RESEARCH CENTER

FIELD
Digital Health, Biology and Earth

Activity Report 2019

Section Software

Edition: 2020-03-21

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

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

BEAGLE Project-Team

6. New Software and Platforms

6.1. aevol

Artificial Evolution

KEYWORDS: Bioinformatics - Genomics - Evolution

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

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

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

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

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

6.2. Treerecs

KEYWORDS: Bioinformatics - Biology - Computational biology

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

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

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

NEWS OF THE YEAR: Release of a 0.1 stable version

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

BIGS Project-Team

6. New Software and Platforms

6.1. 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

6.2. ARMADA

A Statistical Methodology to Select Covariates in High-Dimensional Data under Dependence

KEYWORDS: Biostatistics - Aggregated methods - High Dimensional Data - Personalized medicine - Variable selection

FUNCTIONAL DESCRIPTION: Two steps variable selection procedure in a context of high-dimensional dependent data but few observations. First step is dedicated to eliminate dependence between variables (clustering of variables, followed by factor analysis inside each cluster). Second step is a variable selection using by aggregation of adapted methods. https://hal.archives-ouvertes.fr/hal-02173568

NEWS OF THE YEAR: This package is a new one.

- Participants: Aurélie Muller and Anne Gégout-Petit
- Contact: Aurélie Muller
- Publication: Package 'armada' : A Statistical Methodology to Select Covariates in High-Dimensional Data under Dependence
- URL: https://cran.r-project.org/web/packages/armada/

6.3. kosel

Variable Selection by Revisited Knockoffs Procedures

KEYWORDS: Variable selection - Regression

FUNCTIONAL DESCRIPTION: Performs variable selection for many types of L1-regularised regressions using the revisited knockoffs procedure. This procedure uses a matrix of knockoffs of the covariates independent from the response variable Y. The idea is to determine if a covariate belongs to the model depending on whether it enters the model before or after its knockoff. The procedure suits for a wide range of regressions with various types of response variables. Regression models available are exported from the R packages 'glmnet' and 'ordinalNet'. Based on the paper linked to via the URL below: Gegout A., Gueudin A., Karmann C. (2019) https://arxiv.org/abs/1907.03153

NEWS OF THE YEAR: This package is a new one.

- Participants: Clémence Karmann, Aurélie Muller and Anne Gégout-Petit
- Contact: Aurélie Muller
- Publication: The revisited knockoffs method for variable selection in L_1-penalised regressions.
- URL: https://cran.r-project.org/web/packages/kosel/kosel.pdf

6.4. 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/

6.5. 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

6.6. HSPOR

Hidden Smooth Polynomial Regression for Rupture Detection

KEYWORDS: Polynomial regression - Rupture detection

FUNCTIONAL DESCRIPTION: Several functions that allow by different methods to infer a piecewise polynomial regression model under regularity constraints, namely continuity or differentiability of the link function. The implemented functions are either specific to data with two regimes, or generic for any number of regimes, which can be given by the user or learned by the algorithm.

NEWS OF THE YEAR: This package is a new one

- Participants: Florine Greciet, Romain Azais and Anne Gégout-Petit
- Contact: Florine Greciet
- URL: https://cran.r-project.org/web/packages/HSPOR/

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

6. New Software and Platforms

6.1. lib3Dmol

Library in Rust for manipulating 3D representations of molecules

KEYWORDS: 3D modeling - Proteins - Molecules - Rust

FUNCTIONAL DESCRIPTION: The lib3Dmol library can be called by programs written in Rust for 3D modelling of biomolecules and their interactions.

RELEASE FUNCTIONAL DESCRIPTION: The 0.2.0 version can be used with any type of biomolécule.

- Contact: Philippe Noel
- URL: http://mbi.loria.fr

6.2. QRMSDmap

Parallelized computation of RMSD map of molecular structures after 3D alignment based on the quaternion method.

KEYWORDS: Molecules - RMSD - Rust - Bioinformatics

FUNCTIONAL DESCRIPTION: This program allows fast computing of 3D alignments and 3D distances on a large number of biomolecular structures.

RELEASE FUNCTIONAL DESCRIPTION: This 2.3.2 version improves CPU parallelization and decreases memory consumption.

