



RESEARCH CENTER

FIELD

Digital Health, Biology and Earth

Activity Report 2017

Section Software

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ABS Project-Team

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 2017, major efforts targeted two points. First, the simplification of installation procedures. 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/>

AMIBIO Team (section vide)

BEAGLE Project-Team

5. New Software and Platforms

5.1. aevol

Artificial 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: Carole Knibbe
- URL: <http://www.aevol.fr/>

5.2. 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: [DeCoSTAR: Reconstructing the ancestral organization of genes or genomes using reconciled phylogenies](#)
- URL: <http://pbil.univ-lyon1.fr/software/DeCoSTAR/>

5.3. EvoEvo

Evolution of Evolution

KEYWORDS: Bioinformatics - Biology - Evolution

FUNCTIONAL DESCRIPTION: In the context of the EvoEvo european project we are developing an integrated model of microorganisms evolution. This model will extend the current evolutionary models developed in the team (Aevol and R-Aevol) by adding a metabolic level and an ecosystem level. In 2014, a first version has been developed and released that includes the genomic, genetic and metabolic levels.

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

5.4. 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 aggregate 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

5.5. FluoBacTracker

KEYWORDS: Bioinformatics - Biology - Biomedical imaging

SCIENTIFIC DESCRIPTION: FluoBacTracker is an ImageJ plugin allowing the segmentation 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://fluobacktracker.inrialpes.fr>

5.6. 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/>

BIGS Project-Team

5. New Software and Platforms

5.1. Angio-Analytics

KEYWORDS: Health - Cancer - Biomedical imaging

SCIENTIFIC DESCRIPTION: This tool allows the pharmacodynamic characterization of anti-vascular effects in anti-cancer treatments. It uses time series of in vivo images provided by intra-vital microscopy. Such in vivo images are obtained owing to skinfold chambers placed on mice skin. The automatized analysis is split up into two steps that were completely performed separately and manually before. The first steps corresponds to image processing to identify characteristics of the vascular network. The last step is the system identification of the pharmacodynamic response and the statistical analysis of the model parameters.

FUNCTIONAL DESCRIPTION: Angio-Analytics allows the pharmacodynamic characterization of anti-vascular effects in anti-cancer treatments.

- Participant: Thierry Bastogne
- Contact: Thierry Bastogne

5.2. In silico

In silico design of nanoparticles for the treatment of cancers by enhanced radiotherapy

KEYWORDS: Bioinformatics - Cancer - Drug development

FUNCTIONAL DESCRIPTION: To speed up the preclinical development of medical engineered nanomaterials, we have designed an integrated computing platform dedicated to the virtual screening of nanostructured materials activated by X-ray making it possible to select nano-objects presenting interesting medical properties faster. The main advantage of this in silico design approach is to virtually screen a lot of possible formulations and to rapidly select the most promising ones. The platform can currently handle the accelerated design of radiation therapy enhancing nanoparticles and medical imaging nano-sized contrast agents as well as the comparison between nano-objects and the optimization of existing materials.

- Participant: Thierry Bastogne
- Contact: Thierry Bastogne

5.3. SesIndexCreator

FUNCTIONAL DESCRIPTION: This package allows computing and visualizing socioeconomic indices and categories distributions from datasets of socioeconomic variables (These tools were developed as part of the EquitArea Project, a public health program).

- Participants: Benoît Lalloué, Jean-Marie Monnez, Nolwenn Le Meur and Severine Deguen
- Contact: Benoît Lalloué
- URL: http://www.equitarea.org/documents/packages_1.0-0/

BONSAI Project-Team

6. New Software and Platforms

6.1. 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>

6.2. 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 Violette
- 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>

6.3. 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>

6.4. 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: H  l  ne Touzet, Pierre Pericard, Yoann Dufresne, Samuel Blanquart and Lo  c Couderc
- Contact: H  l  ne 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, 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 translationnal 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 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. Platforms

6.9.1. 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 2017, a Galaxy portal (<https://galaxyproject.org/>) for structural bioinformatics software was added to the platform thanks to funding for an engineer (Antoine Chemardin) from the IFB.

- Contact: Marie-Dominique Devignes

DYLISS Project-Team

6. New Software and Platforms

6.1. AskOmics

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

FUNCTIONAL DESCRIPTION: AskOmics allows to load heterogeneous bioinformatics data (formatted as tabular files) into a Triple Store system using a user-friendly web interface. AskOmics also provides an intuitive graph-based user interface supporting the creation of complex queries that currently require hours of manual searches across tens of spreadsheet files. The elements of interest selected in the graph are then automatically converted into a SPARQL query that is executed on the users' data.

NEWS OF THE YEAR: Several functionalities have been developed: 1) capacity of integrating genomics data (import of GFF and BED files and generation of RDF compliant with the FALDO ontology), 2) integration of data and knowledge in the OWL format to exploit biological information from external repositories, particularly from EBI and NCBI. Notably, this functionality allows AskOmics to support the Gene Ontology, the Taxonomy ontology as well as BioPAX biological networks. 3) improved user interface expressivity for generating SPARQL queries, 4) implementation of a support for multiple concurrent user sessions, with the distinction between public and user-specific datasets 5) deployment of AskOmics on the GenOuest cloud infrastructure to facilitate its release and diffusion 6) interoperability between AskOmics and the Galaxy workflow environment.

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

6.2. PADMet-utils

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

FUNCTIONAL DESCRIPTION: The main concept underlying padmet-utils is to provide solutions that ensure the consistency, the internal standardization and the reconciliation of the information used within any workflow that combines several tools involving metabolic networks reconstruction or analysis.

NEWS OF THE YEAR: In 2017, Padmet-utils was enriched with a RDF export to allow the interoperability of the AuReMe workspace for the reconstruction of metabolic networks with the Askomics Tool for querying heterogeneous data. Padmet-utils was also extended to handle metabolic networks in the SBML3 format.

- Participants: Alejandro Maass, Meziane Aite and Anne Siegel
- Partner: University of Chile
- Contact: Anne Siegel
- URL: <https://gitlab.inria.fr/maite/padmet-utils>

6.3. CADBIOM

Computer Aided Design of Biological Models

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

FUNCTIONAL DESCRIPTION: Based on Guarded transition semantic, this software provides a formal framework to help the modeling of biological systems such as cell signaling network. It allows investigating synchronization events in biological networks. Software development has been restarted since November 2016. The source code is available at the following address: <https://gitlab.irisa.fr/0000B8EG/Cadbiom>

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

6.4. conquests

Crossroads in Metabolic Network from Stoichiometric and Topologic Studies

KEYWORDS: Bioinformatics - ASP - Answer Set Programming - Constraint-based programming

FUNCTIONAL DESCRIPTION: This Python package in systems biology allows the identification of essential metabolites with respect to the production of targeted elements in a metabolic network, by comparing flux and graph-based analysis. Conquests's inputs are a sbml file corresponding to a metabolic network and the biomass reaction name. The outputs are three sets of essential metabolites. They are computed according to three complementary criteria: graph-based accessibility of targeted metabolites, the presence of flux in the biomass reaction and the maximisation of flux in the biomass reaction.

NEWS OF THE YEAR: Conquest was released in 2017.

- Contact: Julie Laniau

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 Deniérou
- 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 find a reconstruction of minimum cost. The main problem with this approach is that the cost of the events strongly influence 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 Sinimeri, Catherine Matias, Christian Baudet, Christian Gautier, Marie-France Sagot and Pierluigi Crescenzi
- Contact: Blerina Sinimeri
- 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

5.6. 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 Sinimeri, Christian Baudet, Marie-France Sagot and Pierluigi Crescenzi
- Contact: Blerina Sinimeri
- URL: <http://eucalypt.gforge.inria.fr/>

5.7. 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>

5.8. 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>

5.9. 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/>

5.10. HgLib

KEYWORD: Graph algorithmics

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.

- Contact: Arnaud Mary
- URL: <https://gitlab.inria.fr/kirikomics/hglib>

5.11. 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://kisssplice.prabi.fr/tools/kissDE/>

5.12. KisSplice

KEYWORDS: Bioinformatics - Bioinformatics 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-Laferrrière, 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://kisssplice.prabi.fr/>

5.13. 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/>

5.14. 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/>

5.15. 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: <http://metexplore.toulouse.inra.fr/metexplore/>

5.16. 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/>

5.17. 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 synthesise 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-Laferrrière, Arnaud Mary, Delphine Parrot, Laurent Bulteau, Leen Stougie, Marie-France Sagot and Susana Vinga
- Contact: Marie-France Sagot
- URL: <http://multipus.gforge.inria.fr/>

5.18. 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/>

5.19. 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/>

5.20. 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>

5.21. 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

5.22. 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

5.23. 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/>

5.24. 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++.

