generalized from the concept of Sparse Variation which combines the L1 norm and Total Variation (TV) to favors the colocalization of high-intensity pixels and high-magnitude gradient. The experiments showed that the proposed regularization approach produces competitive deconvolution results on fluorescence images, compared to those obtained with other approaches such as TV or the Schatten norm of Hessian matrix. The final deconvolution algorithm has been dedicated to large 2D 20 000 x 20 000 images. The method is able to process a 512 x 512 image in 250 ms (Matlab) with a non optimized implementation.

- Participants: Hoai Nam Nguyen and Charles Kervrann
- Partner: Innopsys
- Contact: Charles Kervrann

6.13. Platforms

6.13.1. Mobyle@Serpico plateform and software distribution

*Figure 2. Mobyle@*SERPICO *web portal.*

The objective is to disseminate the distribution of SERPICO image processing software in the community of cell biology and cell imaging.

Free binaries: software packages have been compiled for the main operating systems (Linux, MacOS, Windows) using CMake (see http://www.cmake.org/). They are freely available on the team website under a proprietary license (e.g. ND-SAFIR and HULLKGROUND are distributed this way at http://serpico.rennes.inria.fr/doku.php?id=software:index).

Mobyle@Serpico web portal: An on-line version (http://mobyle-serpico.rennes.inria.fr) of the image processing algorithms has been developped using the Mobyle framework (Institut Pasteur, see http://mobyle.pasteur.fr/). The main role of this web portal (see Fig. 2) is to demonstrate the performance of the programs developed by the team: QUANTEV, C-CRAFT[14], ATLAS[1], HULLKGROUND[38], KLTRACKER[44], MOTION2D[43], MS-DETECT[39], ND-SAFIR[6], OPTICALFLOW and FLUX ESTIMATION [14]. The web interface makes our image processing methods available for biologists at Mobyle@SERPICO (http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#welcome) without any installation or configuration on their own. The size of submitted images is limited to 200 MegaBytes per user and all the results are kept 15 days. The web portal and calculations run on a server with 2 CPU x 8 cores, 64 GigaBytes of RAM (500 MegaBytes for each user / Data is saved for 3 months).

ImageJ plugins: IMAGEJ (see http://rsb.info.nih.gov/ij/) is a widely used image visualization and analysis software for biologist users. We have developed IMAGEJ plug-in JAVA versions of the following software: ND-SAFIR [6], HULLKGROUND [38], MOTION2D [43], ATLAS [1]. The C-CRAFT algorithm [14] has been developped for the image processing ICY platform (http://icy.bioimageanalysis.org/).

- **Contact:** Charles Kervrann, Charles Deltel (Inria Rennes SED).
- **Partner:** UMR 144 CNRS-Institut Curie and France-BioImaging.

6.13.2. IGRIDA-Serpico cluster

The IGRIDA-Serpico cluster of 200 nodes is opened for end-users for large scale computing and data sets processing (200 TeraBytes).

- **Batch Scheduler:** OAR
- **File management:** Puppet / Git / Capistrano
- **OS:** Linux Debian 7
- **User connexion:** public ssh key
- **Contact:** Charles Kervrann, Charles Deltel (Inria Rennes SED).

ARAMIS Project-Team

6. New Software and Platforms

6.1. Brain Networks Toolbox

KEYWORDS: Neuroimaging - Medical imaging

FUNCTIONAL DESCRIPTION: Brain Networks Toolbox is an open-source package of documented routines implementing new graph algorithms for brain network analysis. It mainly contains Matlab code of new methods developed by the team and associated to publications (e.g., brain network thresholding, extraction of the information redundancy, node accessibility, etc). It requires, as input, adjacency matrices representing brain connectivity networks. Thus, it is independent on the specific approach used to construct brain networks and it can be used to extract network properties from any neuroimaging modality in healthy and diseased subjects.

- Participants: Fabrizio De Vico Fallani, Jeremy Guillon and Mario Chavez
- Contact: Fabrizio De Vico Fallani
- URL: https://github.com/brain-network/bnt

6.2. Deformetrica

KEYWORDS: 3D modeling - C++ - Automatic Learning - Mesh - Anatomy - Image analysis

SCIENTIFIC DESCRIPTION: Deformetrica is a software for the statistical analysis of 2D and 3D shape data. It essentially computes deformations of the 2D or 3D ambient space, which, in turn, warp any object embedded in this space, whether this object is a curve, a surface, a structured or unstructured set of points, or any combination of them.

Deformetrica comes with two applications:

registration, which computes the best possible deformation between two sets of objects, atlas construction, which computes an average object configuration from a collection of object sets, and the deformations from this average to each sample in the collection.

Deformetrica has very little requirements about the data it can deal with. In particular, it does not require point correspondence between objects!

FUNCTIONAL DESCRIPTION: Deformetrica is a software for the statistical analysis of 2D and 3D shape data. It essentially computes deformations of the 2D or 3D ambient space, which, in turn, warp any object embedded in this space, whether this object is a curve, a surface, a structured or unstructured set of points, or any combination of them.

Deformetrica comes with two applications:

- Registration, which computes the optimal deformation between two sets of objects,

- Atlas construction, which computes an average object configuration from a collection of object sets, and the deformations from this average to each sample in the collection.

Deformetrica has very little requirements about the data it can deal with. In particular, it does not require point correspondence between objects!

- Participants: Alexandre Routier, Ana Fouquier, Barbara Gris, Benjamin Charlier, Cédric Doucet, Joan Alexis Glaunès, Marcel Prastawa, Michael Bacci, Pietro Gori and Stanley Durrleman
- Partners: University of Utah - Université de Montpellier 2 - Université Paris-Descartes
- Contact: Stanley Durrleman
- URL: http://www.deformetrica.org/

6.3. Clinica

KEYWORDS: Neuroimaging - Brain MRI - MRI - Clinical analysis - Image analysis - Machine learning

SCIENTIFIC DESCRIPTION: Clinica is a software platform for multimodal brain image analysis in clinical research studies. It makes it easy to apply advanced analysis tools to large scale clinical studies. For that purpose, it integrates a comprehensive set of processing tools for the main neuroimaging modalities: currently MRI (anatomical, functional, diffusion) and PET, in the future, EEG/MEG. For each modality, Clinica allows to easily extract various types of features (regional measures, parametric maps, surfaces, curves, networks). Such features are then subsequently used as input of machine learning, statistical modeling, morphometry or network analysis methods. Processing pipelines are based on combinations of freely available tools developed by the community. It provides an integrated data management specification to store raw and processing data. Clinica is written in Python. It uses the Nipype system for pipelining. It combines widely-used software for neuroimaging data analysis (SPM, Freesurfer, FSL, MRtrix...), morphometry (Deformetrica), machine learning (Scikit-learn) and the BIDS standard for data organization.

FUNCTIONAL DESCRIPTION: Clinica is a software platform for multimodal brain image analysis in clinical research studies. It makes it easy to apply advanced analysis tools to large scale clinical studies. For that purpose, it integrates a comprehensive set of processing tools for the main neuroimaging modalities: currently MRI (anatomical, functional, diffusion) and PET, in the future, EEG/MEG. For each modality, Clinica allows to easily extract various types of features (regional measures, parametric maps, surfaces, curves, networks). Such features are then subsequently used as input of machine learning, statistical modeling, morphometry or network analysis methods. Clinica also provides an integrated data management specification to store raw and processing data. Overall, Clinica helps to: i) apply advanced analysis tools to clinical research studies, ii) easily share data and results, iii) make research more reproducible.

NEWS OF THE YEAR: - Three clinical studies made with Clinica Clinica : Bertrand et al, JAMA Neurology, 2018 , Jacquemont et al, Neurobiol Aging, 2017, Wen et al, JNNP, 2018 - Clinica presented at OHBM 2018 conference - Clinica was the support for the tutorial "Pattern Recognition for Neuroimaging" at OHBM 2018

- Participants: Jeremy Guillon, Thomas Jacquemont, Pascal Lu, Arnaud Marcoux, Tristan Moreau, Alexandre Routier, Jorge Samper Gonzalez, Junhao Wen, Olivier Colliot, Stanley Durrleman, Michael Bacci, Simona Bottani, Ninon Burgos, Sabrina Fontanella, Pietro Gori, Mauricio Diaz Melo and Elina Thibeau-Sutre

- Partners: Institut du Cerveau et de la Moelle épinière (ICM) - CNRS - INSERM - UPMC

- Contact: Olivier Colliot

- Publications: Amyloidosis and neurodegeneration result in distinct structural connectivity patterns in mild cognitive impairment - Yet Another ADNI Machine Learning Paper? Paving The Way Towards Fully-reproducible Research on Classification of Alzheimer's Disease - Reproducible evaluation of classification methods in Alzheimer's disease: Framework and application to MRI and PET data - Neurite density is reduced in the presymptomatic phase of C9orf72 disease - Early cognitive, structural and microstructural changes in c9orf72 presymptomatic carriers before 40 years of age

- URL: http://www.clinica.run

6.4. Platforms

6.4.1. *Platform Brain-computer interface*

Our team coordinates the developments of the Brain-Computer Interface (BCI) platform at the Centre EEG/MEG of the neuroimaging core facility of the ICM. Several projects, including our NETBCI NSF/NIH/ANR and ATTACK Big-brain theory funded projects, as well as experiments by different researchers of the Institute, are currently being run. To reinforce the impact of the platform we have recently recruited an engineer (J. Gonzalez-Astudillo) for the software and technical development.

ATHENA Project-Team

5. New Software and Platforms

5.1. BCI-VIZAPP

BCI visual applications

KEYWORDS: Health - Brain-Computer Interface - GUI (Graphical User Interface)

SCIENTIFIC DESCRIPTION: Bci-Vizapp is a library that allows (in interaction with OpenViBE) to build BCI (Brain Computer Interfaces) applications based on the P300 speller principle. Bci-Vizapp provides a library that allows you to create the BCI's stimulation part as part of the Qt toolkit. Being able to use a standard toolkit to make BCI applications is a strong Bci-Vizapp originality. Indeed, in general the use of such toolkits is prohibited by the need for a very precise control of the display timings, which generally eliminates high-level graphic toolkits such as Qt.

FUNCTIONAL DESCRIPTION: BCI-VIZAPP includes a virtual keyboard for typing text, a photodiode monitoring application for checking timing issues. It communicates with the OpenViBE acquisition server for signal acquisition and with the OpenViBE designer for signal processing. The configuration is performed through a wizard.

This software is a new version following the CoAdapt P300 stimulator software.

NEWS OF THE YEAR: Bci-Vizapp is undergoing a profound transmutation with the help of CRISAM's SED in ADT BciBrowser (part of the AMDT). This change aims at integrating the functionality of Bci-Vizapp in third-party applications such as a web browsers.

- Participants: Nathanaël Foy, Romain Lacroix, Maureen Clerc and Théodore Papadopoulo
- Contact: Maureen Clerc

5.2. DIPY

Diffusion Imaging in Python

KEYWORDS: MRI - Medical imaging

FUNCTIONAL DESCRIPTION: Diffusion Imaging in Python (Dipy) is a free and open source software project for computational neuroanatomy, focusing mainly on diffusion magnetic resonance imaging (dMRI) analysis. E. Garyfallidis (now Indiana University) is the founder and lead engineer of this open source project in the development of diffusion MRI methods. We continuously collaborate with this global effort and our effort is combined with Université de Sherbrooke, in Canada and Stanford University among others. See for example our registration, denoising, tractography and microstructures tutorials.

- Participants: Demian Wassermann and Rutger Fick
- Partner: Sherbrooke University
- Contact: Demian Wassermann
- URL: http://nipy.org/dipy/

5.3. High Performance Diffusion MRI

KEYWORDS: Health - Neuroimaging - Medical imaging

FUNCTIONAL DESCRIPTION: This library has been developed and transferred to the Cie Olea Medical currently in charge of its validation and inclusion in its Olea Sphere platform. We have been closely involved in pushing the frontiers of the diffusion MRI (dMRI) in the recent years, especially in the mathematical modelling and processing of the dMRI signal and have developed state-of-the-art software implementations in the form of a C++ library that can be effectively used to infer the complex microstructure of the cerebral white matter. The algorithms and software transfered to Olea Medical fall into four categories : (i) local tissue modelling, which includes both popular 2nd order models and advanced higher than 2nd order models such as DTI, higher order Cartesian tensors (HOTs), ODF, FOD, EAP, maxima extraction, regularization and segmentation, (ii) generation of scalar indices (or biomarkers), which include DTI biomarkers, Diffusion Kurtosis Imaging (DKI) and invariants of 4th order tensors, (iii) global structure estimation, which includes deterministic and probabilistic tractography, and (iv) data visualisation for scalar indices, local models and global structures.

- Participants: Aurobrata Ghosh, Rachid Deriche and Théodore Papadopoulo
- Partner: Olea Medical
- Contact: Rachid Deriche

5.4. OpenMEEG

KEYWORDS: Health - Neuroimaging - Medical imaging

SCIENTIFIC DESCRIPTION: OpenMEEG provides a symmetric boundary element method (BEM) implementation for solving the forward problem of electromagnetic propagation over heterogeneous media made of several domains of homogeneous and isotropic conductivities. OpenMEEG works for the quasistatic regime (frequencies < 100Hz and medium diameter < 1m).

FUNCTIONAL DESCRIPTION: OpenMEEG provides state-of-the art tools for modelling bio-electromagnetic propagation in the quasi-static regime. It is based on the symmetric BEM for the EEG/MEG forward problem, with a distributed source model. OpenMEEG has also been used to model the forward problem of ECoG, for modelling nerves or the cochlea. OpenMEEG is a free, open software written in C++ with python bindings. OpenMEEG is used through a command line interface, but is also interfaced in graphical interfaces such as BrainStorm, FieldTrip or SPM.

RELEASE FUNCTIONAL DESCRIPTION: OpenMEEG has had a large update including notably the parallelisation of some operators and bug corrections. The new version allows in addition the use of non-nested domains.

NEWS OF THE YEAR: OpenMEEG has had a large update including notably the parallelisation of some operators and bug corrections. The new version allows in addition the use of non-nested domains. These improvements have been ditributed with the two new releases (2.4.0 and 2.4.1) made in 2018.

- Participants: Alexandre Gramfort, Emmanuel Olivi, Geoffray Adde, Jan Kybic, Kai Dang, Maureen Clerc, Perrine Landreau, Renaud Keriven and Théodore Papadopoulo
- Contact: Théodore Papadopoulo
- Publications: OpenMEEG: opensource software for quasistatic bioelectromagnetics - Forward Field Computation with OpenMEEG. - Source modeling of ElectroCorticoGraphy (ECoG) data: Stability analysis and spatial filtering
- URL: http://openmeeg.github.io/

BIOVISION Project-Team

5. New Software and Platforms

5.1. Virtual Retina

A biological retina model with contrast gain control for large scale simulations

KEYWORDS: Neurosciences - Simulation - Biology - Health

SCIENTIFIC DESCRIPTION: Virtual Retina has a variety of biological features implemented such as (i) spatio-temporal linear filter implementing the basic center/surround organization of retinal filtering, (ii) non-linear contrast gain control mechanism providing instantaneous adaptation to the local level of contrast, (iii) spike generation by one or several layers of ganglion cells paving the visual field.

FUNCTIONAL DESCRIPTION: Virtual Retina is a simulation software that allows large-scale simulations of biologically-plausible retinas.

- Participants: Adrien Wohrer, Pierre Kornprobst, Bruno Cessac, Maria-Jose Escobar and Thierry Viéville
- Contact: Pierre Kornprobst
- Publication: Virtual Retina: A biological retina model and simulator, with contrast gain control
- URL: https://team.inria.fr/biovision/virtualretina/

5.2. PRANAS

Platform for Retinal ANalysis And Simulation

KEYWORDS: Retina - Neural Code - Data management - Statistics - Modeling - Vision

SCIENTIFIC DESCRIPTION: PRANAS was designed as a user-friendly tool dedicated to neuroscientist community in a large sense, i.e., not only experienced computational neuroscientists. It has two main goals : (i) to analyze retina data, especially spatio-temporal correlations, at single cell but also population levels, (ii) to simulate the spike response of the retina to a visual flow with a customizable retina simulator which evolves in synergy with experimental data analysis. In general, PRANAS allows to explore several aspects of retinal image processing such as understanding how to reproduce accurately the statistics of the spiking activity at the population level, or reconciling connectomics and simple computational rules for visual motion detection. This makes this tool a unique platform to better understand how the retina works.

FUNCTIONAL DESCRIPTION: The retina encodes a visual scene by trains of action potentials sent to the brain via the optic nerve. PRANAS brings to neuroscientists and modelers tools to better understand this coding. It integrates a retina simulator allowing large scale simulations while keeping a strong biological plausibility and a toolbox for the analysis of spike trains population statistics. The statistical method (entropy maximization under constraints) takes into account both spatial and temporal correlations as constraints, allowing to analyze the effects of memory on statistics. PRANAS also integrates a tool computing and representing in 3D (time-space) receptive fields. All these tools are accessible through a friendly graphical user interface. The most CPU-costly of them has been implemented to run in parallel. The actual version simulates healty retinas but the long term goal is to study retinas with a pathology (DMLA, Retinitis Pigmentosa, Glaucoma).

- Authors: Bruno Cessac, Pierre Kornprobst, Sélim Kraria, Hassan Nasser, Daniela Pamplona, Geoffrey Portelli and Adrien Wohrer
- Contact: Bruno Cessac
- Publication: PRANAS: A New Platform for Retinal Analysis and Simulation
- URL: https://team.inria.fr/biovision/pranas-software/

5.3. Platforms

5.3.1. VRead

We are currently developing the VRead platform, a reading platform for digital content. We are now in the phase of building and testing prototypes with low-vision patients. We have started to conduct a qualitative Market research with patients to get a continuous feedback from them, discover their needs and thus better drive the developments. A special care is taken for ergonomics to optimize user experience in virtual reality. This is a crucial aspect in this project, especially because we primarily target a more fragile population so that we have to take into account their vision loss and cognitive skills. As for the technical aspect, we are using the Unity game engine along with the Oculus SDK, allowing us to deploy and test early on the Samsung GearVR mobile platform. For scripting the engine we code in C# using the proprietary directives of Unity. We ship the VRead Viewer with an operator application which allows for supervision and tuning of parameters of the reader in realtime. This application is written using the Unity SDK and is deployable under macOS, Windows and Linux.

This project received financial support from Université Côte d'Azur (France) (duration: 18 months, period: Aug. 2017– Jan. 2019 and Inria (via InriaHUB programme). It is done in collaboration with Aix-Marseille Université (CNRS, Laboratoire de Psychologie Cognitive, Marseille, France), Centre hospitalier Pasteur 2 (service d'ophtalmologie, Nice, France) and University of Genoa (DIBRIS, Genoa, Italy).

5.3.2. *Macular*

We are currently developing the platform Macular, a large-scale simulations platform of impaired retinas, allowing to mimic specific degeneracies or pharmacologically induced impairments, as well as to emulate electric stimulation by prostheses. With this tool scientists will be able to design a simulation gui adapted to their need, so as to test hypotheses, make in-silico experiments prior to real experiments, test models, change the equations of a model and look at the impact of the dynamics. We hope it will become a standard for the community of modelers, experimentalists in the academic word, as well as for companies doing research and development. Macular will also help to better understand how to design algorithms to help visually impaired individuals. Especially, the Biovision team wants to develop computer algorithms for retinal prostheses that reproduce the functions performed by the bypassed parts of the eye: these algorithms can then be used as a "camera to eye translator" in retinal prosthetics.

CAMIN Team

5. New Software and Platforms

5.1. RT_Stim

Real-Time simulation for functional electrical Stimulation

KEYWORDS: Real time - Biomechanics - Control - Co-simulation

FUNCTIONAL DESCRIPTION: Hybrid simulation architecture gathering in a single framework and consistent time scales both the numerical integration of the continuous model of a bio-mechanical system (bones, joints and muscles) and a model of the hardware and software control architecture, including control tasks, communication protocols and real-time schedulers. Simulation run in real-time when possible, and otherwise consistent time scales are generated. The framework is intended to seamlessly evolve from purely software models to hardware-in-the-loop simulation.