- Contact: Philippe Noel
- URL: http://mbi.loria.fr

6.3. EROS-DOCK

Exhaustive Rotational Search using Branch-and-Bound algorithm for rigid docking

KEYWORDS: 3D modeling - Proteins - Docking

FUNCTIONAL DESCRIPTION: EROS-DOCK is a protein-protein docking program for Linux. It takes in input the 3D structures of two proteins in PDB format, and gives as output a list of transformation matrices describing the most probable relative positions of the two proteins in nature, together with a score (approximation of their binding energy for that position). On a modern workstation, docking times is in the order of few hours for a blind global search. The user can also provide nowledge of particular contact points at the surface of each protein, which accelerates the pruning of the solutions space. The underlying algorithm uses a pi-ball representation of the rotational 3D space, to accelerate the search for close-fitting orientations of the two molecules by a branch-and-bound technique.

- Contact: Isaure Chauvot de Beauchêne
- URL: https://erosdock.loria.fr

6.4. NAFRAGDB

Databases of nucleic acids fragments bound to proteins

KEYWORDS: Structural Biology - Nucleic Acids - Data base

FUNCTIONAL DESCRIPTION: NAfragDB is a python-based software for (i) the automated parsing, correction and annotation of all protein - nucleic acid structures in the public Protein Data Bank, (ii) the creation of libraries of non-redundant RNA/DNA structural fragments, (iii) the selection of sets of structures by customized queries, and (iv) the computation of statistics on sets of RNA/DNA - protein structures.

- Contact: Isaure Chauvot de Beauchêne

6.5. RNA-PDBComplete

Completing RNA structures in PDB files

KEYWORDS: Nucleic Acids - Structural Biology

FUNCTIONAL DESCRIPTION: PDBcomplete is a software and a webserver for the completion of missing atoms in an RNA structure provided in PDB format. PDBcomplete is capable of taking into account the presence of other molecules in the overall PDB structure to avoid atoms collisions. It uses as template an in-house library of mono-nucleotide libraries created with the NAfragDB tool.

- Contact: Isaure Chauvot de Beauchêne
- URL: https://pdbcomplete.loria.fr/

6.6. MBI platform for structural bioinformatics

Initiated during the previous CPER projects Intelligence Logicielle (1999-2005) and MISN: Modelisation, Interactions et Systèmes Numériques (2006-2013), the MBI platform (MBI = Modelling Biomolecules and their Interactions) is today part of the SMEC platform coordinated by MD Devignes and M Smaïl-Tabbone (SMEC: Simulation, Modélisation et Extraction de Connaissances), in the frame of the ongoing CPER projet ITM2P (Innovations Technologiques et Modélisation pour la Médecine Personnalisée ; 2015-2020). The MBI platform is composed of several HPC and storage servers that are shared between users mostly for structural bioinformatics usages. The MBI platform is part of the bioinformatic platform network of the French Institute of Bioinformatics (IFB ; http://www.france-bioinformatique.fr.

- Participants: Marie-Dominique Devignes [contact person], Isaure Chauvot de Beauchêne, Sjoerd de Vries, Antoine Moniot, Emmanuel Bresso, Philippe Noel, Patrice Ringot.
- URL: https://mbi.loria.fr

DYLISS Project-Team

6. New Software and Platforms

6.1. AskOmics

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

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

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

NEWS OF THE YEAR: (1) migration to github, (2) complete re-engineering for cleaning the successive layers and accomodating further extensions, (3) integration of the Corese triplestore (https://corese.inria.fr/) in addition to fuseki and virtuoso, (4) improved user interface, (5) capability to save queries for sharing and reusing them, (6) automatic generation of askomics-compliant graph of entity types (abstraction), (7) capability to use askomics to query remote endpoints (including Uniprot and neXtProt), (8) support for federated queries involving remote endpoints and local data

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

6.2. AuReMe

Automatic Reconstruction of Metabolic networks

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

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

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

RELEASE FUNCTIONAL DESCRIPTION: - Reworking padmet and padmet-utils to allow full-python workflow in the future - Adding new script padmet-utils/exploration/prot2genome with exonerate - Fixing minor errors

NEWS OF THE YEAR: (1) Pantograph replaced by OrthoFinder (2) Create a readthedocs for AuReMe, padmet and padmet-utils (3) Reworking padmet and padmet-utils to allow full python workflow (4) Adding new script padmet-utils/exploration/prot2genome with exonerate (5) Modify template data structure (6) Fixing errors

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

6.3. biseau

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

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

NEWS OF THE YEAR: First release.