RELEASE FUNCTIONAL DESCRIPTION: speed up from x2 to x4 for kmer counting and graph construction phases (optimizations based on minimizers and improved Bloom filters). GATB's k-mer counter has been improved using techniques from KMC2, to achieve competitive running times compared to KMC2. ability to store arbitrary information associated to each kmer of the graph, enabled by a minimal perfect hash function (costs only 2.61 bits/kmer of memory) improved API with new possibilities (banks and kmers management) many new snippets showing how to use the library.

- Participants: Charles Deltel, Claire Lemaitre, Dominique Lavenier, Guillaume Rizk, Patrick Durand and Pierre Peterlongo
- Contact: Dominique Lavenier
- URL: <http://gatb.inria.fr/>

6.2. DiscoSnpRad

DISCOVering Single Nucleotide Polymorphism, Indels in RAD seq data

KEYWORD: RAD-seq

FUNCTIONAL DESCRIPTION: Software discoSnpRad is designed for discovering Single Nucleotide Polymorphism (SNP) and insertions/deletions (indels) from raw set(s) of RAD-seq data. Note that number of input read sets is not constrained, it can be one, two, or more. Note also that no other data as reference genome or annotations are needed. The software is composed of several modules. First module, kissnp2, detects SNPs from read sets. A second module, kissreads2, enhances the kissnp2 results by computing per read set and for each variant found i/ its mean read coverage and ii/ the (phred) quality of reads generating the polymorphism. Then, variants are grouped by RAD locus, and a VCF file is finally generated. We also provide several scripts to further filter and select informative variants for downstream population genetics studies.

This tool relies on the GATB-Core library.

- Contact: Pierre Peterlongo
- URL: <https://github.com/GATB/DiscoSnp>

6.3. GWASDM

Genome Wide Association Study using Data Mining strategy

KEYWORDS: GWAS - Data mining

FUNCTIONAL DESCRIPTION: From two cohorts of genotyped individuals (case and control), the GWASDM software performs a Genome Wide Association Study based on data mining techniques and generates several patterns of SNPs that correlate with a given phenotype. The algorithm implemented in GWASDM directly uses relative risk measures such as risk ratio, odds ratio and absolute risk reduction combined with confidence intervals as anti-monotonic properties to efficiently prune the search space. The algorithm discovers a complete set of discriminating patterns with regard to given thresholds or applies heuristic strategies to extract the largest statistically significant discriminating patterns in a given dataset.

- Contact: Dominique Lavenier

6.4. bcool

de Bruijn graph cOrrectiOn from graph aLignment

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

FUNCTIONAL DESCRIPTION: 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

- Partner: Université libre de Bruxelles
- Contact: Pierre Peterlongo
- URL: <http://github.com/Malfoy/BCOOL>

6.5. 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 describes a 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.

- Contact: Camille Marchet

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.

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: New version 2.0 with correction of several bugs.

- 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

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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: New version developed this year, making the tool accessible to a broader 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.

- 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 segmentation 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://fluobacktracker.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: Use for the modeling of the osmotic stress response network in *E. coli*.

- Participants: François Rechenmann, Hidde De Jong and Michel Page
- 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/biocham/>

MORPHEME Project-Team

4. New Software and Platforms

4.1. BioLib

KEYWORD: Biomedical imaging

FUNCTIONAL DESCRIPTION: Library of image analysis for biology: object detection, tracking

- Participants: Étienne Delclaux, Grégoire Malandain, Sylvain Prigent and Xavier Descombes
- Contact: Xavier Descombes

4.2. PIB

Biological imaging platform

FUNCTIONAL DESCRIPTION: This platform, based on the DTK meta-platform, aims at gathering the team software development, and at providing a visual development tool.

- Participants: Étienne Delclaux, Grégoire Malandain and Xavier Descombes
- Contact: Xavier Descombes

4.3. Stracking

KEYWORDS: Bioinformatics - Biology - Biomedical imaging

SCIENTIFIC DESCRIPTION: Head Tracking and Flagellum Tracing for Sperm Motility Analysis : Sperm quality assessment plays an essential role in human fertility and animal breeding. Manual analysis is time-consuming and subject to intra- and inter-observer variability. To automate the analysis process, as well as to offer a means of statistical analysis that may not be achieved by visual inspection, we present a computational framework that tracks the heads and traces the tails for analyzing sperm motility, one of the most important attributes in semen quality evaluation. Our framework consists of 3 modules: head detection, head tracking, and flagellum tracing. The head detection module detects the sperm heads from the image data, and the detected heads are the inputs to the head tracking module for obtaining the head trajectories. Finally, a flagellum tracing algorithm is proposed to obtain the flagellar beat patterns.

FUNCTIONAL DESCRIPTION: This software is developed within the ANR project MOTIMO. It allows to segment and track spermatozoons from confocal microscopy image sequences.

- Participants: Grégoire Malandain, Huei Fang Yang, Sylvain Prigent and Xavier Descombes
- Contact: Xavier Descombes

PLEIADE Team

5. New Software and Platforms

5.1. 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 Alcyon 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>

5.2. Pantograph

KEYWORDS: Systems Biology - Bioinformatics - Genomics - Gene regulatory networks

SCIENTIFIC DESCRIPTION: Pantograph requires a template model in SMBL format, where every reaction is annotated with a gene association that describes its gene-protein-reaction dependencies as a boolean formula over the genes of the organism.

Pantograph uses a consensus procedure to infer relationships between metabolic models, based on several sources of orthology between genomes. These inter-genome relations are used to rewrite the gene associations. Every successful rewrite is used as evidence that the corresponding reaction should be present in the inferred model.

The resulting models can be validated with respect to phenotypic information obtained from experimental results.

FUNCTIONAL DESCRIPTION: Pantograph is a software toolbox to reconstruct, curate and validate genome-scale metabolic models. It uses existing metabolic models as templates, to start a reconstructions process in which new, species-specific reactions are added. Pantograph uses an iterative approach to improve reconstructed models, facilitating manual curation and comparisons between reconstructed model's predictions and experimental evidence.

Pantograph uses a consensus procedure to infer relationships between metabolic models, based on several sources of orthology between genomes. This allows for a very detailed rewriting of reaction's genome associations between template models and the model you want to reconstruct.

NEWS OF THE YEAR: Work is in progress to integrate Razanne Issa's Ab-Pantograph modules into Pantograph. Ab-Pantograph uses abductive logic to invert the inference process: a reaction explains the presence of the genes in its gene-protein-reaction formula, rather than the genes justify the reaction. Ab-Pantograph is driven by the goal of explaining all of the genes in the target organism.

- Participants: Anna Zhukova, David James Sherman, Nicolas Loira and Pascal Durrens
- Partner: University of Chile
- Contact: Nicolas Loira
- Publication: **Pantograph: A template-based method for genome-scale metabolic model reconstruction**
- URL: <http://pathtastic.gforge.inria.fr/>

5.3. 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 a 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 Alcyon 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/>

5.4. 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

5.5. 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](#)

5.6. 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/>

SERPICO Project-Team

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: Patrick Bouthemy, Charles Kervrann, Jean Salamero, Jérôme Boulanger and Antoine Basset
- Partner: UMR 144 CNRS - Institut Curie
- Contact: Patrick Bouthemy
- Publication: [Adaptive spot detection with optimal scale selection in fluorescence microscopy images](#)
- URL: <http://mobyly-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: Patrick Bouthemy, Jean Salamero, Charles Kervrann and Thierry Pécot
- 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://mobyly-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: Frédéric Lavancier, Thierry Pécot 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://mobyte-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 written using the format specified by CWriter::EWriterFormat. Support Fedora 3 (g++ 3.4.2).

- Participants: Charles Kervrann, Fabien Spindler, Jean Marc Odobez, Patrick Bouthemy and Thierry Pécot
- 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-dimensionnal 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: Charles Kervrann, Patrick Bouthemy, Jean Salamero and Jérôme Boulanger
- 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: Ion Grama, Quansheng Liu and Qiyu Jin
- 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: Jean Salamero, Jérôme Boulanger and Liu Zengzhen
- Partner: UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- Publication: [QuantEv: quantifying the spatial distribution of intracellular events](#)
- URL: <http://mobyale-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 using adaptive wavelet transform, segment with parametric active contours and restore (i.e., artifact correction and deconvolution) TMA (Tissue MicroArrays) images.