- Contact: Daniel Simon

5.2. Platforms

5.2.1. *Modular embedded architecture for real time control of a FES system*

Participants: Christine Azevedo Coste, Benoît Sijobert, Ronan Le Guillou.

The results presented in section 6.2 and 6.3 have led to the development of a new hardware and software architecture embedding a network of sensors and actuators interfaced to a controller, as part of Benoît Sijobert's PhD work and ADT STIMBIO (Ronan Le Guillou). In order to solve numerous issues and constraints observed during experiments, a new hardware and software architecture has been elaborated. The decision was made to decentralize the controller (i.e. the computer) directly on the participant, thereby relocating the essential wireless links around the user. For this purpose, a mini low-cost single board computer (Raspberry Pi3) was embedded in a 3D-printed case strapped around the waist of the subject. Using wireless inertial sensors connected as a WBAN, the sink node gets the data from all the IMUs, therefore highly decreasing the data flow when multiple IMUs were transmitting inside the network. To get rid of this limitation and guarantee an overall 100 Hz sampling rate no matter the number of IMUs, the wireless inertial sensors can be replaced by wired ones, low-cost with a high speed ARM Cortex-M0 based processor and a Kalman Filter directly providing quaternion estimation at 100 Hz for each IMU. The use of a multiplexer connected through an I2C interface (Inter Integrated Circuit) enabled to keep a 100 Hz rate using 4 IMUs.

The stimulator used in the experiments was a wireless programmable and controllable device. Latency issues and communication losses were observed when the computer sending the command to the stimulator was too far or if an obstacle was present between the computer and the participant wearing the stimulator. Taking advantage of the FES controller located on the subject to control the stimulator nearby has enabled us to solve this issue.

In this configuration, this autonomous FES controller is able to acquire the data, process them, execute control algorithms and send the appropriate stimulation command to the stimulator. For safety reasons, in order to access to the FES controller and to enable a remote access to the stimulation from a computer, an ad-hoc Wi-Fi network is automatically provided by the Raspberry on start-up. The ad-hoc network enables to be independent of a network infrastructure where the connection is not always possible (e.g. Wi-Fi network from the hospital).

This scalable architecture (Figure 3), developed as a modular system, now allows us to implement various new commands laws for Real Time closed loop control as well as giving us the ability to switch sensors and stimulators to meet the needs of specific applications. As part of making this system available for future projects in the team, the ability to easily change stimulators depending of the requirements was needed. To achieve this and in order for the FES architecture to directly control them, Application Programming Interfaces (APIs) were developed for 3 main commercial stimulators in the team. They each corresponds to a specific need and use case. The Vivaltis Phoenix Stimulator allows for low-weight embedding, wireless network control, but only 2 stimulation channels by pod, while being scalable. The BerkelBike Stimulator v2.0 presents a cumbersome but extended control compromise with 8 independent stimulation channels, which is an ideal solution for recumbent FES-assisted cycling. And finally the Hasomed Rehastim v1.0 allowing fine control but isn't battery powered in its commercial version and is not produced anymore.

This new architecture is currently used in clinical experiments and will continue to evolve with a goal of being easy to use, even by untrained clinicians. A funding (EDF Foundation) has been obtained by our clinical partner "CRF La Châtaigneraie" to perform a clinical protocol including 6 patients from which one will participate in the Cybathlon 2020 using this hardware and software architecture. The inclusions will begin in January 2019.
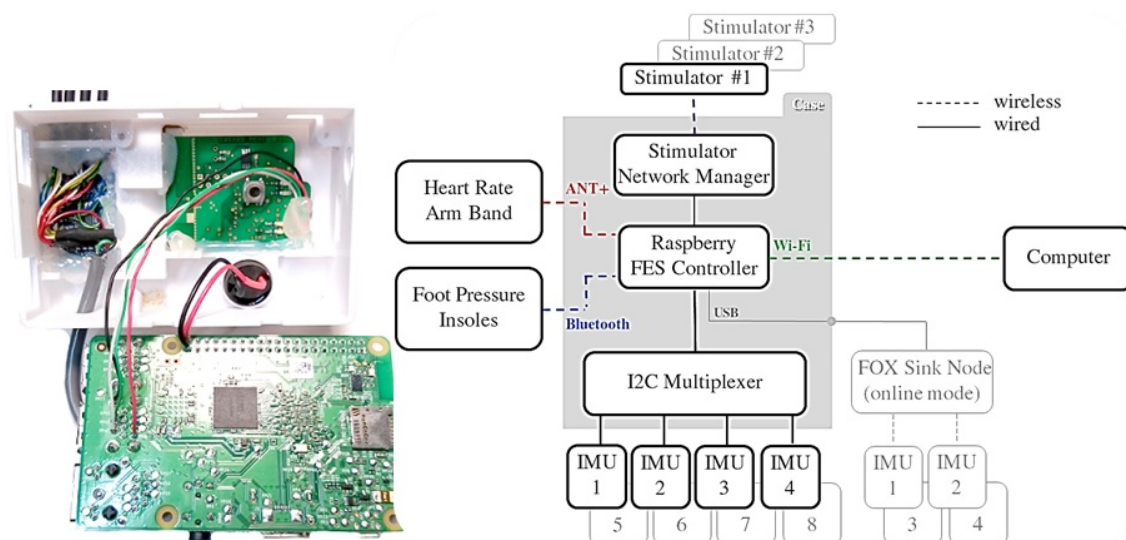
Figure 3. Experimental protocols have led to the development of a scalable hardware architecture decentralized on the subject.

5.2.2. *Tremor monitoring system based on acceleration detection in Parkinson's Disease*
Participants: Christine Azevedo Coste, Ronan Le Guillou.

As part of a preliminary study on the effects of Mindfulness meditation for patients with Parkinson's Disease (PD), an application was developed to monitor the accelerometer of a wrist worn device. The hypothesis being that reducing the cognitive load of a PD patient might reduce the severity of the tremors. We investigated a few devices that might correspond to our requirements : smartwatches, Myo armbands, Inertial Measurement Units,...Having already a Thalmic Myo Armband (Figure 4) we developed a program acquiring the accelerometer data in Real Time and logging it, as well as doing pre-processing and displaying it on the

screen of the clinician to allow him to monitor the session. While this system was ready and already tested, we had to search for another solution due to the termination of the commercial product. We then selected the smartwatch Samsung Gear S3 as a possible alternative and the dedicated application is currently under development.

Figure 4. i) Graphical User Interface of the TREMYO Armband monitoring application during acquisition ii) Baseline test with straight extended arm for temporal comparison of the tremors severity.

<p style="text-align:center;color:red;font-weight:bold;">EPIONE Project-Team</p>

5. New Software and Platforms

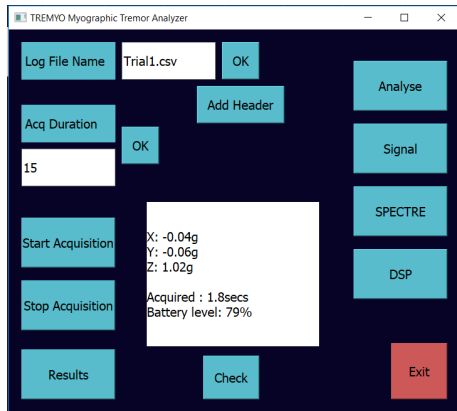## 5.1. CardiacSegmentationPropagation

KEYWORDS: 3D - Segmentation - Cardiac - MRI - Deep learning
FUNCTIONAL DESCRIPTION: Training of a deep learning model which is used for cardiac segmentation in short-axis MRI image stacks.

- Authors: Qiao Zheng, Hervé Delingette, Nicolas Duchateau and Nicholas Ayache
- Contact: Qiao Zheng
- Publication: hal-01753086, version 1

5.2. CardiacMotionFlow

KEYWORDS: 3D - Deep learning - Cardiac - Classification
FUNCTIONAL DESCRIPTION: Creation of a deep learning model for the motion tracking of the heart, extraction of characteristic quantities of the movement and shape of the heart to classify a sequence of cine-MRI cardiac images in terms of the types of pathologies (infarcted heart, dilated , hypertrophied, abnormality of the right ventricle).

- Contact: Qiao Zheng

5.3. MedInria

KEYWORDS: Visualization - DWI - Health - Segmentation - Medical imaging
SCIENTIFIC DESCRIPTION: medInria aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010, renewed in 2012. A fast-track ADT was awarded in 2017 to transition the software core to more recent dependencies and study the possibility of a consortium creation.The Visages team leads this Inria national project and participates in the development of the common core architecture and features of the software as well as in the development of specific plugins for the team's algorithm.
FUNCTIONAL DESCRIPTION: MedInria is a free software platform dedicated to medical data visualization and processing.

- Participants: Maxime Sermesant, Olivier Commowick and Théodore Papadopoulo
- Partners: HARVARD Medical School - IHU - LIRYC - NIH
- Contact: Olivier Commowick
- URL: http://med.inria.fr

5.4. GP-ProgressionModel

GP progression model
KEYWORDS: Data modeling - Data visualization - Data integration - Machine learning - Biostatistics - Statistical modeling - Medical applications - Evolution - Brain - Uncertainly - Uncertainty quantification - Alzheimer's disease - Probability - Stochastic models - Stochastic process - Trajectory Modeling - Marker selection - Health - Statistic analysis - Statistics - Bayesian estimation
FUNCTIONAL DESCRIPTION: Disease progression modeling (DPM) of Alzheimer's disease (AD) aims at revealing long term pathological trajectories from short term clinical data. Along with the ability of providing a data-driven description of the natural evolution of the pathology, DPM has the potential of representing a valuable clinical instrument for automatic diagnosis, by explicitly describing the biomarker transition from normal to pathological stages along the disease time axis.

In this software we reformulate DPM within a probabilistic setting to quantify the diagnostic uncertainty of individual disease severity in an hypothetical clinical scenario, with respect to missing measurements, biomarkers, and follow-up information. The proposed formulation of DPM provides a statistical reference for the accurate probabilistic assessment of the pathological stage of de-novo individuals, and represents a valuable instrument for quantifying the variability and the diagnostic value of biomarkers across disease stages.

This software is based on the publication:

Probabilistic disease progression modeling to characterize diagnostic uncertainty: Application to staging and prediction in Alzheimer's disease. Marco Lorenzi, Maurizio Filippone, Daniel C. Alexander, Sebastien Ourselin Neuroimage. 2017 Oct 24. pii: S1053-8119(17)30706-1. doi: 10.1016/j.neuroimage.2017.08.059. HAL Id : hal-01617750 https://hal.archives-ouvertes.fr/hal-01617750/

- Authors: Marco Lorenzi and Maurizio Filippone
- Contact: Marco Lorenzi
- URL: http://gpprogressionmodel.inria.fr

5.5. Music

Multi-modality Platform for Specific Imaging in Cardiology
KEYWORDS: Medical imaging - Cardiac Electrophysiology - Computer-assisted surgery - Cardiac - Health
FUNCTIONAL DESCRIPTION: MUSIC is a software developed by the Asclepios research project in close collaboration with the IHU LIRYC in order to propose functionalities dedicated to cardiac interventional planning and guidance. This includes specific tools (algorithms of segmentation, registration, etc.) as well as pipelines. The software is based on the MedInria platform.

- Participants: Florent Collot, Mathilde Merle and Maxime Sermesant
- Partner: IHU- Bordeau
- Contact: Maxime Sermesant
- URL: https://team.inria.fr/asclepios/software/music/

5.6. SOFA

Simulation Open Framework Architecture
KEYWORDS: Real time - Multi-physics simulation - Medical applications
FUNCTIONAL DESCRIPTION: SOFA is an Open Source framework primarily targeted at real-time simulation, with an emphasis on medical simulation. It is mostly intended for the research community to help develop new algorithms, but can also be used as an efficient prototyping tool. Based on an advanced software architecture, it allows : the creation of complex and evolving simulations by combining new algorithms with algorithms already included in SOFA, the modification of most parameters of the simulation (deformable behavior, surface representation, solver, constraints, collision algorithm, etc.) by simply editing an XML file, the building of complex models from simpler ones using a scene-graph description, the efficient simulation of the dynamics of interacting objects using abstract equation solvers, the reuse and easy comparison of a variety of available methods.

- Participants: Christian Duriez, François Faure, Hervé Delingette and Stéphane Cotin
- Partner: IGG
- Contact: Stéphane Cotin
- URL: http://www.sofa-framework.org

5.7. geomstats

Computations and statistics on manifolds with geometric structures

KEYWORD: Geometry

FUNCTIONAL DESCRIPTION: Geomstats is a python package that performs computations on manifolds such as hyperspheres, hyperbolic spaces, spaces of symmetric positive definite matrices and Lie groups of transformations. It provides efficient and extensively unit-tested implementations of these manifolds, together with useful Riemannian metrics and associated Exponential and Logarithm maps. The corresponding geodesic distances provide a range of intuitive choices of Machine Learning loss functions. We also give the corresponding Riemannian gradients. The operations implemented in geomstats are available with different computing backends such as numpy, tensorflow and keras. Geomstats manifold computations have are integrated into keras deep learning framework thanks to GPU-enabled implementations.

- Partner: Stanford Department of Statistics
- Contact: Nina Miolane
- URL: https://github.com/geomstats/

<p align="center">**GALEN-POST Team**</p>

6. New Software and Platforms

6.1. Platforms

6.1.1. *The Proximity Operator Repository*

Participants: Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with Giovanni Chierchia, Univ. Paris Est, and Patrick Combettes, North Carolina State University).

link: http://proximity-operator.net/

Proximity operators have become increasingly important tools as basic building blocks of proximal splitting algorithms, a class of algorithms that decompose complex composite convex optimization methods into simple steps involving one of the functions present in the model. This website provides formulas for efficiently computing the proximity operator of various functions, along with the associated codes.

6.1.2. *Kymatio*

Participant: Edouard Oyallon.

link: http://www.kymat.io

The website shares the software `Kymatio` for Scattering Transform, that computes cascade of wavelets and modulus non-linearity. The codes have been optimized for GPUs and work on the open-source framework *PyTorch*.

6.1.3. *Topical Node Embeddings*

Participant: Abdulkadir Çelikkanat

link: https://abdcelikkanat.github.io/projects/TNE/

TNE learns node representations on graphs combining node and topic information, as described in [45]. The framework has been implemented in Python and has been built upon widely used modules, including `networkx`, `scipy`, `gensim` and `scikit-learn`.

6.1.4. *BiasedWalk: Learning latent node features with biased random walks*

Participants: Fragkiskos Malliaros and Duong Nguyen (UC San Diego)

link: https://github.com/duong18/BiasedWalk/

The BiasedWalk network representation learning algorithm, computes latent node features on graphs based on biased random walks [33]. The framework has been implemented in Python and has been built upon widely used modules, including `networkx`, `numpy`, `gensim` and `scikit-learn`.

6.1.5. *DiffuGreedy: Influence maximization in complex networks based on diffusion cascades*

Participants: Fragkiskos Malliaros, Georgios Panagopoulos and Michalis Vazirgiannis (École Polytechnique)

link: https://goo.gl/GpfCVZ

The DiffuGreedy is an algorithm for influence maximization in complex networks, that is based on diffusion cascades. The algorithm implements the methodology described in [35]. It has been implemented in Python and has been built upon widely used modules, including `networkx`, `igraph`, `numpy` and `pandas`.

6.1.6. *Graph-based text categorization*

Participants: Fragkiskos Malliaros, Konstantinos Skianis and Michalis Vazirgiannis (École Polytechnique)

link: https://github.com/y3nk0/Graph-Based-TC/

Graph-based TC is a framework for text categorization that relies on a graph representation of documents. The framework uses various graph centrality criteria to determine the importance of a term within a document. It also makes use of word embeddings to further boost the performance of graph-based methods. The algorithm implements the methodology described in [39]. It has been implemented in Python and has been built upon widely used modules, including `networkx`, `igraph`, `numpy` and `scikit-learn`.

6.1.7. The PINK image library

Participant: Hugues Talbot

link: http://ibipio.hu/joomla/

The PINK image library is a general-purpose, open-source, portable image processing library specializing in discrete geometry and mathematical morphology. It is the result of several decades of research in these domains and features state-of-the art algorithmic implementation of both classical and leading edge DG and MM operators. These include nD parallel thinning and skeletonization methods and efficient hierarchical morphological transforms.

6.1.8. The Vivabrain AngioTK toolkit

Participant: Hugues Talbot

link: https://github.com/vivabrain/angiotk

AngioTK is a toolkit supported by Kitware (the authors of VTK) for the filtering, segmentation, generation and simulation of blood vessels. It was started in the context of the Vivabrain ANR project in 2012, but continues with the same as well as new partners. Applications are numerous, from the simulation and understanding of perfusion (see associated theme) to the simulation of realistic blood flow MRI images with associated ground truth, via the generation of blood vessel atlases.

MATHNEURO Team (section vide)

<p style="text-align:center;color:red;font-weight:bold">MIMESIS Team</p>

6. New Software and Platforms

6.1. SOFA

Simulation Open Framework Architecture

KEYWORDS: Real time - Multi-physics simulation - Medical applications

FUNCTIONAL DESCRIPTION: SOFA is an Open Source framework primarily targeted at real-time simulation, with an emphasis on medical simulation. It is mostly intended for the research community to help develop new algorithms, but can also be used as an efficient prototyping tool. Based on an advanced software architecture, it allows : the creation of complex and evolving simulations by combining new algorithms with algorithms already included in SOFA, the modification of most parameters of the simulation (deformable behavior, surface representation, solver, constraints, collision algorithm, etc.) by simply editing an XML file, the building of complex models from simpler ones using a scene-graph description, the efficient simulation of the dynamics of interacting objects using abstract equation solvers, the reuse and easy comparison of a variety of available methods.

- Participants: Christian Duriez, François Faure, Hervé Delingette and Stéphane Cotin
- Partner: IGG
- Contact: Stéphane Cotin
- URL: http://www.sofa-framework.org

6.2. SofaCV Plugin

Keywords: Simulation - Visualization - Image processing

Functional Description: SofaCV is a plugin for the simulation framework SOFA. Its purpose is to provide computer vision tools to SOFA. More specifically, its goal is to enable the use of SOFA simulations in augmented reality, and virtual reality applications. The SofaCV plugin is not a standalone plugin by itself. Instead it provides an API for submodules (mainly Sofa's ImageProcessing and DataAcquisition plugin) such as base datatypes, Python bindings, SofaQtQuick widgets etc, along with some utility SOFA Components to read, write or display an image in the scene view.

The ImageProcessing plugin is a plugin for the simulation framework SOFA. Its purpose is to provide general purpose Computer vision features to Sofa. More specifically, its goal is to enable the use of SOFA simulations in augmented reality, and virtual reality applications. The ImageProcessing plugin depends on the SofaCV Base plugin. The ImageProcessing plugin doesn't have the ambition to provide cutting-edge computer vision algorithms, but instead, wraps OpenCV's features while taking advantage of SOFA's Component-based API. This plugin also provides useful Camera components, providing on-the-fly conversions from/to OpenGL & OpenCV's camera calibration parameters. (calibrating cameras, modifying both intrinsic and extrinsic camera parameters in OpenGL)

- Author: Bruno Marques
- Contact bruno.josue.marques@inria.fr

6.3. Needle Insertion Plugin

Keywords: Simulation - Needle insertion - Haptic feedback

Functional Description: This plugin contains needle/tissue interaction models for real time simulations of needle insertion in deformable objects using the open-source sofa framework. This allows for modeling the different forces playing a role during the insertion process (penetration forces, friction along the shaft...) using a constrained-based formulation. This formulation provides a fast and stable solution for the simulation of complex insertions (and reinsertion) of the needle in deformable Finite Element models.

- Authors: Hadrien Courtecuisse
- Contact: hcourtecuisse@unistra.fr

6.4. Optimus Plugin

Keywords: Simulation - Stochastic Filtering - Data Assimilation - State Estimation - Medical applications
Functional Description:

The goal of the plugin is to implement a real integration of Verdandi in SOFA in order to provide a complex and efficient tool for data-assimilation and state-estimation based on filtering prediction-correction scheme.