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

6.4. Metage2Metabo

KEYWORDS: Metabolic networks - Microbiota - Metagenomics - Workflow

FUNCTIONAL DESCRIPTION: Metabolic networks are graphs which nodes are compounds and edges are biochemical reactions. To study the metabolic capabilities of microbiota, Metage2Metabo uses multiprocessing to reconstruct metabolic networks at large-scale. The individual and collective metabolic capabilities (number of compounds producible) are computed and compared. From these comparisons, a set of compounds only producible by the community is created. These newly producible compounds are used to find minimal communities that can produce them. From these communities, the keytstone species in the production of these compounds are identified.

NEWS OF THE YEAR: First release.

- Contact: Anne Siegel
- Publication: Metage2Metabo: metabolic complementarity applied to genomes of large-scale microbiotas for the identification of keystone species
- URL: https://github.com/AuReMe/metage2metabo

6.5. Pathmodel

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

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

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

RELEASE FUNCTIONAL DESCRIPTION: Fix an issue with test data.

NEWS OF THE YEAR: (1) Add a container in Singularity Hub (https://singularity-hub.org/collections/3758). (2) Rewrite data files (sterol and MAA). (3) Add creation of pictures of new molecules from MZ. (4) Add new output files to ease understanding of PathModel output. (5) Rewrite the Readme.

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

6.6. CADBIOM

Computer Aided Design of Biological Models

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

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

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

We recently developed a framework that integrates an updated version of the CADBIOM core software and visualization tools. We provided a command line interface allowing users to translate the interactions between biomolecules described in data sources in BioPAX format into the formalism based on the guarded transitions used by CADBIOM. The command line also makes it easy to search for scenarios based on the constraints of a model, to compare scenarios with each other and to visualize interaction graphs facilitating the biologist's expertise (Vignet et al 2019 JOBIM)

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

ERABLE Project-Team

5. New Software and Platforms

5.1. C3Part/Isofun

KEYWORDS: Bioinformatics - Genomics

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

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

5.2. Cassis

KEYWORDS: Bioinformatics - Genomics

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

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

5.3. Coala

CO-evolution Assessment by a Likelihood-free Approach

KEYWORDS: Bioinformatics - Evolution

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

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

5.4. CSC

KEYWORDS: Genomics - Algorithm

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

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

5.5. Cycads

KEYWORDS: Systems Biology - Bioinformatics

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

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

5.6. DBGWAS

KEYWORDS: Graph algorithmics - Genomics

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

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

5.7. Eucalypt

KEYWORDS: Bioinformatics - Evolution

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

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

5.8. Fast-SG

KEYWORDS: Genomics - Algorithm - NGS

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

- Participants: Alex Di Genova, Marie-France Sagot, Alejandro Maass and Gonzalo Ruz Heredia
- Contact: Alex Di Genova
- URL: https://github.com/adigenova/fast-sg

5.9. Gobbolino-Touché

KEYWORDS: Bioinformatics - Graph algorithmics - Systems Biology

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

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

5.10. HapCol

KEYWORDS: Bioinformatics - Genomics

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

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

5.11. HgLib

HyperGraph Library

KEYWORDS: Graph algorithmics - Hypergraphs

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

RELEASE FUNCTIONAL DESCRIPTION: Initial version

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

5.12. KissDE

KEYWORDS: Bioinformatics - NGS

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

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

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

5.13. KisSplice

KEYWORDS: Bioinformatics - Bioinfirmatics search sequence - Genomics - NGS

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

RELEASE FUNCTIONAL DESCRIPTION: Improvements : The 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+.

KISSPLICE was applied to a new application field, virology, through a collaboration with the group of Nadia Naffakh at Institut Pasteur. The goal is to understand how a virus (in this case influenza) manipulates the splicing of its host. This led to new developments in KISSPLICE. Taking into account the strandedness of the reads was required, in order not to mis-interpret transcriptional readthrough. We now use BCALM instead of DBG-V4 for the de Bruijn graph construction and this led to major improvements in memory and time requirements of the pipeline. We still cannot scale to very large datasets like in cancer, the time limiting step being the quantification of bubbles.