- Participants: Cyril Cauchois, Vincent Paveau and Hoai Nam Nguyen
- 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 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>

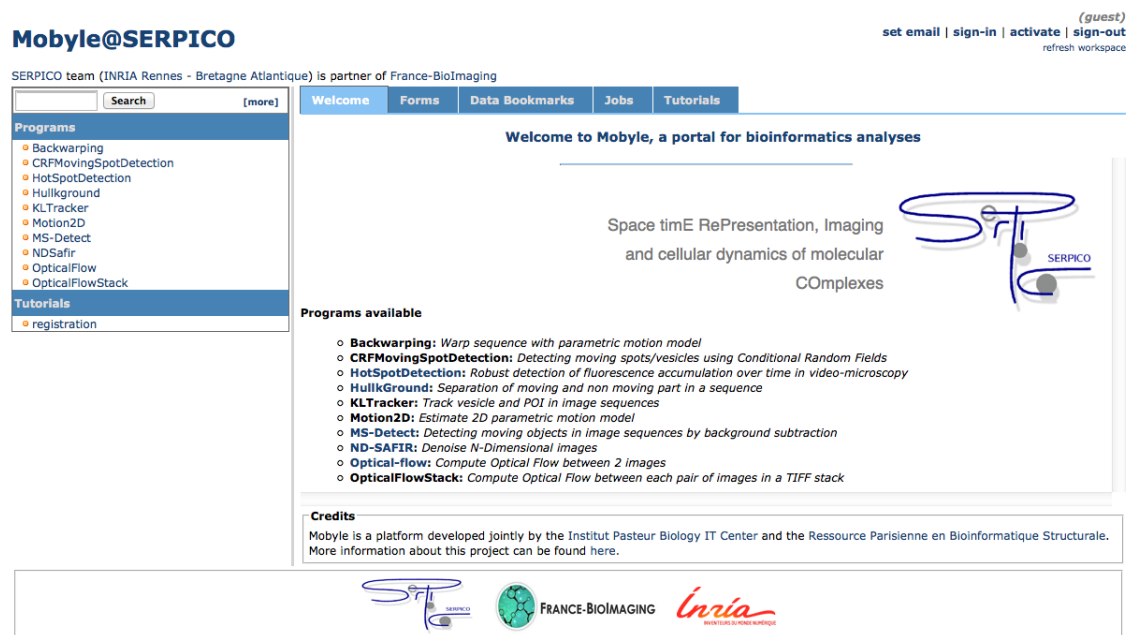


Figure 2. Mobyle@SERPICO web portal.

6.12. Platforms

6.12.1. Mobyle@Serpico platform and software distribution

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[40], KLTRACKER[44], MOTION2D[43], MS-DETECT[41], 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 [40], MOTION2D [43], ATLAS [1]. The C-CRAFT algorithm [14] has been developed 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.

6.12.2. 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).

TAPDANCE Team

5. New Software and Platforms

5.1. Sanakirja

KEYWORD: Databases

FUNCTIONAL DESCRIPTION: Sanakirja is a fully transactional (all operations are atomic) key-value dictionary stored in a file (usable at the low-level layer of a more full-featured database engine), with a zero-copy fork operation (fork is in time and space $O(\log n)$, where n is the number of keys in the file). This project is written in Rust.

- Contact: Pierre-Etienne Meunier
- URL: https://nest.pijul.com/pijul_org/sanakirja

5.2. Thrush

KEYWORD: Security

FUNCTIONAL DESCRIPTION: Purely asynchronous SSH library in Rust.

- Contact: Pierre-Etienne Meunier

5.3. Pijul

KEYWORDS: Data structures - Distributed systems

FUNCTIONAL DESCRIPTION: Patch-based distributed version control system using category theory. This solves a number of problems in other systems (such as Git), like:

- Scaling up to giant repositories (as used by Facebook, Google and Mozilla). - Being easy to understand and use, because based on a solid theory.

- Contact: Pierre-Etienne Meunier
- URL: <https://pijul.org>

5.4. SeqDesign

KEYWORDS: Chemistry - Molecular simulation

FUNCTIONAL DESCRIPTION: SeqDesign is a free energy calculation tool for DNA secondary structures. We use it to design sequences capable of self-assembling in a designed way.

- Contact: Pierre-Etienne Meunier

VIRTUAL PLANTS Project-Team

5. New Software and Platforms

5.1. OpenAlea

KEYWORDS: Bioinformatics - Biology

RELEASE FUNCTIONAL DESCRIPTION: OpenAlea 2.0 adds to OpenAlea 1.0 a high-level formalism dedicated to the modeling of morphogenesis that makes it possible to use several modeling paradigms (Blackboard, L-systems, Agents, Branching processes, Cellular Automata) expressed with different languages (Python, L-Py, R, Visual Programming, ...) to analyse and simulate shapes and their development.

- Participants: Christian Fournier, Christophe Godin, Christophe Pradal, Frédéric Boudon, Guillaume Baty, Julien Coste and Samuel Dufour Kowalski
- Contact: Christophe Pradal

5.2. OpenAlea.Visualea

KEYWORDS: Bioinformatics - Biology

- Participants: Christophe Pradal and Samuel Dufour Kowalski
- Contact: Christophe Pradal

5.3. VPlants

KEYWORDS: Bioinformatics - Biology

FUNCTIONAL DESCRIPTION: Computer algorithms and tools developed by the Virtual Plants team are integrated in the common software suite V-Plants, dedicated to the modeling and analysis of plant development at different scales (e.g. cellular tissue, whole plant, stand). The VPlants packages are integrated into OpenAlea as Python components. General-purpose components (such as PlantGL, MTGs, L-Py) are distributed with the OpenAlea platform and usable through the visual programming environment VisuAlea.

- Contact: Christophe Pradal

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: Anatomy - Mesh - Automatic Learning - C++ - 3D modeling - 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.

- Participants: Junhao Wen, Jorge Samper Gonzalez, Alexandre Routier, Tristan Moreau, Arnaud Marcoux, Pascal Lu, Thomas Jacquemont, Jeremy Guillon, Olivier Colliot, Stanley Durrleman, Michael Bacci, Simona Bottani, Ninon Burgos, Sabrina Fontanella and Pietro Gori
- 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](#)
- URL: <http://www.clinica.run>

6.4. Platforms

6.4.1. Platform Brain-computer interface

Our team has coordinated the implementation 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 funded project, and demos are currently being run by different researchers of the Institute. Such technological advance contributed to the scientific visibility of Inria and ICM with two TV reports (M6 and France 5).

ASCLEPIOS Project-Team

5. New Software and Platforms

5.1. MedInria

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

SCIENTIFIC DESCRIPTION: It 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>

5.2. 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- Bordeaux
- Contact: Maxime Sermesant
- URL: <https://team.inria.fr/asclepios/software/music/>

5.3. 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>

5.4. VP2HF

KEYWORDS: Health - Cardiac - Medical - Image - Processing - Medical imaging

FUNCTIONAL DESCRIPTION: The VP2HF software is developed by the Asclepios team and brings together all the research produced by the VP2HF's partners. It contains MedInria plugins implemented by teams such as UPF Barcelona, KCL, and specific tools provided by Philips (algorithms of segmentation, scar segmentation, ...). It aims at integrating in a single clinical workflow, tools to improve the therapy selection and treatment optimisation for patients suffering from heart failure.

- Participants: Hakim Fadil, Loic Cadour and Maxime Sermesant
- Contact: Maxime Sermesant

5.5. Longitudinal SVF Framework

Longitudinal Stationary Velocity Field (SVF) Framework

KEYWORDS: Image registration - Image analysis - Medical imaging

SCIENTIFIC DESCRIPTION: The pipeline pre-process the images, and then estimates the longitudinal deformation per patient using the log-demons (or more recently the LCC-log-demons), transports the subject-SVF into a common spatial reference and performs group-wise analyses.

FUNCTIONAL DESCRIPTION: The Longitudinal Stationary Velocity Field (SVF) Framework estimates longitudinal brain deformations from image data series, transport them in a common space and perform statistical group-wise analyses.

It is based on freely available softwares and tools, and consists of three main steps: i) Pre-processing, ii) Position correction, iii) Non-linear deformation analysis.

- Authors: Marco Lorenzi, Xavier Pennec, Giovanni Frisoni and Nicholas Ayache
- Partner: IRCCS San Giovanni di Dio Fatebenefratelli
- Contact: Xavier Pennec

5.6. LCC-LogDemos

KEYWORD: Image registration

SCIENTIFIC DESCRIPTION: LCClogDemos is an accurate and robust diffeomorphic registration framework based on the log-Demons. It implements the symmetric Local Correlation Coefficient (LCC) as a similarity measure, and thus it is unbiased with respect to local linear intensity bias of the images.

LCC-LogDemos is suited for both inter and intra-subject registration, and compares well with respect to state-of-art methods. Thanks to the stable and consistent scheme for the computation of the Jacobian determinant of the transformation, LCClogDemos represents a reliable instrument for Tensor Based Morphometry (TBM).