- Main Author: Igor Peterlik
- Collaborators: Sergei Nikolaev, Nava Schulmann, Raffaella Trivisonne
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    - nava.schulmann@inria.fr
    - raffaella.trivisonne@inria.fr

6.5. RGBDTracking Plugin

Keywords: Simulation - RGBD data Processing - Object tracking - data fusion - Numerical simulations
Functional Description: RGBDTracking is a SOFA plugin to register and track deformable objects in real-time using an RGB-D sensor. This frame-by-frame system relies on a prior visual segmentation of the object in the RGB image. The resulting segmented point cloud is then used to register the object, first in a rigid manner, and then by non-rigidly fitting the known mesh, based on the Finite Element Method to model elasticity, and on vision-based external forces exerted on the mesh.

- Author: Antoine Petit
- Contact: antoine.a.petit@inria.fr

<p align="center" style="color:red">MNEMOSYNE Project-Team</p>

6. New Software and Platforms

6.1. DANA

Distributed Asynchronous Numerical and Adaptive computing framework
KEYWORD: Neural networks
FUNCTIONAL DESCRIPTION: DANA is a python framework whose computational paradigm is grounded on the notion of a unit that is essentially a set of time dependent values varying under the influence of other units via adaptive weighted connections. The evolutions of a unit's value are defined by a set of differential equations expressed in standard mathematical notation which greatly ease their definition. The units are organized into groups that form a model. Each unit can be connected to any other unit (including itself) using a weighted connection. The DANA framework offers a set of core objects needed to design and run such models. The modeler only has to define the equations of a unit as well as the equations governing the training of the connections. The simulation is completely transparent to the modeler and is handled by DANA. This allows DANA to be used for a wide range of numerical and distributed models as long as they fit the proposed framework (e.g. cellular automata, reaction-diffusion system, decentralized neural networks, recurrent neural networks, kernel-based image processing, etc.).

- Participant: Nicolas Rougier
- Contact: Nicolas Rougier
- URL: http://dana.loria.fr/

6.2. Virtual Enaction

KEYWORDS: Neurosciences - Simulation - Health
FUNCTIONAL DESCRIPTION: VirtualEnaction: A Platform for Systemic Neuroscience Simulation. The computational models studied in this project have applications that extend far beyond what is possible to experiment yet in human or non-human primate subjects. Real robotics experimentations are also impaired by rather heavy technological constraints, for instance, it is not easy to dismantle a given embedded system in the course of emerging ideas. The only versatile environment in which such complex behaviors can be studied both globally and at the level of details of the available modeling is a virtual environment, as in video games, Such a system can be implemented as "brainy-bot" (a programmed player based on our knowledge of the brain architecture) which goal is to survive in a complete manipulable environment.

In order to attain this rather ambitious objective we both (i) deploy an existing open-source video game middleware in order to be able to shape the survival situation to be studied and (ii) revisit the existing models in order to be able to integrate them as an effective brainy-bot. It consists of a platform associated to a scenario that is the closest possible to a survival situation (foraging, predator-prey relationship, partner approach to reproduction) and in which it is easy to integrate an artificial agent with sensory inputs (visual, touch and smell), emotional and somatosensory cues (hunger, thirst, fear, ..) and motor outputs (movement, gesture, ..) connected to a "brain" whose architecture will correspond to the major anatomical regions involved in the issues of learning and action selection (cortex areas detailed here, basal ganglia, hippocampus, and areas dedicated to sensorimotor processes). The internal game clock can be slowed down enough to be able to run non trivial brainy-bot implementations. This platform has already being used by two students of the team and is now a new deliverable of the KEOpS project.

- Participants: André Garenne, Frédéric Alexandre, Nicolas Rougier and Thierry Viéville
- Contact: Frédéric Alexandre

6.3. Mnemonas

KEYWORDS: Recurrent network - Manifold

FUNCTIONAL DESCRIPTION: This source bundle provides source files of the: - Manifold representation of ontology for machine learning (in progress). - Recurrent neural network weight estimation though backward tuning publication.

- Contact: Thierry Viéville

6.4. ReservoirPy

KEYWORDS: Recurrent network - Artificial intelligence - Reservoir Computing - Multi-label classification - Timeseries Prediction - Time Series - Machine learning - Classification

FUNCTIONAL DESCRIPTION: This toolbox provides a class of Echo State Networks that can be used with Python and its scientific librairies like Numpy, Scipy and Matplolib. It includes useful expertise to train recurrent neural networks of ESN architecture kind.

ESN is a particular kind of recurrent neural network (RNN) with or without leaky neurons. The input stream is projected to a random recurrent layer and a linear output layer (called "read-out") is modified by learning (which can also be done in an online fashion).

Compared to other RNNs, the input layer and the recurrent layer (called "reservoir") do not need to be trained. For other RNNs, the structure of the recurrent layer evolves in most cases by gradient descent algorithms like Backpropagation-Through-Time, which is not biologically plausible and is adapted iteratively to be able to hold a representaion of the input sequence. In contrast, the random weights of the ESN's reservoir are not trained, but adapted to possess the "Echo State Property" (ESP) or at least suitable dynamics (e.g. 'edge of chaos') to generalize, which includes a non-linear transformation of the input that can be learned by a linear classifier. The weights are adapted by scaling the weights based on the maximum absolute eigenvalue (also called spectral radius), which is a hyperparameter specific to the task. The states of the reservoir are linearly separable and can be mapped to the output layer by a computationally cheap linear regression, as no gradient descent is necessary. The weights of the input layer can be scaled by the input scaling hyperparameter, which also depends on the nature of the inputs.

- Partners: Université de Hamburg - University of Hamburg
- Contact: Xavier Hinaut
- URL: https://github.com/neuronalX/reservoirpy

<p style="text-align:center">**NEUROSYS Project-Team**</p>

6. New Software and Platforms

6.1. OpenVIBE

KEYWORDS: Neurosciences - Interaction - Virtual reality - Health - Real time - Neurofeedback - Brain-Computer Interface - EEG - 3D interaction

FUNCTIONAL DESCRIPTION: OpenViBE is a free and open-source software platform devoted to the design, test and use of Brain-Computer Interfaces (BCI). The platform consists of a set of software modules that can be integrated easily and efficiently to design BCI applications. The key features of OpenViBE software are its modularity, its high-performance, its portability, its multiple-users facilities and its connection with high-end/VR displays. The designer of the platform enables to build complete scenarios based on existing software modules using a dedicated graphical language and a simple Graphical User Interface (GUI). This software is available on the Inria Forge under the terms of the AGPL licence, and it was officially released in June 2009. Since then, the OpenViBE software has already been downloaded more than 60000 times, and it is used by numerous laboratories, projects, or individuals worldwide. More information, downloads, tutorials, videos, documentations are available on the OpenViBE website.

- Participants: Cédric Riou, Thierry Gaugry, Anatole Lécuyer, Fabien Lotte, Jussi Tapio Lindgren, Laurent Bougrain, Maureen Clerc and Théodore Papadopoulo
- Partners: INSERM - GIPSA-Lab
- Contact: Anatole Lécuyer
- URL: http://openvibe.inria.fr

6.2. Platforms

6.2.1. EEG experimental room

A room at Inria Nancy - Grand Est is dedicated to electroencephalographic recordings. An umbrella agreement and several additional experiment descriptions have been approved by the Inria Operational Legal and Ethical Risk Assessment Committee (COERLE). A new 64 channels Biosemi EEG amplifier has been added this year to be able to record two experimental campaign in parallel (Regional initiative *Contrat de Projet État Région (CPER) IT2MP* see section 8.1). Specific experimentation have been done in interaction with Pepper, a semi-humanoid robot.

Figure 1. Electroencephalographic Experimental room at Inria Nancy-Grand Est

<p align="center" style="color:red">**PARIETAL Project-Team**</p>

6. New Software and Platforms

6.1. Mayavi

FUNCTIONAL DESCRIPTION: Mayavi is the most used scientific 3D visualization Python software. Mayavi can be used as a visualization tool, through interactive command line or as a library. It is distributed under Linux through Ubuntu, Debian, Fedora and Mandriva, as well as in PythonXY and EPD Python scientific distributions. Mayavi is used by several software platforms, such as PDE solvers (fipy, sfepy), molecule visualization tools and brain connectivity analysis tools (connectomeViewer).

- Contact: Gaël Varoquaux

- URL: http://mayavi.sourceforge.net/

6.2. MedInria

KEYWORDS: Visualization - DWI - Health - Segmentation - Medical imaging
SCIENTIFIC DESCRIPTION: medInria aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010, renewed in 2012. A fast-track ADT was awarded in 2017 to transition the software core to more recent dependencies and study the possibility of a consortium creation.The Visages team leads this Inria national project and participates in the development of the common core architecture and features of the software as well as in the development of specific plugins for the team's algorithm.
FUNCTIONAL DESCRIPTION: MedInria is a free software platform dedicated to medical data visualization and processing.

- Participants: Maxime Sermesant, Olivier Commowick and Théodore Papadopoulo

- Partners: HARVARD Medical School - IHU - LIRYC - NIH

- Contact: Olivier Commowick

- URL: http://med.inria.fr

6.3. Nilearn

NeuroImaging with scikit learn
KEYWORDS: Health - Neuroimaging - Medical imaging
FUNCTIONAL DESCRIPTION: NiLearn is the neuroimaging library that adapts the concepts and tools of scikit-learn to neuroimaging problems. As a pure Python library, it depends on scikit-learn and nibabel, the main Python library for neuroimaging I/O. It is an open-source project, available under BSD license. The two key components of NiLearn are i) the analysis of functional connectivity (spatial decompositions and covariance learning) and ii) the most common tools for multivariate pattern analysis. A great deal of efforts has been put on the efficiency of the procedures both in terms of memory cost and computation time.

- Participants: Alexandre Abraham, Alexandre Gramfort, Bertrand Thirion, Elvis Dohmatob, Fabian Pedregosa Izquierdo, Gaël Varoquaux, Loïc Estève, Michael Eickenberg and Virgile Fritsch

- Contact: Bertrand Thirion

- URL: http://nilearn.github.io/

6.4. PyHRF

KEYWORDS: Medical imaging - Health - Brain - IRM - Neurosciences - Statistic analysis - FMRI

SCIENTIFIC DESCRIPTION: Functional Magnetic Resonance Imaging (fMRI) is a neuroimaging technique that allows the non-invasive study of brain function. It is based on the hemodynamic variations induced by changes in cerebral synaptic activity following sensory or cognitive stimulation. The measured signal depends on the variation of blood oxygenation level (BOLD signal) which is related to brain activity: a decrease in deoxyhemoglobin concentration induces an increase in BOLD signal. The BOLD signal is delayed with respect to changes in synaptic activity, which can be modeled as a convolution with the Hemodynamic Response Function (HRF) whose exact form is unknown and fluctuates with various parameters such as age, brain region or physiological conditions. In this work we propose to analyze fMRI data using a Joint Detection-Estimation (JDE) approach. It jointly detects cortical activation and estimates the HRF. In contrast to existing tools, PyHRF estimates the HRF instead of considering it as a given constant in the entire brain.

FUNCTIONAL DESCRIPTION: As part of fMRI data analysis, PyHRF provides a set of tools for addressing the two main issues involved in intra-subject fMRI data analysis : (i) the localization of cerebral regions that elicit evoked activity and (ii) the estimation of the activation dynamics also referenced to as the recovery of the Hemodynamic Response Function (HRF). To tackle these two problems, PyHRF implements the Joint Detection-Estimation framework (JDE) which recovers parcel-level HRFs and embeds an adaptive spatio-temporal regularization scheme of activation maps.

NEWS OF THE YEAR: The framework to perform software tests has been further developed. Some unitary tests have been set.

- Participants: Aina Frau Pascual, Christine Bakhous, Florence Forbes, Jaime Eduardo Arias Almeida, Laurent Risser, Lotfi Chaari, Philippe Ciuciu, Solveig Badillo, Thomas Perret and Thomas Vincent

- Partners: CEA - NeuroSpin

- Contact: Florence Forbes

- Publications: Frontiers in Neuroinformatics Flexible multivariate hemodynamics fMRI data analyses and simulations with PyHRF - Fast joint detection-estimation of evoked brain activity in event-related fMRI using a variational approach - A Bayesian Non-Parametric Hidden Markov Random Model for Hemodynamic Brain Parcellation

- URL: http://pyhrf.org

6.5. Scikit-learn

KEYWORDS: Regession - Clustering - Learning - Classification - Medical imaging

SCIENTIFIC DESCRIPTION: Scikit-learn is a Python module integrating classic machine learning algorithms in the tightly-knit scientific Python world. It aims to provide simple and efficient solutions to learning problems, accessible to everybody and reusable in various contexts: machine-learning as a versatile tool for science and engineering.

FUNCTIONAL DESCRIPTION: Scikit-learn can be used as a middleware for prediction tasks. For example, many web startups adapt Scikitlearn to predict buying behavior of users, provide product recommendations, detect trends or abusive behavior (fraud, spam). Scikit-learn is used to extract the structure of complex data (text, images) and classify such data with techniques relevant to the state of the art.

Easy to use, efficient and accessible to non datascience experts, Scikit-learn is an increasingly popular machine learning library in Python. In a data exploration step, the user can enter a few lines on an interactive (but non-graphical) interface and immediately sees the results of his request. Scikitlearn is a prediction engine . Scikit-learn is developed in open source, and available under the BSD license.

- Participants: Alexandre Gramfort, Bertrand Thirion, Fabian Pedregosa Izquierdo, Gaël Varoquaux, Loïc Estève, Michael Eickenberg and Olivier Grisel

- Partners: CEA - Logilab - Nuxeo - Saint Gobain - Tinyclues - Telecom Paris

- Contact: Olivier Grisel

- URL: http://scikit-learn.org

6.6. MODL

Massive Online Dictionary Learning

KEYWORDS: Pattern discovery - Machine learning

FUNCTIONAL DESCRIPTION: Matrix factorization library, usable on very large datasets, with optional sparse and positive factors.

- Participants: Arthur Mensch, Gaël Varoquaux, Bertrand Thirion and Julien Mairal

- Contact: Arthur Mensch

- Publications: Subsampled online matrix factorization with convergence guarantees - Stochastic Subsampling for Factorizing Huge Matrices

- URL: http://github.com/arthurmensch/modl

6.7. MNE

MNE-Python

KEYWORDS: Neurosciences - EEG - MEG - Signal processing - Machine learning

FUNCTIONAL DESCRIPTION: Open-source Python software for exploring, visualizing, and analyzing human neurophysiological data: MEG, EEG, sEEG, ECoG, and more.

RELEASE FUNCTIONAL DESCRIPTION: http://martinos.org/mne/stable/what_new.html

- Partners: HARVARD Medical School - New York University - University of Washington - CEA - Aalto university - Telecom Paris - Boston University - UC Berkeley

- Contact: Alexandre Gramfort

- URL: http://martinos.org/mne/

<p align="center" style="color:red">VISAGES Project-Team</p>

6. New Software and Platforms

6.1. Anima

KEYWORDS: Filtering - Medical imaging - Diffusion imaging - Registration - Relaxometry

SCIENTIFIC DESCRIPTION: Anima is a set of libraries and tools developed by the team as a common repository of research algorithms. As of now, it contains tools for image registration, statistical analysis (group comparison, patient to group comparison), diffusion imaging (model estimation, tractography, etc.), quantitative MRI processing (quantitative relaxation times estimation, MR simulation), image denoising and filtering, and segmentation tools. All of these tools are based on stable libraries (ITK, VTK), making it simple to maintain.

- Participants: Aymeric Stamm, Fang Cao, Florent Leray, Guillaume Pasquier, Laurence Catanese, Olivier Commowick, Renaud Hedouin and René-Paul Debroize
- Contact: Olivier Commowick
- URL: https://github.com/Inria-Visages/Anima-Public/wiki

6.2. autoMRI

KEYWORDS: FMRI - MRI - ASL - FASL - SPM - Automation

SCIENTIFIC DESCRIPTION: This software is highly configurable in order to fit to a wide range of needs. Pre-processing includes segmentation of anatomical data, as well as co-registration, spatial normalization and atlas building of all data types. The analysis pipelines perform either within-group analysis or between-group or one subject-versus-group comparison and produce statistical maps of regions with significant differences. These pipelines can be applied to structural data to exhibit patterns of atrophy or lesions, to ASL (both pulsed or pseudo-continuous sequences) or PET data to detect perfusion or metabolic abnormalities, to relaxometry data to detect deviations from a template, to functional data - either BOLD or ASL - to outline brain activations related to block or event-related paradigms. In addition to the standard General Linear Model approach, the ASL pipelines implement an a contrario approach and, for patient-specific perfusion study, an heteroscedastic variance model. Besides, the vascular pipeline processes 4D MRA data and enables accurate assessment of hemodynamic patterns.

FUNCTIONAL DESCRIPTION: AutoMRI Based on MATLAB and the SPM8 toolbox, autoMRI provides complete pipelines to pre-process and analyze various types of images (anatomical, functional, perfusion, metabolic, relaxometry, vascular).

- Participants: Camille Maumet, Cédric Meurée, Elise Bannier, Fang Cao, Isabelle Corouge, Pierre Maurel, Quentin Duche and Julie Coloigner
- Contact: Isabelle Corouge
- URL: https://team.inria.fr/visages/software/

6.3. MedInria

KEYWORDS: Visualization - DWI - Health - Segmentation - Medical imaging

SCIENTIFIC DESCRIPTION: medInria aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010, renewed in 2012. A fast-track ADT was awarded in 2017 to transition the software core to more recent dependencies and study the possibility of a consortium creation.The Visages team leads this Inria national project and participates in the development of the common core architecture and features of the software as well as in the development of specific plugins for the team's algorithm.

FUNCTIONAL DESCRIPTION: MedInria is a free software platform dedicated to medical data visualization and processing.

- Participants: Maxime Sermesant, Olivier Commowick and Théodore Papadopoulo
- Partners: HARVARD Medical School - IHU - LIRYC - NIH
- Contact: Olivier Commowick
- URL: http://med.inria.fr

6.4. QtShanoir

KEYWORDS: Qt - Nifti - Medical imaging - Plug-in - DICOM - Health - C++ - Soap - Webservices - Shanoir
SCIENTIFIC DESCRIPTION: QtShanoir is based on Qt/C++ librairy. It interacts with the Shanoir server using SOAP web services provided. This application queries the server and displays hierarchical data extracted in tree view. Data could also be easily downloaded or uploaded on the server. In order to extend the Shanoir environment, QtShanoir is developed to contain two shared libraries: - « GUI » that represents all user interfaces. - « DAO » that takes in charge the data model. This library assures the connection to the server and provides all QtShanoir services : research, download and upload of Processed Dataset (NIfTI). QtShanoir dynamic libraries are already reused and integrated in other projects: in the software medInria and in an under development command line program.

FUNCTIONAL DESCRIPTION: QtShanoir is a graphical client application of the medical imaging database Shanoir. This application provides various functionalities to satisfy researchers' needs. It allows users to: - explore neuroimaging data derived from multicenter research trials. Through an intuitive user interface, users could easily visualize voluminous amount of structured data: studies, patients and datasets extracted from Shanoir - download and to upload data from the server. This application is available on Windows, UNIX, MacOs X. It is integrated as a plugin in medInria, a multi-plateform for medical image processing and visualization.

- Participants: Alexandre Abadie, Guillaume Renard, Nicolas Wiest Daessle, Olivier Commowick and Wefa Hakem
- Contact: Christian Barillot
- URL: http://qtshanoir.gforge.inria.fr

6.5. Shanoir

SHAring NeurOImaging Resources
KEYWORDS: Neuroimaging - Medical imaging - PACS - Nifti - Data Sharing - DICOM - Health - Shanoir - Webservices - Data base - Biology - Web Application
FUNCTIONAL DESCRIPTION: SHAring NeurOImaging Resources (Shanoir, Previously InriaNeuroTk) is an open source software platform designed to designed to share, archive, search and visualize neuroimaging data.

It provides a user-friendly secure web access and offers an intuitive workflow to facilitate the collecting and retrieving of neuroimaging data from multiple sources and a wizzard to make the completion of metadata easy. Shanoir comes along many features such as anonymization of data, support for multi-centric clinical studies on subjects or group of subjects.