The average registration time for typical 3D images is around 30 minutes for a single core on a Xeon platform 2.66Ghz quad core, 4Gb RAM.

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The average registration time for typical 3D images is around 30 minutes for a single core on a Xeon platform 2.66Ghz quad core, 4Gb RAM.

- Participants: Marco Lorenzi and Xavier Pennec
- Contact: Xavier Pennec
- URL: <https://team.inria.fr/asclepios/software/lcclogdemos/>

5.7. GP-ProgressionModel

GP progression model

KEYWORDS: Data modeling - Data visualization - Data integration - Machine learning - Biostatistics - Statistical modeling - Medical applications - Evolution - Brain - Uncertainty - 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.

Basic usage:

```
model = GP_progression_model.GP_progression_model(input_X,input_N,N_random_features)
```

X and Y should be A list of biomarkers arrays. Each entry "i" of the list is a list of individuals' observations for the biomarker i The monotonicity is enforced by the parameter self.penalty

- The class comes with an external method for transforming a given .csv file in the required input X and Y:

```
X,Y,list_biomarker = GP_progression_model.convert_csv(file_path)
```

- The method Save(folder_path) saves the model parameters to an external folder, that can be subsequently read with the method Load(folder_path)

- Optimization can be done with the method Optimize:

```
model.Optimize()
```

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: <https://team.inria.fr/asclepios/team/marco-lorenzi/>

ATHENA Project-Team

6. New Software and Platforms

6.1. 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 Gallagher and Théodore Papadopoulos
- Contact: Maureen Clerc Gallagher

6.2. 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/>

6.3. 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 transferred 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 Papadopoulos
- Partner: Olea Medical
- Contact: Rachid Deriche

6.4. 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 $< 100\text{Hz}$ and medium diameter $< 1\text{m}$).

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.

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.

- Participants: Alexandre Gramfort, Emmanuel Olivi, Geoffray Adde, Jan Kybic, Kai Dang, Maureen Clerc Gallagher, Perrine Landreau, Renaud Keriven and Théodore Papadopoulos
- Contact: Théodore Papadopoulos
- 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://openmeeeg.github.io/>

BIOVISION Team

6. New Software and Platforms

6.1. Virtual Retina

A biological retina modèle 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.

NEWS OF THE YEAR: Virtual Retina software has been integrated into the platform PRANAS allowing to simulate retinal output via a graphical user interface (see paper published in Frontiers in Neuroinformatics, 2017)

- 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/>

6.2. 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 healthy retinas but the long term goal is to study retinas with a pathology (DMLA, Retinitis Pigmentosa, Glaucoma).

NEWS OF THE YEAR: PRANAS software is described in an article published in Frontiers in Neuroinformatics (2017), and it is available for download.

- 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/>

CAMIN Team

5. New Software and Platforms

5.1. Softwares

5.1.1. HILECOP

Participants: Baptiste Colombani, David Andreu.

High Level hardware Component Programming

Functional Description: Our SENIS (Stimulation Electrique Neurale dIStribuee) based FES architecture relies on distributed stimulation units (DSU) which are interconnected by means of a 2-wire based network. A DSU is a complex digital system since it embeds among others a dedicated processor (micro-machine with a specific reduced instruction set), a monitoring module and a 3-layer protocol stack. To face the complexity of the units digital part and to ease its prototyping on programmable digital devices (e.g. FPGA), we developed an approach for high level hardware component programming (HILECOP). To support the modularity and the reusability of sub-parts of complex hardware systems, the HILECOP methodology is based on components. An HILECOP component has: an Interpreted Time Petri Net (ITPN) based behavior [3](#), a set of functions whose execution is controlled by the PN, and a set of variables and signals. Its interface contains places and transitions from which its PN model can be inter-connected as well as signals it exports or imports. The interconnection of those components, from a behavioral point out view, consists in the interconnection of places and/or transitions according to well-defined mechanisms: interconnection by means of oriented arcs or by means of the "merging" operator (existing for both places and transitions).

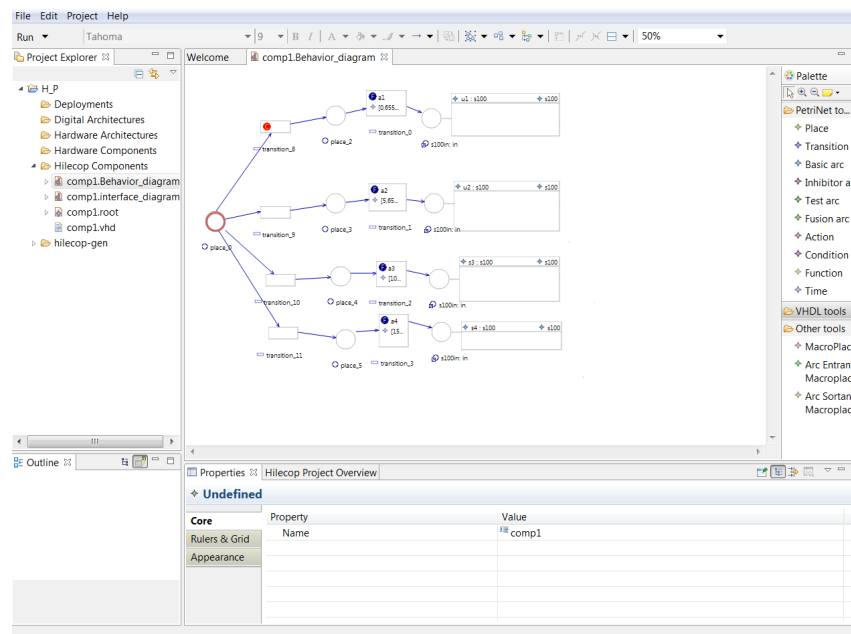


Figure 3. HILECOP screenshot

Several formalism evolutions have been integrated within the HILECOP software, like for instance behavior agregation as well as exception handling, both for analysis and implementation sides. Analysis has also been improved, a new approach for state space generation of synchronously executed ITPN has been designed, validated and then integrated within the software.

The Eclipse-based version of HILECOP (registered at the french Agence de Protection des Programmes (APP)) has been refactored: for instance, the application ECore model, a new Eclipse E4 architecture and a set of new features (new link types and new views to connect components) have been developed.

Specification of GALS systems (Globally Asynchronous Locally Synchronous) and their deployment on the hardware architecture are ongoing works; the aim is to take into account deployment properties like connecting different clocks to HILECOP components within a same FPGA, or on a set of interconnected FPGAs (and thus interconnecting them by means of asynchronous signals).

5.1.2. Sensbiotk

Participants: Christine Azevedo Coste, Roger Pissard-Gibollet, Benoît Sijobert.

Sensbiotk is a toolbox in Python for the calibration, the acquisition, the analysis and visualization of motion capture Inertial Measurement Units (IMU). Motion and Gait parameter reconstruction algorithms are also available. <http://sensbio.github.io/sensbiotk/>

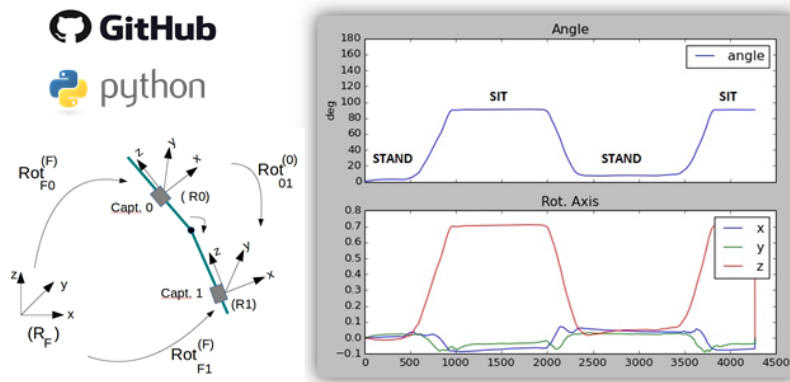


Figure 4. Sensbiotk toolbox for the calibration, the acquisition, the analysis and visualization of motion capture Inertial Measurement Units (IMU)

5.1.3. MOS2SENS

Participants: Mélissa Dali, Olivier Rossel, David Guiraud.

From Model Optimization and Simulation To Selective Electrical Neural Stimulation: it allows to manipulate 3D modeling of nerve and cuff electrodes taking into account anisotropy and the most advanced HH models of the myelinated axons. Based on optimized computing scheme, it allows to predict the activation areas induced by a complex 3D spreading of the current over a multicontact electrodes. Moreover, the tool allows for performing optimization of the needed current to target a specific cross section of the nerve. Version 1.0 (IDDN.FR.001.490036.000.S.P.2014.000.31230) has been released on december 2014 and v2.0 will be released January 2017. The last version includes full interface with OpenMEEG and COMSOL, and many other enhancements concerning both the model itself and the computation scheme.

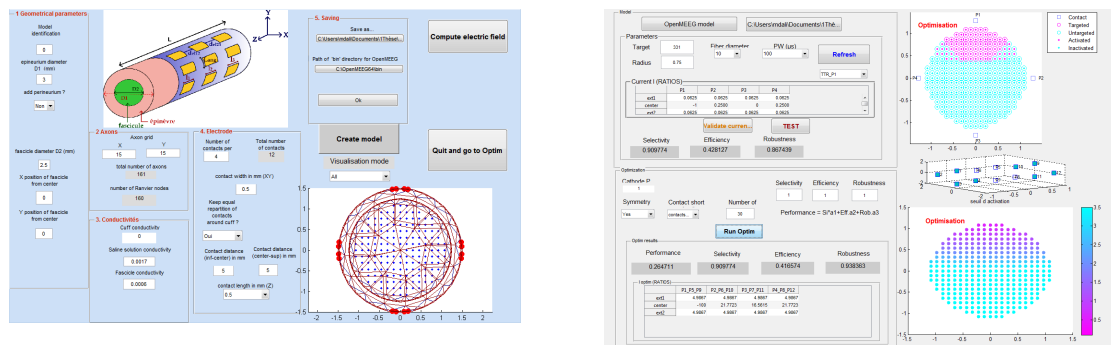


Figure 5. Graphical interface of software MOS2SENS, left: modeling multicontact CUFF electrode, right: optimization for spatial selectivity

GALEN Project-Team

6. New Software and Platforms

6.1. DISD

Dense Image and Surface Descriptors

FUNCTIONAL DESCRIPTION: Scale-Invariant Descriptor, Scale-Invariant Heat Kernel Signatures DISD implements the SID, SI-HKS and ISC descriptors. SID (Scale-Invariant Descriptor) is a densely computable, scale- and rotation- invariant descriptor. We use a log-polar grid around every point to turn rotation/scalings into translation, and then use the Fourier Transform Modulus (FTM) to achieve invariance. SI-HKS (Scale-Invariant Heat Kernel Signatures) extract scale-invariant shape signatures by exploiting the fact that surface scaling amounts to multiplication and scaling of a properly sampled HKS descriptor. We apply the FTM trick on HKS to achieve invariance to scale changes. ISC (Intrinsic Shape Context) constructs a net-like grid around every surface point by shooting outwards and tracking geodesics. This allows us to build a meta-descriptor on top of HKS/SI-HKS that takes neighborhood into account, while being invariant to surface isometries.

- Participants: Eduard Trulls and Iasonas Kokkinos
- Contact: Iasonas Kokkinos
- URL: <http://vision.mas.ecp.fr/Personnel/iasonas/descriptors.html>

6.2. DPMS

FUNCTIONAL DESCRIPTION: Dpms implements branch-and-bound object detection, cutting down the complexity of detection from linear in the number of pixels to logarithmic.

- Participant: Iasonas Kokkinos
- Contact: Iasonas Kokkinos

6.3. DROP

KEYWORDS: Health - Merging - Registration of 2D and 3D multimodal images - Medical imaging

FUNCTIONAL DESCRIPTION: Drop is a software programme that registers images originating from one or more modes by quickly and efficiently calculating a non-rigid / deformable field of deformation. Drop is a new, quick and effective registration tool based on new algorithms that do not require a cost function derivative.

- Partner: Centrale Paris
- Contact: Nikolaos Paragios
- URL: <http://campar.in.tum.de/Main/Drop>

6.4. FastPD

KEYWORD: Medical imaging

FUNCTIONAL DESCRIPTION: FastPD is an optimization platform in C++ for the computer vision and medical imaging community.

- Contact: Nikolaos Paragios
- URL: <http://www.csd.uoc.gr/~komod/FastPD/>

6.5. GraPeS

Grammar Parser for Shapes

FUNCTIONAL DESCRIPTION: It is a software for parsing facade images using shape grammars. Grapes implement a parsing methods based on Reinforcement Learning principles. It optimizes simultaneously the topology of the parse tree as well as the associated parameters. GraPeS comes along with predefined shape grammars as XML files and defines three kinds of rewards. However, it also offers the possibility to create new grammars and to provide custom rewards in text files, widening the scope of potential applications. The name of the software comes from the aspect of the parse tree of the binary split grammars involved in the process.

RELEASE FUNCTIONAL DESCRIPTION: Supports jpg and gif file formats.

- Participant: Iasonas Kokkinos
- Contact: Iasonas Kokkinos

6.6. HOAP-SVM

High-Order Average Precision SVM

SCIENTIFIC DESCRIPTION: We consider the problem of using high-order information (for example, persons in the same image tend to perform the same action) to improve the accuracy of ranking (specifically, average precision). We develop two learning frameworks. The high-order binary SVM (HOB-SVM) optimizes a convex upper bound of the surrogate 0-1 loss function. The high-order average precision SVM (HOAP-SVM) optimizes a difference-of-convex upper bound on the average precision loss function.

Authors of the research paper: Puneet K. Dokania, A. Behl, C. V. Jawahar and M. Pawan Kumar

FUNCTIONAL DESCRIPTION: The software provides a convenient API for learning to rank with high-order information. The samples are ranked according to a score that is proportional to the difference of max-marginals of the positive and the negative class. The parameters of the score function are computed by minimizing an upper bound on the average precision loss. The software also provides an instantiation of the API for ranking samples according to their relevance to an action, using the poselet features. The following learning algorithms are included in the API:

(1) Multiclass-SVM (2) AP-SVM (3) High Order Binary SVM (HOB-SVM) (4) High Order AP-SVM (HOAP-SVM) (5) M4 Learning (unpublished work)

The API is developed in C/C++ by Puneet K. Dokania.

- Participants: Pawan Kumar and Puneet Dokania
- Contact: Puneet Dokania
- URL: <http://puneetkdokania.github.io/projects/ranking-highorder/ranking-highorder.html>

6.7. LBSD

Learning-Based Symmetry Detection

FUNCTIONAL DESCRIPTION: LBSD implements the learning-based approach to symmetry detection. It includes the code for running a detector, alongside with the ground-truth symmetry annotations that we have introduced for the Berkeley Segmentation Dataset (BSD) benchmark.

- Participant: Stavros Tsogkas
- Contact: Stavros Tsogkas
- URL: https://github.com/tsogkas/oid_1.0

6.8. mrf-registration

KEYWORDS: Health - Medical imaging

FUNCTIONAL DESCRIPTION: Deformable image and volume registration, is a deformable registration platform in C++ for the medical imaging community. This is the first publicly available platform which contains most of the existing metrics to perform registration under the same concept. The platform is used for clinical research from approximately 3,000 users worldwide.

RELEASE FUNCTIONAL DESCRIPTION: Bugfix in image resampling Resampling of binary mask is now w.r.t. to target image Added adjustable sigma for Gaussian image pyramid Added level dependent scaling of maximum displacement when linkMax is disabled Changed approximation method for computation of the inverse displacement field (less memory demanding) Bugfix in grid and quiver visualization Added support for compressed MHD Bugfix in 3D thin-plate splines in landmark-based registration

- Participant: Nikolaos Paragios
- Contact: Nikolaos Paragios
- URL: <http://www.mrf-registration.net/>

6.9. TeXMeG

FUNCTIONAL DESCRIPTION: Texture, modulation, generative models, segmentation, TeXMeG is a front-end for texture analysis and edge detection platform in Matlab that relies on Gabor filtering and image demodulation. Includes frequency- and time- based definition of Gabor- and other Quadrature-pair filterbanks, demodulation with the Regularized Energy Separation Algorithm and Texture/Edge/Smooth classification based on MDL criterion.

- Participant: Iasonas Kokkinos
- Contact: Iasonas Kokkinos
- URL: <http://cvsp.cs.ntua.gr/software/texture/>

6.10. Platforms

6.10.1. 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.

MATHNEURO Team (section vide)

MIMESIS Team

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. SofaPardisoSolver

KEYWORDS: Simulation - Linear Systems Solver - Direct solvers - Collision - Numerical simulations

SCIENTIFIC DESCRIPTION: The SofaPardisoSolver allows for fast direct solution of sparse systems of linear equations, using a decomposition (such as LU, LDL and Cholesky) according to the type of the matrix. Moreover, the wrapper allows for employing a partial factorization which brings a significant improvement when solving augmented systems, usually resulting in problems involving collisions and/or domain decomposition.