Shanoir offers an ontology-based data organization (OntoNeuroLOG). Among other things, this facilitates the reuse of data and metadata, the integration of processed data and provides traceability trough an evolutionary approach. Shanoir allows researchers, clinicians, PhD students and engineers to undertake quality research projects with an emphasis on remote collaboration. As a secured J2EE web application, it therefore allows you safely storing and archiving, with no more requirements than a computer with an internet connection!

Furthermore, Shanoir is not only a web application: it is also a complete neuroinformatics platform in which you can easily integrate your existing processing tools or develop your own ones: see ShanoirTk.

The clinical scores resulting from instrument based assessments (e.g. neuropsychological tests) can also be entered and easily retrieved and exported in different formats (Excel, CSV, Xml). Scores and image acquisitions are bound together which makes relationship analysis possible. The instrument database is scalable an new measures can be added in order to meet specific project needs, by use of intuitive graphical interfaces.

Using cross-data navigation and advanced search criteria, the users can quickly point to a subset of data of data to be downloaded. Client side applications have as well been developed to illustrate how to locally access and exploit data through the available web services. With regards to security, the system requires authentication and user rights are tunable for each hosted studies. The person responsible for the study can define which users are allowed to see, download or import data.

Shanoir serves neuroimaging researchers in organizing efficiently their studies while cooperating with other laboratories. By managing patient privacy, Shanoir allows the exploitation of clinical data in a research context. It is finally a handy solution to publish and share data with a broader community.

- Participants: Adrien Férial, Anthony Baire, Bernard Gibaud, Christian Barillot, Guillaume Renard, Justine Guillaumont, Michael Kain and Yao Yao
- Partners: Université de Rennes 1 - CNRS - INSERM
- Contact: Christian Barillot
- URL: http://shanoir.gforge.inria.fr

6.6. ShanoirUploader

KEYWORDS: Webservices - PACS - Medical imaging - Neuroimaging - DICOM - Health - Biology - Java - Shanoir

SCIENTIFIC DESCRIPTION: ShanoirUploader is a desktop application on base of JavaWebStart (JWS). The application can be downloaded and installed using an internet browser. It interacts with a PACS to query and retrieve the data stored on it. After this ShanoirUploader sends the data to a Shanoir server instance in order to import these data. This application bypasses the situation, that in most of the clinical network infrastructures a server to server connection is complicated to set up between the PACS and a Shanoir server instance.

FUNCTIONAL DESCRIPTION: ShanoirUploader is a Java desktop application that transfers data securely between a PACS and a Shanoir server instance (e.g., within a hospital). It uses either a DICOM query/retrieve connection or a local CD/DVD access to search and access images from a local PACS or the local CD/DVD. After having retrieved the data, the DICOM files are locally anonymized and then uploaded to the Shanoir server. A possible integration of a hash creation application for patient identifiers is provided as well. The primary goals of that application are to enable mass data transfers between different remote server instances and therefore reduce the waiting time of the users, when importing data into Shanoir. Most of the time during import is spent with data transfers.

- Participants: Christian Barillot, Ines Fakhfakh, Justine Guillaumont, Michael Kain and Yao Yao
- Contact: Christian Barillot
- URL: http://shanoir.gforge.inria.fr

6.7. Shanoir-NG

KEYWORDS: Neuroimaging - DICOM - Nifti

FUNCTIONAL DESCRIPTION: Shanoir-NG provides a user-friendly secure web access and offers an intuitive workflow to facilitate the collecting and retrieving of neuroimaging data from multiple sources and a wizzard to make the completion of metadata easy. Shanoir-NG comes along many features such as anonymization of data, support for multi-centric clinical studies on subjects or group of subjects.

Shanoir-NG offers an ontology-based data organization (OntoNeuroLOG). Among other things, this facilitates the reuse of data and metadata, the integration of processed data and provides traceability through an evolutionary approach. Shanoir allows researchers, clinicians, PhD students and engineers to undertake quality research projects with an emphasis on remote collaboration. As a secured Jakarta EE web application, it therefore allows you safely storing and archiving, with no more requirements than a computer with an internet connection!

RELEASE FUNCTIONAL DESCRIPTION: Shanoir-NG is a complete technological remake of the first version of the Shanoir application, but maintaining the key concepts of Shanoir.

NEWS OF THE YEAR: Shanoir-NG is a complete technological remake of the first version of the Shanoir application, but maintaining the key concepts of Shanoir.

- Participants: Christian Barillot, Mathieu Simon, Michael Kain, Yao Yao, Aneta Morawin, Arnaud Touboulic, Ines Fakhfakh and Anthony Baire
- Contact: Michael Kain

6.8. Platforms

6.8.1. The Neurinfo Platform

VisAGeS is the founding actor of an experimental research platform which was installed in August 2009 at the University Hospital of Rennes. The University of Rennes 1, Inria, Inserm for the academic side, and the University Hospital of Rennes and the Cancer Institute "Eugene Marquis" for the clinical side, are partners of this neuroinformatics platform called Neurinfo (http://www.neurinfo.org). This platform has been supported under the "Contrat de Projets Etat-Région" (Christian Barillot is the PI) and has received a total amount of 4.01 M€ for the period 2007–2014. European (FEDER), National (through Ministry of research, Inria, Inserm and ANR) and local councils (Brittany Region, Ille et Vilaine, and Rennes Metropole) have joined their effort to support this operation for a total amount of 4 010 k€ (600 k€ for the infrastructures, 2 850 k€ for the equipments and 560 k€ for the functioning). This application was set up through the Regional PIMATGI initiative coordinated by INSERM in Brittany (C. Roux). The PIMATGI initiative participated to the funding of three complementary platforms: Neurinfo, TheraFONC as a technical platform dedicated to therapy guided by functional imaging especially in the oncology domain (Inserm U650 - LaTIM, Dir. Ch. Roux, Brest), and TherA-Image as a platform dedicated to image guided mini-invasive surgery and therapy especially in the domain of cardio-vascular diseases (U642 -LTSI, Dir. L. Senhadji, Rennes).

Concerning the Neurinfo Platform, the activity domain is a continuum between methodological and technological research built around specific clinical research projects. The ambition is to do innovation in science, technology and medical technology transfer for the implementation on the clinical field. On the medical field, the translational research domain mainly concerns medical imaging and more specifically the clinical neurosciences. Among them are multiple sclerosis, epilepsy, neurodegenerative, neurodevelopmental and psychiatric diseases, surgical procedures of brain lesions, neuro-oncology and radiotherapy planning. Beyond these CNS applications, the platform is also open to alternative applications. Neurinfo ambitions to support the emergence of research projects based on their level of innovation, their pluri-disciplinarity and their ability to foster collaborations between different actors (public and private research entities, different medical specialties, different scientific profiles).

In this context, a research 3T MRI system (Siemens Verio) was acquired in summer 2009 in order to develop the clinical research in the domain of morphological, functional, structural and cellular in-vivo imaging. In 2014 a new equipment for simultaneous recording of EEG and MRI images was acquired from Brain Product. In 2015, a mock scanner for experimental set-up was acquired as well as a new High Performance Computing environment made of one large computing cluster and a data center that is shared and operated by the Inria center at IRISA (UMR CNRS 6074). The computation cluster (240 cores) and the data center (up to 50 TB) are dedicated to host and process imaging data produced by the Neurinfo platform, but also by other research partners that share their protocols on the Neurinfo neuroinformatics system (currently more than 30 sites).

VisAGeS and its partners in the Neurinfo project are committed to use this new research platform for developing new regional, national and international collaborations around fundamental and applied clinical research projects dealing with in-vivo medical imaging.

In 2016, VisAGeS has been awarded by IBISA as a "Plateforme d'excellence".

In 2017, funding was collected to replace the 3T Siemens Verio MRI that led to the installation of a new 3T Siemens Prisma in 2018.

In 2018, the INS2I institute of CNRS did awarded the neurinfo platform with a specific support for experimental platform that will be dedicated to the acquisition in 2019 of a EEG-compatible fNIRS system.

AIRSEA Project-Team

5. New Software and Platforms

5.1. AGRIF

Adaptive Grid Refinement In Fortran

KEYWORD: Mesh refinement

SCIENTIFIC DESCRIPTION: AGRIF is a Fortran 90 package for the integration of full adaptive mesh refinement (AMR) features within a multidimensional finite difference model written in Fortran. Its main objective is to simplify the integration of AMR potentialities within an existing model with minimal changes. Capabilities of this package include the management of an arbitrary number of grids, horizontal and/or vertical refinements, dynamic regridding, parallelization of the grids interactions on distributed memory computers. AGRIF requires the model to be discretized on a structured grid, like it is typically done in ocean or atmosphere modelling.

NEWS OF THE YEAR: In 2017, the multiresolution capabilities of the AGRIF software have been extended to be able to treat a much larger number of grids. In particular, the load balancing algorithms have been greatly improved.

- Participants: Roland Patoum and Laurent Debreu
- Contact: Laurent Debreu
- Publications: Numerical and experimental approach for a better physical description of submesoscale processes : A north-western Mediterranean Sea case - AGRIF: Adaptive Grid Refinement in Fortran
- URL: http://www-ljk.imag.fr/MOISE/AGRIF

5.2. BALAISE

Bilbliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement

KEYWORDS: Multi-scale analysis - Data assimilation - Optimal control

FUNCTIONAL DESCRIPTION: BALAISE (Bilbliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement) is a test bed for image data assimilation. It includes a shallow water model, a multi-scale decomposition library and an assimilation suite.

- Contact: Patrick Vidard

5.3. NEMOVAR

Variational data assimilation for NEMO

KEYWORDS: Oceanography - Data assimilation - Adjoint method - Optimal control

FUNCTIONAL DESCRIPTION: NEMOVAR is a state-of-the-art multi-incremental variational data assimilation system with both 3D and 4D var capabilities, and which is designed to work with NEMO on the native ORCA grids. The background error covariance matrix is modelled using balance operators for the multivariate component and a diffusion operator for the univariate component. It can also be formulated as a linear combination of covariance models to take into account multiple correlation length scales associated with ocean variability on different scales. NEMOVAR has recently been enhanced with the addition of ensemble data assimilation and multi-grid assimilation capabilities. It is used operationnaly in both ECMWF and the Met Office (UK)

- Partners: CERFACS - ECMWF - Met Office
- Contact: Patrick Vidard

5.4. Sensitivity

FUNCTIONAL DESCRIPTION: This package is useful for conducting sensitivity analysis of complex computer codes.

- Contact: Laurent Gilquin
- URL: https://cran.r-project.org/web/packages/sensitivity/index.html

ANGE Project-Team

6. New Software and Platforms

6.1. Freshkiss

FREe Surface Hydrodynamics using KInetic SchemeS
KEYWORDS: Finite volume methods - Hydrostatic Navier-Stokes equations - Free surface flows
FUNCTIONAL DESCRIPTION: Freshkiss3D is a numerical code solving the 3D hydrostatic and incompressible Navier-Stokes equations with variable density.

- Participants: Fabien Souille, Emmanuel Audusse, Jacques Sainte Marie and Marie-Odile Bristeau
- Partners: UPMC - CEREMA
- Contact: Jacques Sainte Marie

6.2. TSUNAMATHS

KEYWORDS: Modeling - Tsunamis
FUNCTIONAL DESCRIPTION: Tsunamaths is an educational platform aiming at simulating historical tsunamis. Real data and mathematical explanations are provided to enable people to better understand the overall process of tsunamis.

- Participants: Emmanuel Audusse, Jacques Sainte Marie and Raouf Hamouda
- Contact: Jacques Sainte Marie
- URL: http://tsunamath.paris.inria.fr/

6.3. Verdandi

KEYWORDS: HPC - Model - Software Components - Partial differential equation
FUNCTIONAL DESCRIPTION: Verdandi is a free and open-source (LGPL) library for data assimilation. It includes various such methods for coupling one or several numerical models and observational data. Mainly targeted at large systems arising from the discretization of partial differential equations, the library is devised as generic, which allows for applications in a wide range of problems (biology and medicine, environment, image processing, etc.). Verdandi also includes tools to ease the application of data assimilation, in particular in the management of observations or for a priori uncertainty quantification. Implemented in C++, the library may be used with models implemented in Fortran, C, C++ or Python.

- Participants: Dominique Chapelle, Gautier Bureau, Nicolas Claude, Philippe Moireau and Vivien Mallet
- Contact: Vivien Mallet
- URL: http://verdandi.gforge.inria.fr/

6.4. Polyphemus

KEYWORD: Simulation
FUNCTIONAL DESCRIPTION: Polyphemus is a modeling system for air quality. As such, it is designed to yield up-to-date simulations in a reliable framework: data assimilation, ensemble forecast and daily forecasts. Its completeness makes it suitable for use in many applications: photochemistry, aerosols, radionuclides, etc. It is able to handle simulations from local to continental scales, with several physical models. It is divided into three main parts:

libraries that gather data processing tools (SeldonData), physical parameterizations (AtmoData) and post-processing abilities (AtmoPy),

programs for physical pre-processing and chemistry-transport models (Polair3D, Castor, two Gaussian models, a Lagrangian model),

model drivers and observation modules for model coupling, ensemble forecasting and data assimilation.

- Participants: Sylvain Doré and Vivien Mallet
- Contact: Vivien Mallet
- URL: http://cerea.enpc.fr/polyphemus/

6.5. Urban noise analysis

KEYWORD: Environment perception

FUNCTIONAL DESCRIPTION: This software processes mobile observations collected by the application Ambiciti (previously known as SoundCity). It can merge simulated noise maps with the mobile observations.

- Authors: Raphaël Ventura, Vivien Mallet and Guillaume Cherel
- Contact: Vivien Mallet

6.6. Freshkiss3D

- Authors: Jacques Sainte Marie, Marie-Odile Bristeau, Anne-Céline Boulanger, Raouf Hamouda, Emmanuel Audusse, Alain Dervieux, Bijan Mohammadi and David Froger
- Partner: UPMC
- Contact: Jacques Sainte Marie

<p style="text-align:center">**CASTOR Project-Team**</p>

6. New Software and Platforms

6.1. CEDRES++

KEYWORDS: 2D - Magnetic fusion - Plasma physics

FUNCTIONAL DESCRIPTION: In Tokamaks, at the slow resistive diffusion time scale, the magnetic configuration in the plasma can be described by the MHD equilibirum equations inside the plasma and the Maxwell equations outside. Moreover, the magnetic field is often supposed not to depend on the azimutal angle.

Under this assumption of axisymmetric configuration, the equilibrium in the whole space reduces to solving a 2D problem in which the magnetic field in the plasma is described by the well known Grad Shafranov equation. The unknown of this problem is the poloidal magnetic flux. The P1 finite element code CEDRES++ solves this free boundary equilibrium problem in direct and inverse mode. The direct problem consists in the computation of the magnetic configuration and of the plasma boundary, given a plasma current density profile and the total current in each poloidal field coils (PF coils). The aim of the inverse problem is to find currents in the PF coils in order to best fit a given plasma shape.

- Participants: Blaise Faugeras, Cédric Boulbe, Holger Heumann and Jacques Blum
- Partners: CNRS - CEA - Université de Nice Sophia Antipolis (UNS)
- Contact: Cédric Boulbe

6.2. Equinox

KEYWORDS: 2D - Problem inverse

FUNCTIONAL DESCRIPTION: EQUINOX is a code dedicated to the numerical reconstruction of the equilibrium of the plasma in a Tokamak. The problem solved consists in the identification of the plasma current density, a non-linear source in the 2D Grad-Shafranov equation which governs the axisymmetric equilibrium of a plasma in a Tokamak. The experimental measurements that enable this identification are the magnetics on the vacuum vessel, but also polarimetric and interferometric measures on several chords, as well as motional Stark effect measurements. The reconstruction can be obtained in real-time and the numerical method implemented involves a finite element method, a fixed-point algorithm and a least-square optimization procedure.

- Participants: Blaise Faugeras, Cédric Boulbe and Jacques Blum
- Contact: Blaise Faugeras

6.3. FBGKI

Full Braginskii

FUNCTIONAL DESCRIPTION: The Full Braginskii solver considers the equations proposed by Braginskii (1965), in order to describe the plasma turbulent transport in the edge part of tokamaks. These equations rely on a two fluid (ion - electron) description of the plasma and on the electroneutrality and electrostatic assumptions. One has then a set of 10 coupled non-linear and strongly anisotropic PDEs. FBGKI makes use in space of high order methods: Fourier in the toroidal periodic direction and spectral elements in the poloidal plane. The integration in time is based on a Strang splitting and Runge-Kutta schemes, with implicit treatment of the Lorentz terms (DIRK scheme). The spectral vanishing viscosity (SVV) technique is implemented for stabilization. Static condensation is used to reduce the computational cost. In its sequential version, a matrix free solver is used to compute the potential. The parallel version of the code is under development.

- Contact: Sebastian Minjeaud

6.4. FEEQS.M

Finite Element Equilibrium Solver in MATLAB

KEYWORDS: Finite element modelling - Optimal control - Plasma physics

FUNCTIONAL DESCRIPTION: FEEQS.M (Finite Element Equilibrium Solver in Matlab) is a MATLAB implementation of the numerical methods in [Heumann2015] to solve equilibrium problems for toroidal plasmas. Direct and inverse problems for both the static and transient formulations of plasma equilibrium can be solved. FEEQS.M exploits MATLAB's evolved sparse matrix methods and uses heavily the vectorization programming paradigm, which results in running times comparable to C/C++ implementations. FEEQS.M complements the production code CEDRES++ in being considered as fast prototyping test bed for computational methods for equilibrium problems. This includes aspects of numerics such as improved robustness of the Newton iterations or optimization algorithms for inverse problems. The latest developments aim at incorporating the resistive diffusion equation.

[Heumann2015]: Heumann, H., Blum, J., Boulbe, C., Faugeras, B., Selig, G., Ané, J.-M., Brémond, S., Grandgirard, V., Hertout, P., Nardon, E.: Quasi-static free-boundary equilibrium of toroidal plasma with CEDRES++: Computational methods and applications. In: Journal of Plasma Physics 81 (2015)

- Participant: Holger Heumann
- Contact: Holger Heumann
- URL: https://scm.gforge.inria.fr/svn/holgerheumann/Matlab/FEEQS.M

6.5. Fluidbox

FUNCTIONAL DESCRIPTION: FluidBox is a software dedicated to the simulation of inert or reactive flows. It is also able to simulate multiphase, multi-material and MDH flows. There exist 2D and 3D dimensional versions. The 2D version is used to test new ideas that are later implemented in 3D. Two classes of schemes are available : a classical finite volume scheme and the more recent residual distribution schemes. Several low Mach number preconditioning are also implemented. The code has been parallelized with and without domain overlapping.

- Participants: Boniface Nkonga, Mario Ricchiuto, Michael Papin and Rémi Abgrall
- Contact: Boniface Nkonga

6.6. Jorek-Inria

FUNCTIONAL DESCRIPTION: Jorek-Inria is a new version of the JOREK software, for MHD modeling of plasma dynamic in tokamaks geometries. The numerical approximation is derived in the context of finite elements where 3D basic functions are tensor products of 2D basis functions in the poloidal plane by 1D basis functions in the toroidal direction. More specifically, Jorek uses curved bicubic isoparametric elements in 2D and a spectral decomposition (sine, cosine) in the toroidal axis. Continuity of derivatives and mesh alignment to equilibrium surface fluxes are enforced. Resulting linear systems are solved by the PASTIX software developed at Inria-Bordeaux.

RELEASE FUNCTIONAL DESCRIPTION: The new formulation of the Jorek-Inria code extends this approximation strategy by introducing more flexibility and a variety of finite elements used in the poloidal plane and in the toroidal direction. It also proposes a sparse matrix interface SPM (Sparse Matrix Manager) that allows to develop clean code without a hard dependency on any linear solver library (i.e. PetSc, Pastix, Mumps, ...).

- Participants: Ahmed Ratnani, Boniface Nkonga, Emmanuel Franck and Hervé Guillard
- Contact: Hervé Guillard
- URL: https://gforge.inria.fr/projects/jorek/

6.7. Plato

A platform for Tokamak simulation

FUNCTIONAL DESCRIPTION: PlaTo (A platform for Tokamak simulation) is a suite of data and softwares dedicated to the geometry and physics of Tokamaks. Plato offers interfaces for reading and handling distributed unstructured meshes, numerical templates for parallel discretizations, interfaces for distributed matrices and linear and non-linear equation solvers. Plato provides meshes and solutions corresponding to equilibrium solutions that can be used as initial data for more complex computations as well as tools for visualization using Visit or Paraview.