FUNCTIONAL DESCRIPTION: The SofaPardisoSolver plugin contains a wrapper allowing for an efficient direct solution of a system of linear equations. It also contains an advanced feature which exploits an algorithm of partial decomposition available in Pardiso. This feature significantly accelerates the computation of Schur complement, typically needed to solve linear complementarity problems (LCP). Example of use: collision and contacts.

- Author: Igor Peterlik
- Contact: Igor Peterlik

6.3. SOFA Xray rendering

KEYWORDS: Simulation - Realistic rendering - Real-time rendering - Medical imaging - Medical applications

FUNCTIONAL DESCRIPTION: This work allows to emulate a X-ray scan image within the simulation platform SOFA. By defining the position of an emitter and receptor in the 3D space, an image is rendered. A realistic medical image of organs can thus be obtained from surface meshes (triangulated or quadrangulated) in real-time.

Version compatible with SOFA v17.06

- Authors: Stéphane Cotin and Frédérick Roy
- Contact: Stéphane Cotin

MNEMOSYNE Project-Team

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. ENAS

Event Neural Assembly Simulation

KEYWORDS: Neurosciences - Health - Physiology

SCIENTIFIC DESCRIPTION: As one gains more intuitions and results on the importance of concerted activity in spike trains, models are developed to extract potential canonical principles underlying spike coding. These methods shed a new light on spike train dynamics. However, they require time and expertise to be implemented efficiently, making them hard to use in a daily basis by neuroscientists or modelers. To bridge this gap, we developed the license free multiplatform software ENAS (<https://enas.inria.fr>) integrating tools for individual and collective spike analysis and simulation, with some specificities devoted to the retina. The core of ENAS is the statistical analysis of population codes. One of its main strength is to provide statistical analysis of spike trains using Maximum Entropy-Gibbs distributions taking into account both spatial and temporal correlations as constraints, allowing to introduce causality and memory in statistics. ENAS also generates simulated spike trains. On one hand, one can draw a population raster from an user-specified Gibbs distribution. On the other hand, we have integrated in ENAS our retina simulator VIRTUAL RETINA, extended here to include lateral connections in the IPL. We hope that ENAS will become a useful tool for neuroscientists to analyse spike trains and we hope to improve it thanks to user feedback. Our goal is to progressively enrich it with the latest research results, in order to facilitate transfer of new methods to the community.

FUNCTIONAL DESCRIPTION: As one gains more intuitions and results on the importance of concerted activity in spike trains, models are developed to extract potential canonical principles underlying spike coding. These methods shed a new light on spike train dynamics. However, they require time and expertise to be implemented efficiently, making them hard to use in a daily basis by neuroscientists or modelers. To bridge this gap, we developed the license free multiplatform software ENAS integrating tools for spike trains analysis and simulation. These tools are accessible through a friendly Graphical User Interface that avoids any scripting or writing code from the user. Most of them have been implemented to run in parallel to reduce the time and memory consumption. ENAS offers basic visualizations and classical analysis for statistics of spike trains analysis. It also proposes statistical analysis with Maximum Entropy-Gibbs distributions taking into account both spatial and temporal correlations as constraints, allowing to introduce causality and memory in statistics. ENAS also includes specific tools dedicated to the retina: Receptive Field computation and a virtual retina simulator. Finally, ENAS generates synthetic rasters, either from known statistics or from the VIRTUAL RETINA simulator. We expect ENAS to become a useful tool for neuroscientists to analyse spike trains and we hope to improve it thanks to users feedback. From our perspective, our goal is to progressively enrich ENAS with the latest research results, in order to facilitate transfer of new methods to the community.

- Participants: Bruno Cessac, Daniela Pamplona, Geoffrey Portelli, Hassan Nasser, Pierre Kornprobst, Rodrigo Cofre Torres, Sélim Kraria, Theodora Karvouniari and Thierry Viéville
- Contact: Bruno Cessac
- URL: <https://enas.inria.fr>

6.3. 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 been 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

NEUROSYS Project-Team

6. New Software and Platforms

6.1. BrianModel

Library of Brian Neuron Models

KEYWORDS: Spiking neural networks - Neurosciences - Numerical simulations

FUNCTIONAL DESCRIPTION: BrianModel is a library of neuron models and ionic currents for the BRIAN simulator. The purpose of BrianModel is to speed up simulation set-up and reduce code duplication across simulation scripts. Template neurons are defined by the ionic currents that flow through their membrane. Implemented templates include: Hodgkin-Huxley pyramidal neuron, Hodgkin-Huxley pyramidal neuron with CAN receptors, Hodgkin-Huxley fast-spiking inhibitory hippocampal. The current library is easily extensible by third-party users due to its hierarchical design. The template neurons and their currents are defined as YAML files, which are conveniently parsed by a Python library which acts as an interface to the BRIAN simulator API's.

- Contact: Francesco Giovannini
- URL: <https://github.com/JoErNanO/brianmodel>

6.2. 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 40000 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 Gallagher and Théodore Papadopoulo
- Partners: INSERM - CEA-List - GIPSA-Lab
- Contact: Anatole Lécuyer
- URL: <http://openvibe.inria.fr>

6.3. Platforms

6.3.1. 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). Our Biosemi EEG amplifier has been extended this year to record 128 channels (Regional initiative *Contrat de Projet État Région (CPER) IT2MP* see section 8.1).

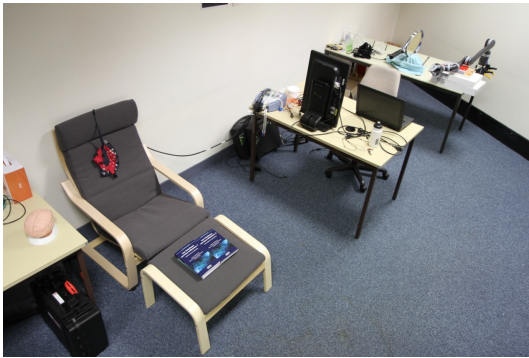


Figure 1. Electroencephalographic Experimental room at Inria Nancy-Grand Est

PARIETAL Project-Team

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: It 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 Papadopoulos
- 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: Health - Brain - IRM - Neurosciences - Statistic analysis - FMRI - Medical imaging

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.

- 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
- URL: <http://pyhrf.org>

6.5. Scikit-learn

KEYWORDS: Regression - 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.

- Contact: Alexandre Gramfort
- URL: <http://martinos.org/mne/>

VISAGES Project-Team

6. New Software and Platforms

6.1. Anima

KEYWORDS: Registration - Diffusion imaging - Medical imaging - Filtering - 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 and Pierre Maurel
- Contact: Isabelle Corouge
- URL: <http://www.irisa.fr/visages/>

6.3. MedInria

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

SCIENTIFIC DESCRIPTION: It 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.

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

6.4. QtShanoir

KEYWORDS: Webservices - Soap - C++ - Health - DICOM - Plug-in - Medical imaging - Qt - Shanoir - Nifti

SCIENTIFIC DESCRIPTION: QtShanoir is based on Qt/C++ librairie. 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 structure, manage, archive, visualize and share neuroimaging data with an emphasis on multi-centric collaborative research projects. It provides common features of neuroimaging data management systems along with research-oriented data organization and enhanced accessibility.

Shanoir is a secured J2EE application running on a JBoss server, reachable via graphical interfaces in a browser or by third party programs via web services. It behaves as a repository of neuroimaging files coupled with a relational database hoding meta-data. The data model, based on OntoNeurolog, an ontology devoted to the neuroimaging field, is structured around research studies where of involved patients have examinations which either produce image acquisitions or clinical scores. Each image acquisition is composed of datasets represented by their acquisition parameters and image files. The system only keeps anonymous data.

Image files imports are possible from various sources (DICOM CDs, PACs, image files in NIfTI / Analyze format) using either online wizards, with completions of related meta-data, or commande line tools. Once de-identified during the import phase, DICOM header's customizable feature. Shanoir can also record any executed processing allowing to retrieve workflows applied to a particular dataset along with the intermediate data.

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 and 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. A study responsible can thereby define the users allowed to see, download or import data into his study or simply make it public.

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.

Shanoir integrates the enterprise search platform, Apache Solr, to provide the users a vast array of advanced features such as near real-time indexing and queries, full-text search, faceted navigation, autosuggestion and autocomplete.

- 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: PACS - Medical imaging - Neuroimaging - DICOM - Health - Biology - Java - Webservices - 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. Platforms

6.7.1. 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 Neurinfo⁰. 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 overall PIMATGI initiative served for the financing of three distinct, but 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. A 3T Siemens Prisma will be installed early 2018.