- Participants: Afeintou Sangam, Boniface Nkonga, Elise Estibals, Giorgio Giorgiani and Hervé Guillard
- Contact: Hervé Guillard

6.8. VacTH

KEYWORD: Problem inverse

FUNCTIONAL DESCRIPTION: VacTH implements a method based on the use of toroidal harmonics and on a modelization of the poloidal field coils and divertor coils to perform the 2D interpolation and extrapolation of discrete magnetic measurements in a tokamak and the identification of the plasma boundary. The method is generic and can be used to provide the Cauchy boundary conditions needed as input by a fixed domain equilibrium reconstruction code like EQUINOX. It can also be used to extrapolate the magnetic measurements in order to compute the plasma boundary itself. The method is foreseen to be used in the real-time plasma control loop on the WEST tokamak.

- Contact: Blaise Faugeras

6.9. NICE

Newton direct and Inverse Computation for Equilibrium

KEYWORDS: 2D - C++ - Scientific computing - Finite element modelling - Plasma physics - Optimal control - Optimization - Identification

FUNCTIONAL DESCRIPTION: The NICE code is under development. Its goal is to gather in a single modern, modular and evolutionary C++ code, the different numerical methods and algorithms from VACTH, EQUINOX and CEDRES++ which share many common features. It also integrates new methods as for example the possibility to use the Stokes model for equilibrium reconstruction using polarimetry measurements.

- Contact: Blaise Faugeras

COFFEE Project-Team

6. New Software and Platforms

6.1. AP_PartFlow

FUNCTIONAL DESCRIPTION: We are developing experimental codes, mainly based on Finite Differences, for the simulation of particulate flows. A particular attention is paid to guaranty the asymptotic properties of the scheme, with respect to relaxation parameters.

- Contact: Thierry Goudon

6.2. Mka3d

KEYWORDS: Scientific computing - Elasticity - Elastodynamic equations
FUNCTIONAL DESCRIPTION: The Mka3d method simulates an elastic solid by discretizing the solid into rigid particles. An adequate choice of forces and torques between particles allows to recover the equations of elastodynamics.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: http://cermics.enpc.fr/~monassel/Mka3D/

6.3. Compass

Computing Architecture to Speed up Simulation
KEYWORDS: Finite volume methods - Porous media - High performance computing
FUNCTIONAL DESCRIPTION: Compass is a parallel code initiated in 2012 and co-developed by LJAD-Inria Coffee and BRGM since 2015. It is devoted to the simulation of multiphase flows in porous media, it accounts for non isothermal and compositional flows and includes complex network of fractures or faults represented as interfaces of co-dimension one coupled to the surrounding matrix. The discretization is based on vertex and cell unknowns and is adapted to polyhedral meshes and heterogeneous media. The ComPASS code is co-developed since december 2016 by the partners of the ANR CHARMS project including BGRM, LJAD-Inria Coffee, Storengy, MdS and LJLL with the objective to develop a new generation simulator for geothermal systems focusing on fluids and accounting for complex fault networks and wells.

- Participants: Simon Lopez, Farid Smai, Michel Kern, Yacine Ould Rouis, Nabil Birgle, Laurence Beaude, Konstantin Brenner and Roland Masson
- Partners: Université de Nice Sophia Antipolis (UNS) - BRGM
- Contact: Roland Masson
- URL: http://www.anr-charms.org/page/compass-code

6.4. NS2DDV-M

2D Navier-Stokes equations with variable density
KEYWORDS: Partial differential equation - Finite volume methods - Finite element modelling

FUNCTIONAL DESCRIPTION: The NS2DDV Matlab toolbox is an open-source program written in Matlab for simulating 2D viscous, incompressible and inhomogeneous flows. The computation kernel of the code is based on Finite Elements - Finite Volumes hybrid methods applied on the 2D Navier-Stokes equations. It works on unstructured meshes and can include mesh refinements strategies. We develop and freely distribute a new version of the Matlab code NS2DDV-M (equipped with a graphic interface and an accurate documentation) to promote new collaborations in the domain, allow some easy comparisons with concurrent codes on the same benchmark cases, and compare alternative numerical solution methods.

- Partner: Laboratoire Paul Painlevé
- Contact: Caterina Calgaro-Zotto
- URL: https://wikis.univ-lille1.fr/painleve/ns2ddv

6.5. SimBiof

KEYWORDS: Bioinformatics - Chemistry
FUNCTIONAL DESCRIPTION: We are developing numerical methods, currently by using Finite Differences approaches, for the simulation of biofilms growth. The underlying system of PDEs takes the form of multiphase flows equations with conservation constraints and vanishing phases. The numerical experiments have permitted to bring out the influence of physical parameters on the multidimensional growth dynamics.

- Contact: Thierry Goudon

6.6. CELIA3D

KEYWORDS: Fluid mechanics - Multi-physics simulation
FUNCTIONAL DESCRIPTION: The CELIA3D code simulates the coupling between a compressible fluid flow and a deformable structure. The fluid is handled by a Finite Volume method on a structured Cartesian grid. The solid is handled by a Discrete Element method (Mka3d scheme). The solid overlaps the fluid grid and the coupling is carried out with immersed boundaries (cut cells) in a conservative way.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: http://cermics.enpc.fr/~monassel/CELIA3D/

<p style="text-align: center; color: red;">**FLUMINANCE Project-Team**</p>

5. New Software and Platforms

5.1. 2DLayeredMotion

Estimation of 2D independent mesoscale layered atmospheric motion fields

FUNCTIONAL DESCRIPTION: This software enables to estimate a stack of 2D horizontal wind fields corresponding to a mesoscale dynamics of atmospheric pressure layers. This estimator is formulated as the minimization of a global energy function. It relies on a vertical decomposition of the atmosphere into pressure layers. This estimator uses pressure data and classification clouds maps and top of clouds pressure maps (or infra-red images). All these images are routinely supplied by the EUMETSAT consortium which handles the Meteosat and MSG satellite data distribution. The energy function relies on a data model built from the integration of the mass conservation on each layer. The estimator also includes a simplified and filtered shallow water dynamical model as temporal smoother and second-order div-curl spatial regularizer. The estimator may also incorporate correlation-based vector fields as additional observations. These correlation vectors are also routinely provided by the Eumetsat consortium.

- Participant: Étienne Mémin
- Contact: Étienne Mémin
- URL: http://fluid.irisa.fr/index.html

5.2. 3DLayeredMotion

Estimation of 3D interconnected layered atmospheric motion fields

FUNCTIONAL DESCRIPTION: This software extends the previous 2D version. It allows (for the first time to our knowledge) the recovery of 3D wind fields from satellite image sequences. As with the previous techniques, the atmosphere is decomposed into a stack of pressure layers. The estimation relies also on pressure data and classification clouds maps and top of clouds pressure maps. In order to recover the 3D missing velocity information, physical knowledge on 3D mass exchanges between layers has been introduced in the data model. The corresponding data model appears to be a generalization of the previous data model constructed from a vertical integration of the continuity equation.

- Contact: Étienne Mémin
- URL: http://fluid.irisa.fr

5.3. DenseMotion

Estimation of 2D dense motion fields

FUNCTIONAL DESCRIPTION: This code allows the computation from two consecutive images of a dense motion field. The estimator is expressed as a global energy function minimization. The code enables the choice of different data models and different regularization functionals depending on the targeted application. Generic motion estimators for video sequences or fluid flows dedicated estimators can be set up. This software allows in addition the users to specify additional correlation based matching measurements. It enables also the inclusion of a temporal smoothing prior relying on a velocity vorticity formulation of the Navier-Stoke equation for Fluid motion analysis applications.

- Participant: Étienne Mémin
- Contact: Étienne Mémin
- URL: http://fluid.irisa.fr/index.html

5.4. Low-Order-Motion

Estimation of low order representation of fluid motion

FUNCTIONAL DESCRIPTION: This code enables the estimation of a low order representation of a fluid motion field from two consecutive images.The fluid motion representation is obtained using a discretization of the vorticity and divergence maps through regularized Dirac measure. The irrotational and solenoidal components of the motion fields are expressed as linear combinations of basis functions obtained through the Biot-Savart law. The coefficient values and the basis function parameters are formalized as the minimizer of a functional relying on an intensity variation model obtained from an integrated version of the mass conservation principle of fluid mechanics.

- Participants: Anne Cuzol and Étienne Mémin
- Contact: Étienne Mémin
- URL: http://fluid.irisa.fr

5.5. TYPHOON

- Participants: Christopher Mauzey, Étienne Mémin and Pierre Dérian
- Partner: CSU Chico
- Contact: Étienne Mémin
- URL: http://phys.csuchico.edu/lidar/typhoon/

5.6. H2OLab

KEYWORDS: Simulation - Energy - Contamination - Groundwater - Hydrogeology - Heterogeneity - Uncertainly - Multiscale

SCIENTIFIC DESCRIPTION: The software platform contains a database which is interfaced through the web portal H2OWeb. It contains also software modules which can be used through the interface H2OGuilde. The platform H2OLab is an essential tool for the dissemination of scientific results. Currently, software and database are shared by the partners of the h2mno4 project.

FUNCTIONAL DESCRIPTION: The software platform H2OLab is devoted to stochastic simulations of groundwater flow and contaminant transport in highly heterogeneous porous and fractured geological media.

-Modeling and numerical simulation of aquifers -Porous and fractured heterogeneous media -Flow with mixed finite elements -Solute transport with a Lagrangian method -Stochastic modeling for data uncertainty.

- Participants: Géraldine Pichot, Grégoire Lecourt, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Partners: Université de Rennes 1 - CNRS - Université de Lyon - Université de Poitiers
- Contact: Jocelyne Erhel
- URL: http://h2olab.inria.fr/

5.7. PALMTREE

KEYWORD: Monte-Clarlo

FUNCTIONAL DESCRIPTION: We present an easy-to-use package for the parallelization of Lagrangian methods for partial differential equations. In addition to the reduction of computation time, the code aims at satisfying three properties:

simplicity: the user just has to add the algorithm governing the behaviour of the particles. portability: the possibility to use the package with any compiler and OS. action-replay: the ability of the package to replay a selected batch of particles.

The last property allows the user to replay and capture the whole sample path for selected particles of a batch. This feature is very useful for debugging and catching some relevant information.

- Authors: Lionel Lenôtre, Géraldine Pichot, Lionel Lenôtre and Lionel Lenôtre
- Contact: Géraldine Pichot

5.8. GRT3D

Global Reactive Transport in 3D
KEYWORDS: Geochemistry - Dispersion - Scientific calculation - Simulation - Advection
SCIENTIFIC DESCRIPTION: Participants : Édouard Canot, Jocelyne Erhel [correspondant] .

Version: version 2.0, April 2014

APP: registered

Programming language: C

Abstract: Reactive transport modeling has become an essential tool for understanding complex environmental problems. It is an important issue for MoMaS and C2S@EXA partners (see sections 8.2.5 , 8.2.3), in particular Andra. We have developed a method coupling transport and chemistry, based on a method of lines such that spatial discretization leads to a semi-discrete system of algebraic differential equations (DAE system). The main advantage is to use a complex DAE solver, which controls simultaneously the timestep and the convergence of Newton algorithm. The approach SIA uses a fixed-point method to solve the nonlinear system at each timestep, whereas the approach SNIA uses an explicit scheme.

The software suite GRT3D has four executable modules:

SIA1D: Sequential Iterative Approach for 1D domains,

GDAE1D: Global DAE approach for 1D domains,

SNIA3D: Sequential Non Iterative Approach for 1D, 2D or 3D domains.

GDAE3D: Global DAE approach for 1D, 2D or 3D domains. This module has three variants: the original one with logarithms, an optimized one still with logarithms, an optimized one which does not use logarithms.

Current work: extension of the chemistry module and parallelization.
FUNCTIONAL DESCRIPTION: Reactive transport modeling has become an essential tool for understanding complex environmental problems. It is an important issue for MoMaS and C2S@EXA partners, in particular Andra. We have developed a method coupling transport and chemistry, based on a method of lines such that spatial discretization leads to a semi-discrete system of algebraic differential equations (DAE system). The main advantage is to use a complex DAE solver, which controls simultaneously the timestep and the convergence of Newton algorithm. The approach SIA uses a fixed-point method to solve the nonlinear system at each timestep, whereas the approach SNIA uses an explicit scheme.

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SNIA3D: Sequential Non Iterative Approach for 1D, 2D or 3D domains.

GDAE3D: Global DAE approach for 1D, 2D or 3D domains. This module has three variants: the original one with logarithms, an optimized one still with logarithms, an optimized one which does not use logarithms.

- Participants: Caroline De Dieuleveult, Édouard Canot, Jocelyne Erhel, Nadir Soualem and Souhila Sabit
- Partner: ANDRA
- Contact: Jocelyne Erhel

LEMON Team

6. New Software and Platforms

6.1. SW2D

Shallow Water 2 Dimensions

KEYWORDS: Numerical simulations - Shallow water equations

FUNCTIONAL DESCRIPTION: Urban floods are usually simulated using two-dimensional shallow water models. A correct representation of the urban geometry and hydraulics would require that the average computational cell size be between 0.1 m and 1 m. The meshing and computation costs make the simulation of entire districts/conurbations impracticable in the current state of computer technology.

An alternative approach consists in upscaling the shallow water equations using averaging techniques. This leads to introducing storage and conveyance porosities, as well as additional source terms, in the mass and momentum balance equations. Various versions of porosity-based shallow water models have been proposed in the literature. The Shallow Water 2 Dimensions (SW2D) computational code embeds various finite volume discretizations of these models. Ituses fully unstructured meshes with arbitrary numbers of edges. The key features of the models and numerical techniques embedded in SW2D are :

- specific momentum/energy dissipation models that are active only under transient conditions. Such models, that are not present in classical shallow water models, stem from the upscaling of the shallow water equations and prove essential in modeling the features of fast urban flow transients accurately

- modified HLLC solvers for an improved discretization of the momentum source terms stemming from porosity gradients

- higher-order reconstruction techniques that allow for faster and more stable calculations in the presence of wetting/drying fronts.

- Participant: Vincent Guinot
- Contact: Vincent Guinot

6.2. WindPoS-SDM-LAM

KEYWORDS: Numerical simulations - 3D - Fluid mechanics

FUNCTIONAL DESCRIPTION: Software platform for wind modeling.

- Authors: Antoine Rousseau, Cristian Paris Ibarra, Jacques Morice, Mireille Bossy and Sélim Kraria
- Contact: Mireille Bossy
- URL: https://windpos.inria.fr

6.3. SDM

Stochastic Downsaling Method

FUNCTIONAL DESCRIPTION: The computation of the wind at small scale and the estimation of its uncertainties is of particular importance for applications such as wind energy resource estimation. To this aim, starting in 2005, we have developed a new method based on the combination of an existing Numerical Weather Prediction model providing a coarse prediction, and a Lagrangian Stochastic Model for turbulent flows. This Stochastic Downscaling Method (SDM) requires a specific modeling of the turbulence closure, and involves various simulation techniques whose combination is totally original (such as Poisson solvers, optimal transportation mass algorithm, original Euler scheme for confined Langevin stochastic processes, and stochastic particle methods).

- Participants: Antoine Rousseau, Antoine Rousseau, Claire Chauvin, Frederic Bernardin and Mireille Bossy
- Contact: Mireille Bossy

6.4. OceaPoS-SDM

KEYWORDS: 3D - Turbulence - Oceanography - Numerical simulations - Stochastic models - Marine Energies
FUNCTIONAL DESCRIPTION: Simulation platform for ocean turbulence and interaction with hydroturbines

- Partner: MERIC
- Contact: Mireille Bossy

<p style="text-align:center">**MAGIQUE-3D Project-Team**</p>

5. New Software and Platforms

5.1. Elasticus

KEYWORDS: Discontinuous Galerkin - Acoustic equation - Elastodynamic equations - Elastoacoustic - 2D - 3D - Time Domain

SCIENTIFIC DESCRIPTION: Elasticus simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

FUNCTIONAL DESCRIPTION: Elasticus is a sequential library, independent of Total plateform and developed in Fortran, to simulate wave propagation in geophysical environment, based on a DG method. It is meant to help PhD students and post-doctoral fellows to easily implement their algorithms in the library. Thus, readability of the code is privileged to optimization of its performances. Developed features should be easily transferred in the computing platform of Total. Elasticus manages arbitrary orders for the spatial discretization with DG method.

NEWS OF THE YEAR: In 2018, we implemented the coupling between hexahedra and tetrahedra and the coupling between Discontinuous Galerkin methods and Spectral Element methods in 2D and in 3D. We also introduced Perfectly Matched layers in the Spectral Element kernel.

- Participants: Julien Diaz, Lionel Boillot and Simon Ettouati
- Contact: Julien Diaz
- Publications: Spectral Element Method and Discontinuous Galerkin approximation for elasto-acoustic problems - Hybrid space discretization to solve elasto-acoustic coupling - On the coupling of Spectral Element Method with Discontinuous Galerkin approximation for elasto-acoustic problems - SEM-DG Approximation for elasto-acoustics

5.2. Hou10ni

KEYWORDS: 2D - 3D - Elastodynamic equations - Acoustic equation - Elastoacoustic - Frequency Domain - Time Domain - Discontinuous Galerkin

SCIENTIFIC DESCRIPTION: Hou10ni simulates acoustic and elastic wave propagation in time domain and in harmonic domain, in 2D and in 3D. It is also able to model elasto acoustic coupling. It is based on the second order formulation of the wave equation and the space discretization is achieved using Interior Penalty Discontinuous Galerkin Method. Recently, the harmonic domain solver has been extended to handle Hybridizable Discontinuous Galerkin Methods.

FUNCTIONAL DESCRIPTION: This software simulates the propagation of waves in heterogeneous 2D and 3D media in time-domain and in frequency domain. It is based on an Interior Penalty Discontinuous Galerkin Method (IPDGM) and allows for the use of meshes composed of cells of various order (p-adaptivity in space).

NEWS OF THE YEAR: In 2018, we have finished scalablity tests and performance comparison of Hou10ni/Mumps vs Hou10ni/Maphys on Plafrim, in the framework of the european project HPC4E. The code is now being ported on Turing, in order to extend the scability tests to the time-domain problem.

- Participants: Conrad Hillairet, Elodie Estecahandy, Julien Diaz, Lionel Boillot and Marie Bonnasse Gahot

- Contact: Julien Diaz

- Publications: Hybridizable discontinuous Galerkin method for the two-dimensional frequency-domain elastic wave equations - Convergence of seismic full waveform inversion and extension to Cauchy data - Convergence Analysis for Seismic Full Waveform Inversion - Stability and convergence analysis for seismic depth imaging using FWI - On the use of a laser ablation as a laboratory seismic source - Towards Energy-Efficient Storage Servers - Equivalent Robin Boundary Conditions for Acoustic and Elastic Media - Comparison of solvers performance when solving the 3D Helmholtz elastic wave equations over the Hybridizable Discontinuous Galerkin method - Comparison of solvers performance when solving the 3D Helmholtz elastic wave equations using the Hybridizable Discontinuous Galerkin method - Resolution strategy for the Hybridizable Discontinuous Galerkin system for solving Helmholtz elastic wave equations - Seismic imaging in laboratory trough laser Doppler vibrometry - Absorbing Boundary Conditions for 3D Elastic TTI Modeling, Application to Time-Based and Time-Harmonic Simulations - Shape and material parameter reconstruction of an isotropic or anisotropic solid immersed in a fluid - Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media. - Multi-level explicit local time-stepping methods for second-order wave equations - Absorbing Boundary Conditions for 3D elastic TTI modeling - Modeling of elastic Helmholtz equations by hybridizable discontinuous Galerkin method (HDG) for geophysical applications - Performance Assessment on Hybridizable Dg Approximations for the Elastic Wave Equation in Frequency Domain - High-Order IPDG Approximations for Elasto-Acoustic Problems - High-order Discontinuous Galerkin approximations for elasto-acoustic scattering problems - Modelling of seismic waves propagation in harmonic domain by hybridizable discontinuous Galerkin method (HDG) - Absorbing Boundary Conditions for 3D Tilted Transverse Isotropic media - Performance comparison between hybridizable DG and classical DG methods for elastic waves simulation in harmonic domain - Polynomial speeds in a Discontinuous Galerkin code - Hybridizable Discontinuous Galerkin method for the simulation of the propagation of the elastic wave equations in the frequency domain - Discontinuous Galerkin methods for the simulation of the propagation of the elastic wave equations in the frequency domain - High order discontinuous Galerkin methods for time-harmonic elastodynamics - Hybridizable discontinuous Galerkin method for the two-dimensional frequency-domain elastic wave equations - Efficient DG-like formulation equipped with curved boundary edges for solving elasto-acoustic scattering problems - Numerical schemes for the simulation of seismic wave propagation in frequency domain - Performance analysis of DG and HDG methods for the simulation of seismic wave propagation in harmonic domain - Hybridizable Discontinuous Galerkin method for solving Helmholtz elastic wave equations - Discontinuous Galerkin methods for solving Helmholtz elastic wave equations for seismic imaging - Performance comparison of HDG and classical DG method for the simulation of seismic wave propagation in harmonic domain - Contributions to the mathematical modeling and to the parallel algorithmic for the optimization of an elastic wave propagator in anisotropic media - Contribution to the mathematical analysis and to the numerical solution of an inverse elasto-acoustic scattering problem

- URL: https://team.inria.fr/magique3d/software/hou10ni/

5.3. MONTJOIE

KEYWORDS: High order finite elements - Edge elements - Aeroacoustics - High order time schemes

SCIENTIFIC DESCRIPTION: Montjoie is designed for the efficient solution of time-domain and time-harmonic linear partial differential equations using high-order finite element methods. This code is mainly written for quadrilateral/hexahedral finite elements, partial implementations of triangular/tetrahedral elements are provided. The equations solved by this code, come from the "wave propagation" problems, particularly acoustic, electromagnetic, aeroacoustic, elastodynamic problems.

FUNCTIONAL DESCRIPTION: Montjoie is a code that provides a C++ framework for solving partial differential equations on unstructured meshes with finite element-like methods (continuous finite element, discontinuous Galerkin formulation, edge elements and facet elements). The handling of mixed elements (tetrahedra, prisms, pyramids and hexahedra) has been implemented for these different types of finite elements methods. Several applications are currently available : wave equation, elastodynamics, aeroacoustics, Maxwell's equations.

- Participants: Gary Cohen, Juliette Chabassier, Marc Duruflé and Morgane Bergot
- Contact: Marc Duruflé
- URL: http://montjoie.gforge.inria.fr/

5.4. tmodeling-DG

Time-domain Wave-equation Modeling App

KEYWORDS: 2D - 3D - Elastoacoustic - Elastodynamic equations - Discontinuous Galerkin - Time Domain

SCIENTIFIC DESCRIPTION: tmodeling-DG simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

FUNCTIONAL DESCRIPTION: tmodelling-DG is the follow up to DIVA-DG that we develop in collaboration with our partner Total. Its purpose is more general than DIVA-DG and should contains various DG schemes, basis functions and time schemes. It models wave propagation in acoustic media, elastic (isotropic and TTI) media and elasto-acoustic media, in two and three dimensions.

NEWS OF THE YEAR: In 2018, we have coupled the code with a Reverse Time Migration algorithm.

- Participants: Julien Diaz, Lionel Boillot, Simon Ettouati and Hélène Barucq
- Partner: TOTAL
- Contact: Julien Diaz

5.5. OpenWind

Open Wind Instrument Design

KEYWORDS: Wave propagation - Inverse problem - Experimental mechanics - Image processing

FUNCTIONAL DESCRIPTION: -Computes resonating pipes' impedance using one-dimensional nite element method and the transfer matrix method -sound synthesis in the time domain (FDTD and FEM in space) - informatic interface for the usage of an input impedance measurement setup. -instrument bore extraction using tomographical image processing -inverse problem solving

- Contact: Juliette Chabassier

5.6. ffwi

Frequency-domain Full Waveform Inversion

KEYWORDS: 2D - 3D - Discontinuous Galerkin - Inverse problem - Frequency Domain - Acoustic equation - Elasticity

FUNCTIONAL DESCRIPTION: ffwi is developed in partnership with Total in the context of the Depth Imaging Partnership (DIP). It is devoted to perform seismic imaging using the Full Waveform Inversion method, in the frequency domain. It is based upon the software Fmodeling, which is itself dedicated to the forward problem. In FWI, the forward problem is solved using Hybridizable Discontinuous Galerkin Methods. The reconstruction of medium parameter is conducted with an iterative minimization scheme, which uses gradient descent techniques. The software can work with acoustic and elastic media, in two and three dimensions.

- Partner: TOTAL
- Contact: Florian Faucher

SERENA Project-Team

6. New Software and Platforms

6.1. CELIA3D

KEYWORDS: Fluid mechanics - Multi-physics simulation

FUNCTIONAL DESCRIPTION: The CELIA3D code simulates the coupling between a compressible fluid flow and a deformable structure. The fluid is handled by a Finite Volume method on a structured Cartesian grid. The solid is handled by a Discrete Element method (Mka3d scheme). The solid overlaps the fluid grid and the coupling is carried out with immersed boundaries (cut cells) in a conservative way.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: http://cermics.enpc.fr/~monassel/CELIA3D/

6.2. DiSk++

KEYWORDS: High order methods - Polyhedral meshes - C++

SCIENTIFIC DESCRIPTION: Discontinuous Skeletal methods approximate the solution of boundary-value problems by attaching discrete unknowns to mesh faces (hence the term skeletal) while allowing these discrete unknowns to be chosen independently on each mesh face (hence the term discontinuous). Cell-based unknowns, which can be eliminated locally by a Schur complement technique (also known as static condensation), are also used in the formulation. Salient examples of high-order Discontinuous Skeletal methods are Hybridizable Discontinuous Galerkin methods and the recently-devised Hybrid High-Order methods. Some major benefits of Discontinuous Skeletal methods are that their construction is dimension-independent and that they offer the possibility to use general meshes with polytopal cells and non-matching interfaces. The mathematical flexibility of Discontinuous Skeletal methods can be efficiently replicated in a numerical software: by using generic programming, the DiSk++ library offers an environment to allow a programmer to code mathematical problems in a way completely decoupled from the mesh dimension and the cell shape.

FUNCTIONAL DESCRIPTION: The software provides a numerical core to discretize partial differential equations arising from the engineering sciences (mechanical, thermal, diffusion). The discretization is based on the "Hybrid high-order" or "Discontinuous Skeletal" methods, which use as principal unknowns polynomials of arbitrary degree on each face of the mesh. An important feature of these methods is that they make it possible to treat general meshes composed of polyhedral cells. The DiSk ++ library, using generic programming techniques, makes it possible to write a code for a mathematical problem independently of the mesh. When a user writes the code for his problem using the basic operations offered by DiSk ++, that code can be executed without modifications on all types of mesh already supported by the library and those that will be added in the future.

- Author: Matteo Cicuttin
- Partner: CERMICS
- Contact: Matteo Cicuttin
- Publication: Implementation of Discontinuous Skeletal methods on arbitrary-dimensional, polytopal meshes using generic programming
- URL: https://github.com/wareHHOuse/diskpp

6.3. GENFIELD

KEYWORDS: Hydrogeology - Algorithm - Heterogeneity

SCIENTIFIC DESCRIPTION: GENFIELD implements a parallel version of the algorithm initially proposed by [E. Pardo-Iguzquiza and M. Chica-Olmo, Mathematical Geology, 25(2):177-217, 1993].

FUNCTIONAL DESCRIPTION: GENFIELD allows the generation of gaussian correlated fields. It is based on the circulant embedding method. Parallelism is implemented using MPI communications. GENFIELD is used in hydrogeology to model natural fields, like hydraulic conductivity or porosity fields.

NEWS OF THE YEAR: In 2018, we have performed scaling tests on ADA cluster. They have revealed that the symmetry of the phases required by this algorithm penalized a lot the parallel efficiency of GENFIELD (cf poster hal-01960444, version 1). We have decided to stop the development of GENFIELD. In 2018, we have developed a complete new software (cf BIL Inria ParaCIRCE) based on another algorithm initially proposed by [C. R. Dietrich and G. N. Newsam. A fast and exact method for multidimensional gaussian stochastic simulations. Water Resources Research, 29(8):2861-2869, 1993].

- Participants: Géraldine Pichot, Simon Legrand, Grégoire Lecourt, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Contact: Géraldine Pichot
- Publications: GENFIELD: A parallel software for the generation of stationary Gaussian random fields - Algorithms for stationary Gaussian random field generation
- URL: https://gitlab.inria.fr/slegrand/Genfield_dev

6.4. Mka3d

KEYWORDS: Scientific computing - Elasticity - Elastodynamic equations

FUNCTIONAL DESCRIPTION: The Mka3d method simulates an elastic solid by discretizing the solid into rigid particles. An adequate choice of forces and torques between particles allows to recover the equations of elastodynamics.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: http://cermics.enpc.fr/~monassel/Mka3D/

6.5. NEF-Draw

Numerical Experiments involving Fractures -Visualisation

KEYWORD: Fracture network

FUNCTIONAL DESCRIPTION: This software is a visualization tool of discrete fractured networks. It allows the visualization of the network geometry, the mesh of the network together with several quantities of interest (mesh quality, flow solution including wells) computed with the software NEF-Flow.

NEWS OF THE YEAR: This version includes Matlab vectorization of the operations which makes it possible to load flow solution on meshes with more than one million of fractures. It includes a text menu allowing the user to choose between different visualisation options (geometry, mesh together with the aspect ratio or together with the flow solution) A selective visualisation of fractures is also possible, loading only the fractures that carry most of the flow.

- Participant: Géraldine Pichot
- Contact: Géraldine Pichot
- URL: https://gitlab.inria.fr/gpichot/NEF

6.6. NEF-Flow

KEYWORDS: Hydrogeology - Numerical simulations - 3D

SCIENTIFIC DESCRIPTION: NEF-Flow is a Matlab software for the simulation of steady state single phase flow in Discrete Fracture Networks (DFNs) using the Mixed Hybrid Finite Element (MHFEM) method for conforming and non conforming discretizations.

FUNCTIONAL DESCRIPTION: The software NEF-Flow solves the problem of an incompressible fluid flowing through a network of fractures. The software is interfaced with different mesh generators, among which BLSURF from the GAMMA3 team. A mixed hybrid finite element method is implemented.

NEWS OF THE YEAR: The last version includes new feature: - wells, sink/source terms boundary conditions - Implementation of P1 non conforming finite elements - New data structures to save the information local to each fracture - New tests per fracture have been added to check the solution - Add wells and sink/sources boundary conditions in the function that check the solution.

- Participants: Géraldine Pichot, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Contact: Géraldine Pichot
- Publication: A mixed hybrid Mortar method for solving flow in discrete fracture networks
- URL: https://gitlab.inria.fr/gpichot/NEF

6.7. ParaCirce

Parallel Circulant Embedding

KEYWORDS: 2D - 3D - Hydrogeology - Gaussian random fields - MPI

SCIENTIFIC DESCRIPTION: ParaCirce implements the algorithm proposed by [C. R. Dietrich and G. N. Newsam. A fast and exact method for multidimensional gaussian stochastic simulations. Water Resources Research, 29(8):2861-2869, 1993].

FUNCTIONAL DESCRIPTION: ParaCirce implements a parallel Circulant Embedding method for the generation in parallel of 2D or 3D Gaussian Random Fields (second order stationary).

NEWS OF THE YEAR: - MPI implementation - Dedicated C++ classes to allow a user-friendly and safe usage of the library - Efficient use of the external library RngStream (L'Ecuyer) for a guarantee of independent realizations and reproductibility. - Splitting of the domain along one direction. The repartition of the field is automatic or defined by the user. - Automatic computation of the padding

- Participants: Géraldine Pichot and Simon Legrand
- Contact: Géraldine Pichot
- URL: https://gitlab.inria.fr/slegrand/paracirce

6.8. PRune

ParserRUNnEr

KEYWORD: Test

FUNCTIONAL DESCRIPTION: Python tool to parse single or multi configurations parameters files and to automatically run a program and store the results in a predefined tree.

- Participants: Simon Legrand and Géraldine Pichot
- Contact: Simon Legrand

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STEEP Project-Team

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5. New Software and Platforms

5.1. Software tools for the TRANUS LUTI Model

KEYWORDS: Urban planning - Transport model - LUTI

FUNCTIONAL DESCRIPTION: This year, we have consolidated and extended our software tools for the TRANUS LUTI model, thanks to support by Inria allowing to hire an engineer for one year Emna Jribi (ADT TRACAV project). Various tasks have been accomplished, concerning three types of functionality, these are as follows. First, calibration of TRANUS. The software implementation of our methods for calibrating the TRANUS land-use component has been cleaned up. It has been encapsulated such as to be seamlessly integrated within the TRANUS workflow (consisting of a sequence of executables, exchanging data through binary and other files). Second, graphical user interfaces to facilitate the repeated execution of TRANUS executables, for generating reports on results or for the exploration of the space of some critical model parameters. Third, we have continued to work on the embedding of TRANUS within the open source QGIS platform (a widely used Geographic Information System).

- Participants: Emna Jribi, Thomas Capelle and Peter Sturm
- Contact: Peter Sturm
- URL: https://gitlab.inria.fr/tranus

5.2. USAT

Urban Sprawl Analysis Toolkit

KEYWORDS: Urban sprawl - Urban planning

FUNCTIONAL DESCRIPTION: This software allows to calculate and analyse indices of urban sprawl from open data (OpenStreetMap), aimed to be used by urban scientists and urban planners. A spatialized version of indices measuring the accessibility, dispersion and land use mix is calculated. The implemented methods are described in [9].

- Participants: Luciano Gervasoni, Serge Fenet and Peter Sturm
- Partner: LIRIS
- Contact: Peter Sturm
- URL: https://github.com/lgervasoni/urbansprawl

5.3. USAT WEB

Urban Sprawl Analysis Toolkit Web-service

KEYWORDS: Urban planning - Urban sprawl

FUNCTIONAL DESCRIPTION: This is a web-service on top of the software USAT described above. The web-service will allow any user to select a region of interest and to launch the calculation and display of sprawl indices using USAT. It is in the process of being hosted on the HPC platform of IN2P3, after which it will be made open to the public. The source code for this web-service is already available at the below site.

The web-service is described in [10].

- Participants: Lucas Rezakhanlou, Peter Sturm, Luciano Gervasoni and Serge Fenet
- Contact: Peter Sturm
- Publication: USAT (Urban Sprawl Analysis Toolkit) : une plateforme web d'analyse de l'étalement urbain à partir de données massives ouvertes
- URL: https://gitlab.inria.fr/lrezakha/usat-web

5.4. InterfacesTRANUS

FUNCTIONAL DESCRIPTION: This software contains two interfaces dedicated to facilitating the usage of the TRANUS integrated land use and transport model+software. The first interface is dedicated to enabling the execution of the TRANUS binary programs without the need to use the console or the TRANUS GUI. The second interface provides an aid for calibrating a TRANUS model, by interactively exploring ranges of different parameters of a TRANUS model and visualising model outputs across these ranges.

- Participants: Julien Armand, Peter Sturm and Thomas Capelle
- Contact: Peter Sturm
- URL: https://gitlab.inria.fr/tranus/TRANUS_Interfaces

5.5. LUM_OSM

Land Use Mix calculation from OpenStreepMap data
FUNCTIONAL DESCRIPTION: The software uses Mapzen Metro Extracts to retrieve the OpenStreetMap data of a given region in the PostgreSQL format. Afterwards, a continuous representation of residential and activity land uses is created. Finally, a GIS output containing the degree of land use mixture is calculated by means of using the land uses maps. The implemented approach is documented in the paper "A framework for evaluating urban land use mix from crowd-sourcing data", http://hal.inria.fr/hal-01396792

- Participants: Luciano Gervasoni, Marti Bosch Padros, Peter Sturm and Serge Fenet
- Partners: EPFL - Ecole Polytechnique Fédérale de Lausanne - LIRIS
- Contact: Peter Sturm
- URL: http://github.com/martibosch/landusemix

5.6. QGIS_Tranus_Reports

FUNCTIONAL DESCRIPTION: This software allows to graphically visualise data output by the TRANUS LUTI model (and possibly, of any other data of the same structure). In particular, this concerns any data items defined per zone of a modelled territory (productions, indicators, etc.). The software is designed as a plugin for the geographical information system platform QGIS and can be run interactively as well as by the command line or by a call from within another software. The interactive mode (within QGIS) allows the user to define graphical outputs to be generated from TRANUS output files (type of graphs to be generated – 2D or 3D – color coding to be used, choice of data to be displayed, etc.). Visualisation of data is done in the form of 2D graphs or 3D models defined using java-script.

- Participants: Fausto Lo Feudo, Huu Phuoc Nguyen, Patricio Inzaghi, Peter Sturm and Thomas Capelle
- Contact: Peter Sturm
- URL: https://gitlab.inria.fr/tranus/QGIS_Tranus_Reports

5.7. Comptabilité Ecologique

FUNCTIONAL DESCRIPTION: Databases, database handling tools and data visualization tools (on the website). Databases include socio-economic and environmental datasets. Visualization tools include interactive piecharts, maps and Sankey diagrams.

- Participants: Jean-Yves Courtonne and Pierre-Yves Longaretti
- Contact: Jean-Yves Courtonne
- URL: http://www.eco-data.fr

TONUS Team

6. New Software and Platforms

6.1. CLAC

Conservation Laws Approximation on many Cores

SCIENTIFIC DESCRIPTION: It is clear now that future computers will be made of a collection of thousands of interconnected multicore processors. Globally it appears as a classical distributed memory MIMD machine. But at a lower level, each of the multicore processors is itself made of a shared memory MIMD unit (a few classical CPU cores) and a SIMD unit (a GPU). When designing new algorithms, it is important to adapt them to this kind of architecture. Our philosophy will be to program our algorithms in such a way that they can be run efficiently on this kind of computers. Practically, we will use the MPI library for managing the coarse grain parallelism, while the OpenCL library will efficiently operate the fine grain parallelism.

We have invested for several years until now into scientific computing on GPUs, using the open standard OpenCL (Open Computing Language). We were recently awarded a prize in the international AMD OpenCL innovation challenge thanks to an OpenCL two-dimensional Vlasov-Maxwell solver that fully runs on a GPU. OpenCL is a very interesting tool because it is an open standard now available on almost all brands of multicore processors and GPUs. The same parallel program can run on a GPU or a multicore processor without modification.

Because of the envisaged applications of CLAC, which may be either academic or commercial, it is necessary to conceive a modular framework. The heart of the library is made of generic parallel algorithms for solving conservation laws. The parallelism can be both fine-grained (oriented towards GPUs and multicore processors) and coarse-grained (oriented towards GPU clusters). The separate modules allow managing the meshes and some specific applications. In this way, it is possible to isolate parts that should be protected for trade secret reasons.

FUNCTIONAL DESCRIPTION: CLAC is a generic Discontinuous Galerkin solver, written in C/C++, based on the OpenCL and MPI frameworks.

- Partner: AxesSim
- Contact: Philippe Helluy
- URL: http://clac.gforge.inria.fr/

6.2. Selalib

SEmi-LAgrangian LIBrary

KEYWORDS: Plasma physics - Semilagrangian method - Parallel computing - Plasma turbulence

SCIENTIFIC DESCRIPTION: The objective of the Selalib project (SEmi-LAgrangian LIBrary) is to develop a well-designed, organized and documented library implementing several numerical methods for kinetic models of plasma physics. Its ultimate goal is to produce gyrokinetic simulations.

Another objective of the library is to provide to physicists easy-to-use gyrokinetic solvers, based on the semi-lagrangian techniques developed by Eric Sonnendrücker and his collaborators in the past CALVI project. The new models and schemes from TONUS are also intended to be incorporated into Selalib.

FUNCTIONAL DESCRIPTION: Selalib is a collection of modules conceived to aid in the development of plasma physics simulations, particularly in the study of turbulence in fusion plasmas. Selalib offers basic capabilities from general and mathematical utilities and modules to aid in parallelization, up to pre-packaged simulations.