⁰<http://www.neurinfo.org>

AIRSEA Project-Team

6. New Software and Platforms

6.1. 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>

6.2. BALAISE

Bibliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement

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

FUNCTIONAL DESCRIPTION: BALAISE (Bibliothèque 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

6.3. DassFlow

- Participants: Jerome Monnier, Joel Marin and Marc Honnorat
- Contact: Eric Blayo-Nogret

6.4. DiceDesign

Designs of Computer Experiments

FUNCTIONAL DESCRIPTION: This package is useful for conducting design and analysis of computer experiments.

- Contact: Céline Hartweg
- URL: <https://cran.r-project.org/web/packages/DiceDesign/index.html>

6.5. DiceEval

Construction and Evaluation of Metamodels

FUNCTIONAL DESCRIPTION: This package is useful for conducting design and analysis of computer experiments. Estimation, validation and prediction of models of different types : linear models, additive models, MARS, PolyMARS and Kriging.

- Contact: Céline Hartweg
- URL: <https://cran.r-project.org/web/packages/DiceEval/index.html>

6.6. 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

6.7. 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 ChereI
- Contact: Vivien Mallet

CASTOR Project-Team

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 equilibrium equations inside the plasma and the Maxwell equations outside. Moreover, the magnetic field is often supposed not to depend on the azimuthal 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

5. New Software and Platforms

5.1. 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

5.2. 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: Chang Yang, Cindy Guichard, Robert Eymard, Roland Masson and Thierry Goudon
- Partners: Université de Nice Sophia Antipolis (UNS) - BRGM
- Contact: Roland Masson

5.3. NS2DDV

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: Creusé Emmanuel
- URL: <https://wikis.univ-lille1.fr/painleve/ns2ddv>

5.4. 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

5.5. 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/>

5.6. 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/>

FLUMINANCE Project-Team

6. New Software and Platforms

6.1. 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>

6.2. 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>

6.3. 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>

6.4. 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>

6.5. TYPHOON

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

6.6. H2OLab

KEYWORDS: Energy - Contamination - Groundwater - Hydrogeology - Heterogeneity - Uncertainty - Multi-scale - Simulation

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 H2OGuille. 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/>

6.7. PALMTREE

KEYWORD: Monte-Carlo

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

6.8. GRT3D

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.

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.

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

LEMON Team

5. New Software and Platforms

5.1. Action Dépollution

FUNCTIONAL DESCRIPTION: Action Dépollution is a serious game made for learning how to purify fast and well a water reservoir, such as lakes. In the scope of the international initiative Mathematics of Planet Earth, this game shows an application of mathematics related to environmental education and sustainable development. The player can act as a researcher, that compares different strategies and looks for the best solution.

- Participants: Alain Rapaport, Alexis Pacholik and Antoine Rousseau
- Contact: Antoine Rousseau
- URL: <https://depollution.inria.fr/>

5.2. 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. It uses 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

5.3. 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>

MAGIQUE-3D Project-Team

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 platform 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 2017, we implemented the coupling between triangles and quadrangles, and we started the implementation of coupling between Discontinuous Galerkin methods and Spectral Element methods

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

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 2017, we have completed the implementation of hybridizable DG for 3D anisotropic elastic, and we have coupled Hou10ni with Maphys (developed by Inria team project Hiepac). We have begun scalability tests and performance comparison of Hou10ni/Mumps vs Hou10ni/Maphys, in the framework of the european project HPC4E.

- 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 2017, we have completed the implementation of Lagrange and Jacobi polynomials and we have released the 3D elastodynamic version and the 3D elasto-acoustic coupling.

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

5.5. fmodeling

Frequency-domain Wave-equation Modeling App (fModeling)

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

SCIENTIFIC DESCRIPTION: FModelling simulates acoustic and elastic wave propagation in frequency domain, in 2D and in 3D, using Discontinuous Galerkin Methods and Hybridizable Discontinuous Galerkin Methods. The space discretization is based on Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with two linear solvers (Mumps and Maphys).

FUNCTIONAL DESCRIPTION: fmodeling is developed in partnership with Total in the context of the Depth Imaging Partnership (DIP). It is the equivalent of Tmodeling for frequency domain. The software deals with wave equation in the frequency domain and solves the forward problem using Discontinuous Galerkin methods or Hybridizable Discontinuous Galerkin Methods. In particular, acoustic and elastic (isotropic and TTI) media are considered in two and three dimensions. It is planned to implement and to test various kind of basis function and to couple the code with various linear solvers (such as Mumps or Maphys). The software is coupled to the Inversion solver of Total to conduct Seismic Imaging using iterative minimization with the Full Waveform Inversion method.

NEWS OF THE YEAR: In 2017, we completed the implementation of Hybridizable Discontinuous Galerkin Methods and we started the validation of the code in an industrial context. We have also coupled the code with the Full Waveform Inversion solver of Total.

- Partner: TOTAL
- Contact: Julien Diaz

SERENA Project-Team

6. New Software and Platforms

6.1. GEOFRAC

GEOFRACFLOW

KEYWORDS: Hydrogeology - Numerical simulations - 3D

SCIENTIFIC DESCRIPTION: GEOFRACFLOW 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 GEOFRACFLOW 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.

RELEASE FUNCTIONAL DESCRIPTION: The last version includes optimisations of the code, mainly with an efficient upload of the mesh data generated with BLSURF and vectorization of the operations.

- 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](#)

6.2. Ref-indic

Refinement indicators

KEYWORD: Inverse problem

SCIENTIFIC DESCRIPTION: The refinement indicator algorithm is suited for the estimation of a distributed parameter occurring in a mathematical simulation model, typically a set of partial differential equations. When the numerical simulation model must be solved on a fine grid, the refinement indicator algorithm provides an adaptive parameterization of the sought parameter that avoids overparameterization difficulties. In each grid cell, the estimated parameter may be of dimension greater than one, i.e. the algorithm is able to estimate several scalar distributed parameters.

Ref-indic implements a generic version of the refinement indicator algorithm that can dock specific programs provided they conform to the generic algorithm API.

The API of Ref-indic requires four main functionalities (called tasks) for the user specific program, it must be able: * to initialize, i.e. to open all necessary data files, to perform all necessary preliminary computation, and to return an initial coarse parameterization (giving a zone number between 0 and the initial number of zones minus one for each cell of the fine grid), * to compute the gradient on the fine grid for a given fine parameterization, * to optimize the problem for a given coarse parameterization, * and to finalize, i.e. to store the resulting coarse parameterization.

Given any such user specific program, the inversion platform automatically provides a program that solves the corresponding user inverse problem using the refinement indicator algorithm.

FUNCTIONAL DESCRIPTION: Ref-indic is an adaptive parameterization platform using refinement indicators. Slogan is “invert details only where they are worth it”. Ref-indic implements a generic version of the refinement indicator algorithm that can dock specific programs provided they conform to the generic algorithm API.

NEWS OF THE YEAR: In its current implementation, the inversion platform can only build coarse parameterizations for a distributed parameter defined on a fine rectangular grid. From version 1.5+pl0, the user has the possibility to specify masked cells in the fine rectangular grid that will be ignored by the algorithm (with the use of the specific zone number -1 in the initial coarse parameterization). This allows for the treatment of inverse problems defined on unstructured meshes. The handling of both-way interpolations must be taken care of by the gradient computation and optimization tasks. The masked cells must be the same for all components of the parameter.

- Contact: François Clément
- Publications: [Image Segmentation with Multidimensional Refinement Indicators](#) - [The Multidimensional Refinement Indicators Algorithm for Optimal Parameterization](#)
- URL: <http://refinement.inria.fr/ref-indic/>

6.3. Sklml

The OCaml parallel skeleton system

KEYWORDS: Parallel programming - Functional programming

SCIENTIFIC DESCRIPTION: Writing parallel programs is not easy, and debugging them is usually a nightmare. To cope with these difficulties, the skeleton programming approach uses a set of predefined patterns for parallel computations. The skeletons are higher order functional templates that describe the program underlying parallelism.

Sklml is a new framework for parallel programming that embeds an innovative compositional skeleton algebra into the OCaml language. Thanks to its skeleton algebra, Sklml provides two evaluation regimes to programs: a regular sequential evaluation (merely used for prototyping and debugging) and a parallel evaluation obtained via a recompilation of the same source program in parallel mode.

Sklml was specifically designed to prove that the sequential and parallel evaluation regimes coincide.

FUNCTIONAL DESCRIPTION: Sklml is a functional parallel skeleton compiler and programming system for OCaml programs. Slogan is “easy coarse grain parallelization”.

NEWS OF THE YEAR: Caml preprocessors are no longer needed.

- Participants: François Clément and Pierre Weis
- Contact: François Clément
- URL: <http://sklml.inria.fr>

6.4. GENFIELD

KEYWORDS: Hydrogeology - Algorithm - Heterogeneity

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.