- Partners: Max Planck Insitute - Garching - Université de Strasbourg
- Contact: Philippe Helluy
- URL: http://selalib.gforge.inria.fr/

6.3. SCHNAPS

Solver for Conservative Hyperbolic Nonlinear Applications for PlasmaS
KEYWORDS: Discontinuous Galerkin - StarPU - Kinetic scheme
FUNCTIONAL DESCRIPTION: Generic systems of conservation laws. Specific models: fluids, Maxwell, Vlasov, acoustics (with kinetic representation). Multitasking with StarPU. Explicit solvers (RK2, RK3, RK4): accelerated with OpenCL Implicit solvers: through kinetic representations and palindromic time integration.

- Contact: Philippe Helluy
- URL: http://schnaps.gforge.inria.fr/

6.4. Slappy

KEYWORDS: Python - Opencl
FUNCTIONAL DESCRIPTION: The code Slappy solves the advection equations on multi-patch and non-conform complex geometries with the Semi-Lagrangian method. Using this we can also treat some hyperbolic/parabolic PDE with the Approximate BGK method which, allows to write a PDE as a transport plus a local relaxation step. The code is written in PyOpcenCL and can be used on CPU/GPU.

- Contact: Emmanuel Franck

6.5. Patapon

Parallel Task in Python
KEYWORDS: Python - Parallel computing - High order time schemes
FUNCTIONAL DESCRIPTION: Patapon is a code in PyOpenCL which allows to solve PDE like MHD using the vectorial Lattice Boltzmann method on Cartesian grids.

- Contact: Philippe Helluy

BIOCORE Project-Team

6. New Software and Platforms

6.1. In@lgae

Numerical simulator of microalgae based processes

KEYWORDS: Simulation - Microalgae system - Productivity

FUNCTIONAL DESCRIPTION: In@lgae simulates the productivity of a microalgae production system, taking into account both the process type and its location and time of the year. The process is mainly defined by its thermal dynamics and by its associated hydrodynamics. For a given microalgal strain, a set of biological parameters describe the response to nitrogen limitation, temperature and light. As a result, the biomass production, CO_2 and nitrogen fluxes, lipid and sugar accumulation are predicted.

RELEASE FUNCTIONAL DESCRIPTION: The In@lgae platform has been optimised to make it faster. Some of the key models have been rewritten in C++ to allow a faster computation. Models have been improved to include, in the growth rate computation, the composition of the light spectrum. The graphical user interface has been enhanced and several sets of parameters describing different microalgal species have been stored.

- Participants: Étienne Delclaux, Francis Mairet, Olivier Bernard and Quentin Béchet
- Contact: Olivier Bernard

6.2. Odin

Platform for advanced monitoring, control and optimisation of bioprocesses

KEYWORDS: Bioinformatics - Biotechnology - Monitoring - Automatic control

SCIENTIFIC DESCRIPTION: This C++ application enables researchers and industrials to easily develop and deploy advanced control algorithms through the use of a Scilab interpreter. It also contains a Scilab-based process simulator which can be harnessed for experimentation and training purposes. ODIN is primarily developed in the C++ programming language and uses CORBA to define component interfaces and provide component isolation. ODIN is a distributed platform, enabling remote monitoring of the controlled processes as well as remote data acquisition.It is very modular in order to adapt to any plant and to run most of the algorithms, and it can handle the high level of uncertainties that characterises the biological processes through explicit management of confidence indexes.

FUNCTIONAL DESCRIPTION: ODIN is a software framework for bioprocess control and supervision. ODIN is a distributed platform, where algorithms are described with a common structure easy to implement. Finally, ODIN can perform remote data acquisition and process these data to compute the signals to be applied to the actuators, together with estimates of state variables or process state. ODIN can handle the high level of uncertainties that characterises the biological processes through explicit management of confidence indexes.

- Participants: Fabien Dilet, Florian Guenn, Francesco Novellis, Mathieu Lacage, Melaine Gautier, Olivier Bernard, Olivier Calabro, Romain Primet and Serigne Sow
- Contact: Olivier Bernard
- URL: https://team.inria.fr/biocore/software/odin/

<h1 style="text-align:center;color:red">CARMEN Project-Team</h1>

5. New Software and Platforms

5.1. CEPS

Cardiac ElectroPhysiology Simulation

KEYWORDS: Simulation - Health - Mesh - Cardiac - 3D - Cardiac Electrophysiology

SCIENTIFIC DESCRIPTION: As compared to other existing softwares, CEPS aims at providing a more general framework of integration for new methods or models and a better efficiency in parallel. CEPS is designed to run on massively parallel architectures, and to make use of state-of-the-art and well known computing libraries to achieve realistic and complex heart simulations. CEPS also includes software engineering and validation tools.

FUNCTIONAL DESCRIPTION: CEPS is a numerical simulation tool focused on the modeling of cardiac electrophysiology. The goal of CEPS is to easily allow the development of new numerical methods and new physical models.

- Participants: Mehdi Juhoor, Nejib Zemzemi, Antoine Gerard, Charlie Douanla Lontsi, Pierre-Elliott Bécue, Marc Fuentes and Yves Coudière
- Partners: Université de Bordeaux - Fondation Bordeaux Université - CHU de Bordeaux - Inria
- Contact: Yves Coudière
- URL: https://gforge.inria.fr/projects/ceps/

5.2. Platforms

5.2.1. CEMPACK

CEMPACK is a new collection of software that was previously archived in different places. It includes the high-performance simulation code Propag and a suite of software for the creation of geometric models, preparing inputs for Propag, and analysing its outputs. In 2017 the code was collected in an archive on Inria's GitLab platform, and a public website was created for documentation (http://cempack.gforge.inria.fr). The main components of CEMPACK are the following.

Propag-5.1   Applied modeling studies performed by the Carmen team in collaboration with IHU Liryc and foreign partners [7] [65], [56], [55], [53] rely on high-performance computations on the national supercomputers Irene, Occigen, and Turing. The Propag-5 code is optimized for these systems. It is the result of a decades-long development first at the *Université de Montréal* in Canada, then at Maastricht University in the Netherlands, and finally at the Institute of Computational Science of the *Università della Svizzera italiana* in Lugano, Switzerland. Since 2016 most of the development on Propag has been done by M. Potse at the Carmen team [27]. The code scales excellently to large core counts and, as it is controlled completely with command-line flags and configuration files, it can be used by non-programmers. It also features

- a plugin system for membrane models,
- a completely parallel workflow, including the initial anatomy input and mesh partitioning, which allows it to work with meshes of more than 10^9 nodes,
- a flexible output scheme allowing hundreds of different state variables and transient variables to be output to file, when desired, using any spatial and temporal subsampling,
- a configurable, LUSTRE-aware parallel output system in which groups of processes write HDF5/netCDF files, and
- CWEB documentation of the entire code base.

The code has been stable and reliable for several years. It can be considered the workhorse for our HPC work until CEPS takes over.

Gepetto   The Gepetto suite, named after a famous model maker, transforms a surface mesh of the heart into a set of (semi-)structured meshes for use by the Propag software or others. It creates the different fiber orientations in the model, including the transmurally rotating ventricular fibers and the various bundle structures in the atria (figure 2), and creates layers with possibly different electrophysiological properties across the wall. A practically important function is that it automatically builds the matching heart and torso meshes that Propag uses to simulate potentials in the torso (at a resolution of 1 mm) after projecting simulation results from the heart model (at 0.1 to 0.2 mm) on the coarser torso mesh [64]. Like Propag, the Gepetto software results from a long-term development that started in Montreal, Canada, around 2002. The code for atrial fiber structure was developed by our team.

Blender plugins   Blender (https://www.blender.org) is a free software package for the production of 3-D models, renderings, and animations, comparable to commercial software such as Cinema4D. CEMPACK includes a set of plugins for Blender that facilitate the production of anatomical models and the visualization of measured and simulated data. It uses the MMG remeshing library, which is developed by the CARDAMOM team at Inria Bordeaux.
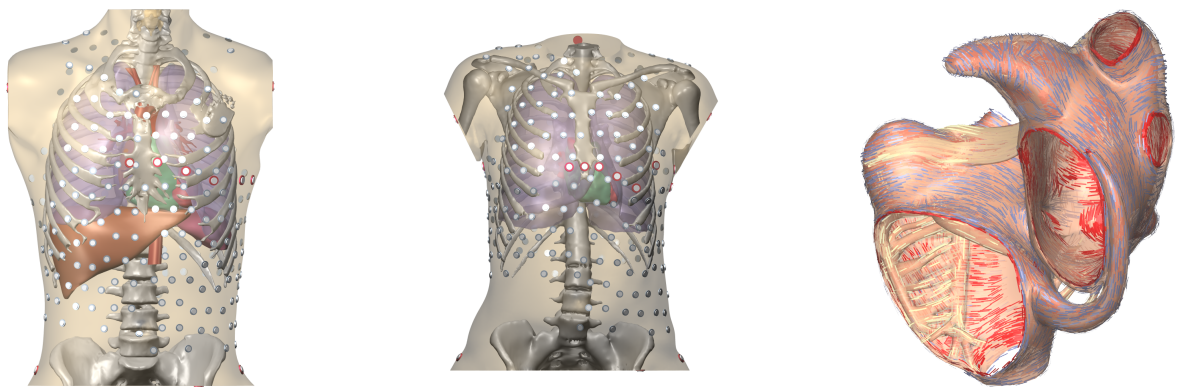

A   *B*   *C*

*Figure 2. **A and B:** Complete heart-torso geometries created with CEMPACK tools. **C:** Bundle structures and different layers of fiber orientation created by the Gepetto software.*

5.2.2. MUSIC

MUSIC is a multimodal platform for cardiac imaging developed by the imaging team at IHU LIRYC in collaboration with the Inria team Asclepios (https://bil.inria.fr/fr/software/view/1885/tab). It is based on the medInria software also developed by the Asclepios team. MUSIC is a cross-platform software for segmentation of medical imaging data, meshing, and ultimately also visualization of functional imaging data and model results.

Several members of the Carmen team use MUSIC for their work, and the team contributes to the software through the IDAM project.

<p align="center" style="color:red">DRACULA Project-Team</p>

4. New Software and Platforms

4.1. CelDyn

KEYWORDS: Modeling - Bioinformatics - Biology

FUNCTIONAL DESCRIPTION: Software "Celdyn" is developed in order to model cell population dynamics for biological applications. Cells are represented either as soft spheres or they can have more complex structure. Cells can divide, move, interact with each other or with the surrounding medium. Different cell types can be introduced. When cells divide, the types of daughter cells are specified. A user interface is developed.

- Participants: Alen Tosenberger, Laurent Pujo-Menjouet, Nikolai Bessonov and Vitaly Volpert
- Contact: Vitaly Volpert

M3DISIM Project-Team

6. New Software and Platforms

6.1. HeartLab

KEYWORDS: Computational geometry - Image analysis - Cardiac - Health - Simulation
FUNCTIONAL DESCRIPTION: The heartLab software is a library designed to perform both simulation and estimation of the heart mechanical behavior (based on various types of measurements, e.g. images).

Also included are geometric data and tools in the code to define cardiac anatomical models compatible with the simulation requirements in terms of mesh quality, fiber direction data defined within each element, and the referencing necessary for handling boundary conditions and estimation, in particular. These geometries are analytical or come from computerized tomography (CT) or magnetic resonance (MR) image data of humans or animals.

- Participants: Radomir Chabiniok, Gautier Bureau, Martin Genet, Federica Caforio, Ustim Khristenko, Dominique Chapelle and Philippe Moireau
- Contact: Philippe Moireau
- URL: https://raweb.inria.fr/rapportsactivite/RA2013/m3disim/uid14.html

6.2. Verdandi

KEYWORDS: HPC - Model - Software Components - Partial differential equation
FUNCTIONAL DESCRIPTION: Verdandi is a free and open-source (LGPL) library for data assimilation. It includes various such methods for coupling one or several numerical models and observational data. Mainly targeted at large systems arising from the discretization of partial differential equations, the library is devised as generic, which allows for applications in a wide range of problems (biology and medicine, environment, image processing, etc.). Verdandi also includes tools to ease the application of data assimilation, in particular in the management of observations or for a priori uncertainty quantification. Implemented in C++, the library may be used with models implemented in Fortran, C, C++ or Python.

- Participants: Dominique Chapelle, Gautier Bureau, Nicolas Claude, Philippe Moireau and Vivien Mallet
- Contact: Vivien Mallet
- URL: http://verdandi.gforge.inria.fr/

6.3. CardiacLab

KEYWORDS: Cardiovascular and respiratory systems - Matlab - Real time
FUNCTIONAL DESCRIPTION: CardiacLab is a MATLAB toolbox allowing to perform "real-time" cardiac simulations using 0D models of the cardiovascular systems. Its modular development includes (1) a module integrating the mechanical dynamics of the cavity taking into account its particular geometry, (2) a module allowing to choose a micro-model of the cardiac contraction, (3) a module of phase management, (4) a circulation module based on Windkessel models or more advanced 1D flows models, and (5) a perfusion module. The objective of this code is threefold: (1) demonstrate to students, engineers, medical doctors, the interest of modeling in cardiac applications, (2) unify our original modeling developments with the possibility to evaluate them with previous team developments before integrating them into 3D complex formulations, and (3) explore some avenues pertaining to real-time simulat

- Participants: Sebastien Impériale, Martin Genet, Federica Caforio, Ustim Khristenko, Peter Baumgartner, Radomir Chabiniok, François Kimmig and Arthur Le Gall
- Contact: Philippe Moireau
- URL: https://gitlab.inria.fr/M3DISIM/CardiacLab

6.4. MoReFEM

Modeling Research with the Finite Element Method

KEYWORDS: HPC - Multiphysics modelling - Data assimilation

FUNCTIONAL DESCRIPTION: MoReFEM is a HPC finite element library for simulating multiphysics evolution problems like the ones encounter in cardiac modeling (electrophysiology, structure and fluid mechanics, transport-diffusion, wave equations)

- Participants: Philippe Moireau, Patrick Le Tallec, Antoine Olivier, Dominique Chapelle, Ustim Khristenko, François Kimmig, Gautier Bureau and Sébastien Gilles

- Contact: Sébastien Gilles

- URL: https://gitlab.inria.fr/MoReFEM

<div align="center">

MAMBA Project-Team

</div>

6. New Software and Platforms

6.1. TiQuant

Tissue Quantifier

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

FUNCTIONAL DESCRIPTION: Systems biology and medicine on histological scales require quantification of images from histological image modalities such as confocal laser scanning or bright field microscopy. The latter can be used to calibrate the initial state of a mathematical model, and to evaluate its explanatory value, which hitherto has been little recognized. We generated a software for image analysis of histological material and demonstrated its use in analysing liver confocal micrografts, called TiQuant (Tissue Quantifier). The software is part of an analysis chain detailing protocols of imaging, image processing and analysis in liver tissue, permitting 3D reconstructions of liver lobules down to a resolution of less than a micrometer.

- Author: Dirk Drasdo
- Contact: Dirk Drasdo

6.2. TiSim

Tissue Simulator

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

SCIENTIFIC DESCRIPTION: TiSim (Tissue Simulator) is a versatile and efficient simulation environment for tissue models. TiSim is a software for agent-based models of multicellular systems. It permits model development with center-based models and deformable cell models, it contains modules for monolayer and multicellular spheroid simulations as well as for simulations of liver lobules. Besides agent-based simulations, the flow of blood and the transport of molecules can be modelled in the extracellular space, intracellular processes such as signal transduction and metabolism can be simulated, for example over an interface permitting integration of SBML-formulated ODE models. TiSim is written in modern C++ , keeping central model constituents in modules to be able to reuse them as building blocks for new models. For user interaction, the GUI Framework Qt is used in combination with OpenGL for visualisation. The simulation code is in the process of being published. The modeling strategy and approaches slowly reach systems medicine and toxicology. The diffusion of software is a fundamental component as it provides the models that are complex and difficult to implement (implementing a liver lobule model from scratch takes about 2-2.5yrs) in form of a software to the developer and users who like to build upon them. This increases significantly the speed of implementing new models. Moreover, standardization is indispensible as it permits coupling different software tools that may have implemented models at different scales / levels.

FUNCTIONAL DESCRIPTION: TiSim is a software that permits agent-based simulations of multicellular systems. - center-based lattice-free agent-based model - modular - C++, Qt, OpenGL, GUI, batch mode - permits multiscale simulations by integration of molecular pathways (for signaling, metabolisms, drug) into each individual cell - applications so far: monolayer growth, multicellular spheroids - Boolean networks (development time = coding time (60 MMs) + model development time (264 MMs)) - in follow-up version 1: - liver lobule regeneration - SBML interface - in follow-up version 2: - deformable cell model (by triangulation of cell surface) - deformable rod models - extracellular matrix - vascular flow and transport TiSim can be directly fed by processed image data from TiQuant.

- Participants: Andreas Buttenschoen, Dirk Drasdo, Eugenio Lella, Géraldine Cellière, Johannes Neitsch, Margaretha Palm, Nick Jagiella, Noémie Boissier, Paul Van Liedekerke, Stefan Hoehme and Tim Johann
- Partner: IZBI, Université de Leipzig
- Contact: Dirk Drasdo

6.3. Platforms

6.3.1. TiSim

New side branches have been developed that integrate the deformable cell model and extracellular matrix model in the TiSim software.

6.3.2. TiQuant

The software has been further extended for machine learning components.

MONC Project-Team

6. New Software and Platforms

6.1. Nenuphar

KEYWORDS: Modeling - Oncologie - Cancer - Partial differential equation - Medical - Medical imaging
FUNCTIONAL DESCRIPTION: The goal of project is to evaluate the aggressiveness of a tumor or its response to therapy. For that purpose, we use a mathematical model based on a set of nonlinear partial differential equations. This model is calibrated on patient data using a longitudinal sequence of CT Scan or MRI of the patient. This approach has been validated on about 35 clinical cases of lung metastases from various primary tumors (kidney, bladder, thyroid). Using two initial images showing the targeted lesion, we recover the patient-specific parameters of the model. The evolution of the disease is then predicted by letting the model run for later times with these parameters.

- Partners: CNRS - INP Bordeaux - Université Bordeaux 1
- Contact: Olivier Saut
- URL: https://team.inria.fr/monc/software/

6.2. papriK

KEYWORDS: Medical imaging - DICOM - Image registration - Image segmentation - 2D - 3D - Image analysis - Image processing - Medical applications - Radiomics
SCIENTIFIC DESCRIPTION: PapriK is the team toolkit devoted to processing and analyzing medical images. It currently wraps VTK and ITK and contains our own algorithms as well : - images input/output (including DICOM) - filtering, rescaling, resampling - segmentation/registration - radiomics computation: histogram, texture, shape
NEWS OF THE YEAR: - add python3 support - work on registration - simplify the library - fix bugs

- Participants: Cynthia Perier, Olivier Saut and Erwan Le Masson
- Partners: Institut Bergonié - Université de Bordeaux
- Contact: Cynthia Perier
- Publications: T2-based MRI Delta-Radiomics Improve Response Prediction in Soft-Tissue Sarcomas Treated by Neoadjuvant Chemotherapy - Pre-treatment magnetic resonance-based texture features as potential imaging biomarkers for predicting event free survival in anal cancer treated by chemoradiotherapy
- URL: https://team.inria.fr/monc/software/

6.3. NENUCORE

KEYWORDS: Image segmentation - Biomedical imaging - Image processing - Real-time rendering
SCIENTIFIC DESCRIPTION: Standalone application for visualization, manipulation and segmentation of 2D and 3D images. The software has been developed for application to medical imaging. The visualization is done in real time and the segmentation can be manual or semi-automatic. The software contains a database including medical images of patients, the segmentation data of these images as well as the associated meta-data.

- Participants: Benjamin Taton, Boris Raymond, Jean Mercat and Vivien Pianet
- Contact: Boris Raymond

6.4. metamats_burden

KEYWORDS: Metastasis - Cancer - Data assimilation - Regression - Biostatistics - Mechanistic modeling - Simulation

SCIENTIFIC DESCRIPTION: This Matlab software is a minimal code for fitting simultaneously primary tumor growth and metastatic burden data using nonlinear mixed-effects modeling.

FUNCTIONAL DESCRIPTION: Set of functions for calibration of models of metastatic burden and primary tumor growth to empirical population data

NEWS OF THE YEAR: Submission to the French agency of software protection (APP). Inclusion of a new model for pre-operative anti-angiogenic treatment. Validation of the previous models on large databases (400+ animals)

- Participants: Sébastien Benzekry and Chiara Nicolo
- Partner: Roswell Park Comprehensive Cancer Center
- Contact: Sébastien Benzekry
- Publications: Modeling Spontaneous Metastasis following Surgery: An In Vivo-In Silico Approach - Computational Modelling of Metastasis Development in Renal Cell Carcinoma
- URL: http://metamats.bordeaux.inria.fr/

6.5. metamats_core

KEYWORDS: Metastasis - Cancer - Mechanistic modeling - Simulation - Modeling

SCIENTIFIC DESCRIPTION: This code is devoted to the simulation of partial differential equation (PDE) based models for the time development of a population of secondary tumors (metastases).

FUNCTIONAL DESCRIPTION: Metamats_core simulates a partial differential equation (PDE)-based model for the time development of a population of secondary tumors (metastases).

NEWS OF THE YEAR: Submission to the French agency of software protection (APP)

- Participant: Sébastien Benzekry
- Contact: Sébastien Benzekry
- Publications: Modeling Spontaneous Metastasis following Surgery: An In Vivo-In Silico Approach - Passing to the limit 2D-1D in a model for metastatic growth - Mathematical analysis of a two-dimensional population model of metastatic growth including angiogenesis - Modeling the impact of anticancer agents on metastatic spreading - Global Dormancy of Metastases due to Systemic Inhibition of Angiogenesis
- URL: http://benzekry.perso.math.cnrs.fr/

6.6. IRENA

Numerical Assessment of IRreversible Electroporation ablation

KEYWORDS: Cancer - Numerical electroporation

SCIENTIFIC DESCRIPTION: The C++ software IRENA developed by O. Gallinato and C. Poignard within the Inria team Monc enable sto compute the static electric field distribution in the clinical configuration of IRE ablation of liver tumors. The code is based on the finite volume method on Cartesian grid. The needles and the liver boundary are determined as the zero of a level-set function. Close to the boundaries, the first and second order derivatives are computed with the standard Ghost Fluid Method. The equivalent conductivities at half points are computed thanks to harmonic mean (additivity law of resistivity). In order to maintain a reasonable computation time, the refinement is low enough (1 mm3 grid voxels). As the mesh does not pick up the very fine needles, the Dirichlet conditions imposed on the active parts of the electrodes and the Neumann conditions imposed on the insulated parts are changed into Robin conditions on the first layer of points around the needles, thanks to a second order development. This results in a numerical scheme, which is computationally efficient and accurate enough.

FUNCTIONAL DESCRIPTION: Digital simulation tool for the assessment of irreversible electroporation clinical process

- Authors: Olivier Gallinato and Clair Poignard
- Contact: Clair Poignard

6.7. metamats_size

Fitting longitudinal data of size and number of metastases using mechanistic models

KEYWORDS: Cancer - Mechanistic modeling - Metastasis - Regression - Simulation - Data assimilation

SCIENTIFIC DESCRIPTION: This software fits models of metastatic development to longitudinal data of metastatic sizes and provides simulation and visualization tools for metastatic modeling.

NEWS OF THE YEAR: Establishment of a first clean and minimal version. Validation of the software on clinical data of brain metastases from non-small cell lung cancer. Submission to the French agency of software protection (APP).

- Participants: Sébastien Benzekry and Mariia Bilous
- Partners: Centre de Recherches en Cancérologie de Marseille - Institut Bergonié - Assistance Publique - Hôpitaux de Marseille
- Contact: Sébastien Benzekry
- Publication: Computational modeling reveals dynamics of brain metastasis in non-small cell lung cancer and provides a tool for personalized therapy
- URL: http://metamats.bordeaux.inria.fr/

6.8. Carcinom

Computer-Assisted Research about Cancer growth and INsights on Oncological Mechanisms

KEYWORDS: Cancer - Regression - Tumor growth

SCIENTIFIC DESCRIPTION: This software is primarily designed to perform a modeling analysis of tumor growth kinetics. Given a data set of longitudinal measurements of tumor size in a population, it fits multiple models of tumor growth (either user-defined or selected from a library of classical models), computes goodness-of-fit statistical metrics, identifies the parameters of the models and estimates associated standard errors. Fits of the data can be performed either individual per individual or using a population approach (nonlinear mixed-effects).

FUNCTIONAL DESCRIPTION: Software for modeling and fitting tumor growth kinetics. Given a data set of longitudinal measurements of tumor size in a population, it fits multiple models of tumor growth (either user-defined or selected from a library of classical models), computes goodness-of-fit statistical metrics, identifies the parameters of the models and estimates associated standard errors. Fits of the data can be performed either on an individual basis or using a population approach (nonlinear mixed-effects).

Graphical and statistical tools of use when analyzing growth curves are also included.

NEWS OF THE YEAR: Submission to the French agency of software protection (APP). Development of a python module for interaction with Monolix.

- Participants: Simon Evain, Vivien Pianet and Cristina Vaghi
- Partner: Roswell Park Comprehensive Cancer Center
- Contact: Sébastien Benzekry
- Publication: Classical Mathematical Models for Description and Forecast of Experimental Tumor Growth
- URL: https://team.inria.fr/monc/software/

6.9. Platforms

6.9.1. Transport Equation Solver v1

Submission to the French agency of software protection of the software "Transport Equation Solver v1".

Ce logiciel répond aux besoins liés à l'analyse fonctionnelle de la vascularisation d'un organe par imagerie dynamique et en particulier il concerne l'analyse de la vascularisation placentaire qui est destinée au diagnostic d'anomalies d'invasion placentaire par échographie dynamique de contraste. De manière plus précise, ce logiciel permet, à partir d'un modèle physique d'écoulement des fluides, d'estimer et de quantifier le transport du produit de contraste injecté lors d'une imagerie par échographie dynamique de contraste.

NUMED Project-Team

4. New Software and Platforms

4.1. Bingham flows

FUNCTIONAL DESCRIPTION: A 1D and 2D code with a new method for the computation of viscoplatic flows with free-surface. It essentially couples Optimization methods and Well-Balanced Finite-Volumes schemes for viscous shallow-water equations (induced by the viscoplastic nature of the fluid). Currently applied to avalanches of dense snow, it is a private code currently actively developed (in C++). One of the key feature is that its well-balanced property allows to obtained the stationary states which are linked to the stopping of the snow avalanche for this highly non-linear type of fluid.

- Contact: Emmanuel Grenier

4.2. OptimChemo

FUNCTIONAL DESCRIPTION: OptimChemo is a userfriendly software designed to study numerically the effect of multiple chemotherapies on simple models of tumour growth and to optimize chemotherapy schedules.

- Participants: Ehouarn Maguet, Emmanuel Grenier, Paul Vigneaux and Violaine Louvet
- Contact: Emmanuel Grenier

4.3. SETIS

KEYWORDS: Health - DICOM - Medical imaging - Drug development
FUNCTIONAL DESCRIPTION: SETIS software is a GUI allowing to treat DICOM medical images to extract pathological data. These data can then be exported and used in a SAEM software (including Monolix (Inria & Lixoft)) for the parameters' estimation of models in the context of population approaches. As an example SETIS can be used to segment and compute the tumor size of a patients from MRI scans taken at different times. The software is sufficiently general to be used in various situations by clinicians (already done by colleagues in Lyon Hospital).

- Participants: Ehouarn Maguet and Paul Vigneaux
- Partner: ENS Lyon
- Contact: Paul Vigneaux

4.4. SIMPHYT

KEYWORDS: Bioinformatics - Cancer - Drug development
FUNCTIONAL DESCRIPTION: SimPHyt is an implementation in Python of the low grad glioma model. The aim is to predict the evolution of the glioma size of patients.

- Participant: Benjamin Ribba
- Contact: Benjamin Ribba

4.5. SITLOG

- Participants: Benjamin Ribba and Morgan Martinet
- Contact: Emmanuel Grenier

4.6. VAXSIMSTAB

KEYWORDS: Bioinformatics - Health - Drug development
FUNCTIONAL DESCRIPTION: VAXSIMSTAB is a modeler stability prediction of vaccine software.

- Participants: Benjamin Ribba, Emmanuel Grenier and Vincent Calvez
- Contact: Benjamin Ribba

REO Project-Team

6. New Software and Platforms

6.1. FELiScE

Finite Elements for Life SCiences and Engineering problems
KEYWORDS: Finite element modelling - Cardiac Electrophysiology - Cardiovascular and respiratory systems
FUNCTIONAL DESCRIPTION: FELiScE is a finite element code which the M3DISIM and REO project-teams have decided to jointly develop in order to build up on their respective experiences concerning finite element simulations. One specific objective of this code is to provide in a unified software environment all the state-of-the-art tools needed to perform simulations of the complex respiratory and cardiovascular models considered in the two teams – namely involving fluid and solid mechanics, electrophysiology, and the various associated coupling phenomena. FELISCE is written in C++, and may be later released as an opensource library. FELiScE was registered in July 2014 at the Agence pour la Protection des Programmes under the Inter Deposit Digital Number IDDN.FR.001.350015.000.S.P.2014.000.10000.

- Participants: Axel Fourmont, Benoit Fabreges, Damiano Lombardi, Dominique Chapelle, Irène Vignon-Clementel, Jean-Frédéric Gerbeau, Marina Vidrascu, Matteo Aletti, Miguel Angel Fernandez Varela, Mikel Landajuela Larma, Philippe Moireau and Sébastien Gilles
- Contact: Miguel Angel Fernandez Varela
- URL: http://felisce.gforge.inria.fr

6.2. SHELDDON

SHELls and structural Dynamics with DOmain decomposition in Nonlinear analysis
FUNCTIONAL DESCRIPTION: SHELDDON is a finite element library based on the Modulef package which contains shell elements, nonlinear procedures and PVM subroutines used in domain decomposition or coupling methods, in particular fluid-structure interaction.

- Participants: Dominique Chapelle, Marina Vidrascu and Patrick Le Tallec
- Contact: Marina Vidrascu
- URL: https://gforge.inria.fr/projects/shelddon/

6.3. DCIMaL

KEYWORD: Cardiac Electrophysiology
FUNCTIONAL DESCRIPTION: DCIMaL is a Python and C++ software for safety pharmacology studies and particularly field potentials signals measured with micro-electrode array (MEA). The software includes a solver for field potential simulations and a dictionary of entries corresponding to features which can be extracted from real or simulated potential signals. It also includes an algorithm for drug classification (channel blockade or torsadogenic risk) and a tool for estimating ion channel activity (based on the CMAES library). DCIMaL was registered in 2018 at the Agence pour la Protection des Programmes Inter Deposit Digital Number IDDN.FR.001.270003.000.S.P.2018.000.31230

- Participants: Fabien Raphel, Jean-Frédéric Gerbeau and Damiano Lombardi
- Contact: Damiano Lombardi

6.4. FELiScE-NS

KEYWORDS: Incompressible flows - Thin-walled solids

FUNCTIONAL DESCRIPTION: FELiScE-NS is a set finite elements solvers for incompressible fluids (fractional-step schemes) and non-linear thin-walled structures (3D shells, and 2D curved beams) developed in the framework of the FELiScE library. FELiSCe-NS was registered in 2018 at the Agence pour la Protection des Programmes Inter Deposit Digital Number IDDN.FR.001.270015.000.S.A.2018.000.31200.

- Participants: Benoit Fabreges, Miguel Angel Fernandez Varela, Axel Fourmont, Jean-Frédéric Gerbeau and Marina Vidrascu
- Contact: Miguel Angel Fernandez Varela

SISTM Project-Team

6. New Software and Platforms

6.1. marqLevAlg

KEYWORDS: Optimization - Biostatistics

FUNCTIONAL DESCRIPTION: An R package for function optimization. Available on CRAN, this package performs a minimization of function based on the Marquardt-Levenberg algorithm. This package is really useful when the surface to optimize is non-strictly convex or far from a quadratic function. A new convergence criterion, the relative distance to maximum (RDM), allows the user to have a better confidence in the stopping points, other than basic algorithm stabilization.

- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/marqLevAlg/index.html

6.2. VSURF

Variable Selection Using Random Forests

KEYWORDS: Classification - Statistics - Machine learning - Regression

FUNCTIONAL DESCRIPTION: An R package for Variable Selection Using Random Forests. Available on CRAN, this package performs an automatic (meaning completely data-driven) variable selection procedure. Originally designed to deal with high dimensional data, it can also be applied to standard datasets.

- Contact: Robin Genuer
- URL: https://github.com/robingenuer/VSURF

6.3. NPflow

Bayesian Nonparametrics for Automatic Gating of Flow-Cytometry Data

KEYWORDS: Bayesian estimation - Bioinformatics - Biostatistics

FUNCTIONAL DESCRIPTION: Dirichlet process mixture of multivariate normal, skew normal or skew t-distributions modeling oriented towards flow-cytometry data pre-processing applications.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/NPflow/

6.4. COVVSURF

Combination of Clustering Of Variables and Variable Selection Using Random Forests

KEYWORDS: Classification - Statistics - Cluster - Machine learning - Regression

- Contact: Robin Genuer
- URL: https://github.com/robingenuer/CoVVSURF

6.5. clogitLasso

KEYWORDS: Biostatistics - Bioinformatics - Machine learning - Regression

FUNCTIONAL DESCRIPTION: R package to fit a sequence of conditional logistic regression models with lasso, for small to large sized samples.

RELEASE FUNCTIONAL DESCRIPTION: Optimisation

- Partner: DRUGS-SAFE
- Contact: Marta Avalos Fernandez
- URL: https://cran.r-project.org/web/packages/clogitLasso/index.html

6.6. TcGSA

Time-course Gene Set Analysis
KEYWORDS: Bioinformatics - Genomics
FUNCTIONAL DESCRIPTION: An R package for the gene set analysis of longitudinal gene expression data sets. This package implements a Time-course Gene Set Analysis method and provides useful plotting functions facilitating the interpretation of the results.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/TcGSA/index.html

6.7. NIMROD

Normal approximation Inference in Models with Random effects based on Ordinary Differential equations
KEYWORDS: Ordinary differential equations - Statistical modeling
FUNCTIONAL DESCRIPTION: We have written a specific program called NIMROD for estimating parameter of ODE based population models.

- Contact: Melanie Prague
- URL: http://etudes.isped.u-bordeaux2.fr/BIOSTATISTIQUE/NIMROD/documentation/html/index.html

6.8. tcgsaseq

Time-Course Gene Set Analysis for RNA-Seq Data
KEYWORDS: Genomics - Biostatistics - Statistical modeling - RNA-seq - Gene Set Analysis
FUNCTIONAL DESCRIPTION: Gene set analysis of longitudinal RNA-seq data with variance component score test accounting for data heteroscedasticity through precision weights.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/tcgsaseq/index.html

6.9. cytometree

KEYWORDS: Clustering - Biostatistics - Bioinformatics
FUNCTIONAL DESCRIPTION: Given the hypothesis of a bimodal distribution of cells for each marker, the algorithm constructs a binary tree, the nodes of which are subpopulations of cells. At each node, observed cells and markers are modeled by both a family of normal distributions and a family of bimodal normal mixture distributions. Splitting is done according to a normalized difference of AIC between the two families.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/cytometree/index.html

6.10. CRTgeeDR

KEYWORDS: Missing data - Statistics - Regression

FUNCTIONAL DESCRIPTION: The CRTgeeDR package allows you to estimates parameters in a regression model (with possibly a link function). It allows treatment augmentation and IPW for missing outcome. It is particularly of use when the goal is to estimate the intervention effect of a prevention strategy agains epidemics in cluster randomised trials.

- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/CRTgeeDR/index.html

6.11. ludic

KEYWORDS: Probability - Biostatistics
FUNCTIONAL DESCRIPTION: An R package to perform probabilistic record Linkage Using only DIagnosis Codes without direct identifiers, using C++ code to speed up computations. Available on CRAN, development version on github.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/ludic/index.html

6.12. CoDaPCA

KEYWORDS: Unsupervised learning - PCA
FUNCTIONAL DESCRIPTION: R functions associated to the article Avalos et al. Representation Learning of Compositional Data. NeurIPS 2018 http://papers.nips.cc/paper/7902-representation-learning-of-compositional-data

- Contact: Marta Avalos Fernandez
- URL: https://github.com/sistm/CoDa-PCA

6.13. Left-censored Lasso

KEYWORDS: Biostatistics - Machine learning
FUNCTIONAL DESCRIPTION: R function associatied to the article Soret et al. Lasso regularization for left-censored Gaussian outcome and high-dimensional predictors. BMC Medical Research Methodology (2018) 18:159 https://doi.org/10.1186/s12874-018-0609-4

RELEASE FUNCTIONAL DESCRIPTION: https://github.com/psBiostat/left-censored-Lasso

- Contact: Marta Avalos Fernandez

6.14. dd-sPLS

Data-Driven Sparse PLS
KEYWORDS: Marker selection - Classification - Regression - Missing data - Multi-Block - High Dimensional Data - PLS - SVD
FUNCTIONAL DESCRIPTION: Allows to build Multi-Data-Driven Sparse PLS models. Multi-blocks with high-dimensional settings are particularly sensible to this. Whatsmore it deals with missing samples (entire lines missing per block) thanks to the Koh-Lanta algorithm. SVD decompositions permit to offer a fast and controlled method.

- Contact: Hadrien Lorenzo
- URL: https://hadrienlorenzo.netlify.com/projects/ddspls/

6.15. kernscr

KEYWORDS: Genomics - Biostatistics

FUNCTIONAL DESCRIPTION: An R package to perform KERNel machine score test for pathway analysis in the presence of Semi-Competing Risks

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=kernscr

6.16. phenotypr

KEYWORDS: Phenotyping - Automatic labelling - Automatic Learning
FUNCTIONAL DESCRIPTION: Machine learning prediction algorithm for predicting a clinical phenotype from structured diagnostic data and CUI occurrence data collected from medical reports, previously processed by NLP approaches.

- Contact: Boris Hejblum
- URL: https://github.com/borishejblum/phenotypr

6.17. R2GUESS

Graphical processing Unit Evolutionary Stochastic Search
FUNCTIONAL DESCRIPTION: R2GUESS package is a wrapper of the GUESS (Graphical processing Unit Evolutionary Stochastic Search) program. GUESS is a computationally optimised C++ implementation of a fully Bayesian variable selection approach that can analyse, in a genome-wide context, single and multiple responses in an integrated way. The program uses packages from the GNU Scientific Library (GSL) and offers the possibility to re-route computationally intensive linear algebra operations towards the Graphical Processing Unit (GPU) through the use of proprietary CULA-dense library.

- Contact: Rodolphe Thiebaut

XPOP Project-Team

6. New Software and Platforms

6.1. mlxR

KEYWORDS: Simulation - Data visualization - Clinical trial simulator
FUNCTIONAL DESCRIPTION: The models are encoded using the model coding language 'Mlxtran', automatically converted into C++ codes, compiled on the fly and linked to R using the 'Rcpp' package. That allows one to implement very easily complex ODE-based models and complex statistical models, including mixed effects models, for continuous, count, categorical, and time-to-event data.

- Contact: Marc Lavielle
- URL: http://simulx.webpopix.org/

6.2. Rsmlx

R speaks Monolix
KEYWORDS: Data modeling - Nonlinear mixed effects models - Statistical modeling
FUNCTIONAL DESCRIPTION: Among other tasks, 'Rsmlx' provides a powerful tool for automatic PK model building, performs statistical tests for model assessment, bootstrap simulation and likelihood profiling for computing confidence intervals. 'Rsmlx' also proposes several automatic covariate search methods for mixed effects models.

- Partner: Lixoft
- Contact: Marc Lavielle

6.3. SPIX

KEYWORDS: Data modeling - Mass spectrometry - Chemistry
FUNCTIONAL DESCRIPTION: SPIX allows you to - To automatically identify, on the basis of statistical approaches, small but significant differences in spectra measured under different conditions, - Model the kinetics of entities that evolve over time

- Partner: Laboratoire de Chimie Moléculaire - Ecole Polytechnique
- Contact: Marc Lavielle