RELEASE FUNCTIONAL DESCRIPTION: The new version includes: - The use of the FFTW3-mpi library for discrete Fourier transform - Non regression tests (and continuous integration through gitlab.inria.fr) - Debugging of the parallel algorithm

- Participants: Géraldine Pichot, Simon Legrand, Grégoire Lecourt, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Contact: Géraldine Pichot
- Publication: [Algorithms for Gaussian random field generation](#)
- URL: https://gitlab.inria.fr/slegrand/Genfield_dev

6.5. 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/datafl4sh/diskpp>

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/>

6.7. 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/>

STEPP Project-Team

6. New Software and Platforms

6.1. 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>

6.2. 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 [14].

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

6.3. 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 [15].

- 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>

6.4. 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

6.5. 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>

6.6. 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

6.7. Comptabilité Ecologique

FUNCTIONAL DESCRIPTION: Databases, database handling tools and data visualization tools (on the web-site). 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 Institute - 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/>

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, CO₂ 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 industrialists 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/>

CARMEN Project-Team

6. New Software and Platforms

6.1. CEPS

Cardiac ElectroPhysiology Simulation

KEYWORDS: 3D - Cardiac - Mesh - Health - Simulation - 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 and Nejib Zemzemi
- Partners: Université de Bordeaux - CNRS - INP Bordeaux - IHU - LIRYC
- Contact: Yves Coudière
- URL: <https://gforge.inria.fr/projects/ceps/>

6.2. Platforms

6.2.1. 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 the course of 2017 the code was collected in an archive on Inria's GitLab platform, and a public website was created where documentation will be placed (<http://cempack.gforge.inria.fr>).

The main components of CEMPACK are the following.

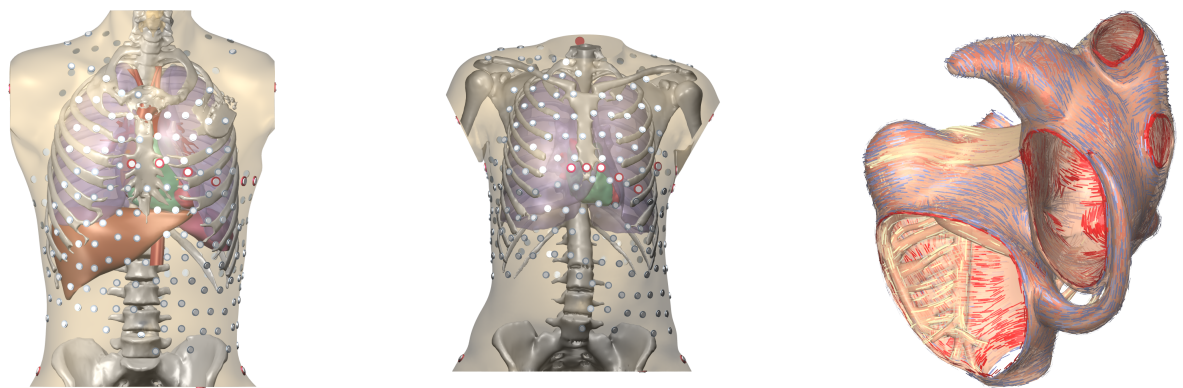
Propag-5.1 Applied modeling studies performed by the Carmen team, especially M. Potse and M. Kania, in collaboration with IHU Liryc and foreign partners [17] [7] [61], [51] [43] rely to a great extent on high-performance computations on the national supercomputers Curie, Occigen, and Turing. The Propag-5 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. 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, and only minor changes are being made currently. 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 [60]. 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 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.

6.2.2. 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.

DRACULA Project-Team

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

4.2. SiMuScale

We have developed within the team the *SiMuScale* platform, a software dedicated to exploring multi-scale population models ("SiMuScale" on researchgate, <https://gforge.inria.fr/projects/simuscale>). Coded in C++, *SiMuScale* is in active development since 2014. *SiMuScale* has been primarily developed to answer the need for an all-purpose, fast and flexible modeling tool for multiscale cell population dynamics. Biological agents (cells) are modeled by visco-elastic spheres, which are subject to mechanical constraints. Each cell possesses its own intracellular dynamics, coupled to other cells through bimolecular signals expressed at the surface of the cell. The internal state of the cell is also coupled to a behavioral state of the cell, which control the macroscopic fate: motility, growth, proliferation, death, etc. Mechanical interactions provide a 3D environment in which cells interact locally. *SiMuScale* is based on a core containing the simulator, and on plug-ins that contain the biological specifications of each cell. The core+plug-ins architecture makes it easier for the researcher to focus on the model and to capitalise on existing models, which all share the same framework and are compatible with each other. That way, *SiMuScale* makes the work of model writing and re-writing minimal and fits into reproducible research.

M3DISIM 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 IDD.N.FR.001.350015.000.S.P.2014.000.10000.

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

6.2. HeartLab

KEYWORDS: Computational geometry - Image analysis - Cardiac - Health - Simulation

SCIENTIFIC 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.

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 Khris-tenko, Dominique Chapelle and Philippe Moireau
- Contact: Philippe Moireau
- URL: <https://raweb.inria.fr/rapportsactivite/RA2013/m3disim/uid14.html>

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. 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 simulation

- 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>

MAMBA Project-Team

5. New Software and Platforms

5.1. 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

5.2. 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 indispensable 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

5.3. Platforms

TiQuant and TiSim The software for tissue image analysis (**Tissue Quantifier**) and simulation (**Tissue Simulator**) has been enriched. In more details,

5.3.1. *TiQuant*

TiQuant [94], [91] is implemented in portable object-oriented ISO C++. The GUI is based on QT and supports real-time visualisation using OpenGL. TiQuant is embedded in the tissue modelling framework CellSys and thus is tightly linked with TiSim, a versatile and efficient simulation environment for tissue models. TiQuant provides an interface to VolView and further complements its functionality by linking to the open-source libraries ITK and VTK (itk/vtk.org). The image/volume processing chains currently implemented in TiQuant for example include techniques to segment conduit and cell segmentation from 3D confocal micrographs of liver tissue based on the Adaptive Otsu Thresholding method and a number of morphological operators. TiQuant was currently extended by a machine-learning component, largely replacing the manual image-processing pipeline.

5.3.2. *TiSim*

TiSim permits agent-based simulations of multicellular systems. It is modular, in object-oriented ISO C++, the GUI based on Qt and OpenGL, while also allowing for batch mode runs. The software permits multi-scale simulations by integration of molecular pathways (for signalling, metabolisms, drug) into each individual cell. Applications so far are monolayer growth, multicellular spheroids, liver regeneration, TRAIL-treatment simulations. It has an SBML interface. In a largely finished follow-up version it will integrate a deformable cell model by triangulation of cell surface, deformable rod models, extracellular matrix and vascular flow and transport. TiSim can be directly fed by structures synthesised from processed image data from TiQuant.

Impact: The tool is used by our collaborators in liver biology, medicine and toxicology. We recently trained a PhD student from P. Segers (Ghent Univ.) on TiQuant and from T. Hillen (Univ. Alberta, Ca) on TiSim and organised a workshop on benchmarking and comparing agent-based models and tools (workshop Leipzig, volet 5).

MONC Project-Team (section vide)

MYCENAE Project-Team

6. New Software and Platforms

6.1. DynPeak

KEYWORDS: Biology - Health - Physiology

SCIENTIFIC DESCRIPTION: DynPeak is an algorithm for pulse detection and frequency analysis in hormonal time series.

- Participants: Alexandre Vidal, Claire Médigue, Frédérique Clément, George Rosca, Qinghua Zhang and Serge Steer
- Partner: INRA
- Contact: Frédérique Clément
- URL: <https://team.inria.fr/mycenae/en/software/>

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 viscoplastic 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 IDD.N.FR.001.350015.000.S.P.2014.000.10000.

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

6.2. MODULEF

FUNCTIONAL DESCRIPTION: The numerical method to approximate the constitutive laws for rubber elasticity derived from polymer physics are implemented in the Inria software Modulef.

It is based on : - algorithms from stochastic geometry to generate suitable polymer networks, - Delaunay tessellation algorithms to deal with steric effects (courtesy of the Inria project-team GAMMA2), - the introduction of 1-dimensional finite elements for the polymer-chains in Modulef.

- Participants: Antoine Gloria and Marina Vidrascu
- Contact: Marina Vidrascu
- URL: <https://www.rocq.inria.fr/modulef/>

6.3. SHELDDON

SHELLs and structural Dynamics with DOnain 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/shelldon/>

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.

- 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 estimate 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 against 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>

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/>