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

5.14. KisSplice2RefGenome

KEYWORDS: Bioinformatics - NGS - Transcriptomics

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

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

5.15. KisSplice2RefTranscriptome

KEYWORDS: Bioinformatics - NGS - Transcriptomics

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

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

5.16. MetExplore

KEYWORDS: Systems Biology - Bioinformatics

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

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

5.17. Mirinho

KEYWORDS: Bioinformatics - Computational biology - Genomics - Structural Biology

FUNCTIONAL DESCRIPTION: Predicts, at a genome-wide scale, microRNA candidates.

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

5.18. Momo

Multi-Objective Metabolic mixed integer Optimization

KEYWORDS: Metabolism - Metabolic networks - Multi-objective optimisation

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

- Participants: Ricardo Luiz de Andrade Abrantes, Nuno Mira, Susana Vinga and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: http://momo-sysbio.gforge.inria.fr

5.19. Moomin

Mathematical explOration of Omics data on a MetabolIc Network

KEYWORDS: Metabolic networks - Transcriptomics

FUNCTIONAL DESCRIPTION: MOOMIN is a tool for analysing differential expression data. It takes as its input a metabolic network and the results of a DE analysis: a posterior probability of differential expression and a (logarithm of a) fold change for a list of genes. It then forms a hypothesis of a metabolic shift, determining for each reaction its status as "increased flux", "decreased flux", or "no change". These are expressed as colours: red for an increase, blue for a decrease, and grey for no change. See the paper for full details: https://doi.org/10.1093/bioinformatics/btz584

- Participants: Henri Taneli Pusa, Mariana Ferrarini, Ricardo Luiz de Andrade Abrantes, Arnaud Mary, Alberto Marchetti-Spaccamela, Leen Stougie and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: https://github.com/htpusa/moomin

5.20. MultiPus

KEYWORDS: Systems Biology - Algorithm - Graph algorithmics - Metabolic networks - Computational biology

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

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

5.21. 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.

- Participants: Vicente Acuna Aguayo, Paulo Vieira Milreu, Alberto Marchetti-Spaccamela, Leen Stougie, Martin Wannagat and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: http://gforge.inria.fr/projects/pitufo/

5.22. Sasita

KEYWORDS: Bioinformatics - Graph algorithmics - Systems Biology

FUNCTIONAL DESCRIPTION:SASITA is a software for the exhaustive enumeration of minimal precursor sets in metabolic networks.

- Participants: Vicente Acuna Aguayo, Ricardo Luiz de Andrade Abrantes, Paulo Vieira Milreu, Alberto Marchetti-Spaccamela, Leen Stougie, Martin Wannagat and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: http://sasita.gforge.inria.fr/

5.23. 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

5.24. 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

5.25. Rime

KEYWORDS: Bioinformatics - Genomics - Sequence alignment

FUNCTIONAL DESCRIPTION: Detects long similar fragments occurring at least twice in a set of biological sequences.

- Participants: Nadia Pisanti and Marie-France Sagot
- Contact: Nadia Pisanti

5.26. 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.

- Participants: Alice Julien-Laferrière, Ricardo Luiz de Andrade Abrantes, Arnaud Mary, Mariana Ferrarini, Susana Vinga, Irene Ziska and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: http://hyperstories.gforge.inria.fr/

5.27. VG-Flow

Viral haplotype reconstruction from contigs using variation graphs

KEYWORD: Haplotyping

FUNCTIONAL DESCRIPTION: The goal of haplotype-aware genome assembly is to reconstruct all individual haplotypes from a mixed sample and to provide corresponding abundance estimates. VG-FLOW provides a reference-genome-independent solution based on the construction of a variation graph, capturing all quasispecies diversity present in the sample. We solve the contig abundance estimation problem and propose a greedy algorithm to efficiently build full-length haplotypes. Finally, we obtain accurate frequency estimates for the reconstructed haplotypes through linear programming techniques.

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

5.28. Virus-VG

Viral haplotype reconstruction from contigs using variation graphs

KEYWORD: Haplotyping

FUNCTIONAL DESCRIPTION: Viruses populate their hosts as a viral quasispecies: a collection of genetically related mutant strains. Viral quasispecies assembly refers to reconstructing the strain-specific haplotypes from read data, and predicting their relative abundances within the mix of strains, an important step for various treatment-related reasons. Reference-genome-independent (de novo) approaches have yielded benefits over reference-guided approaches, because reference-induced biases can become overwhelming when dealing with divergent strains. While being very accurate, extant de novo methods only yield rather short contigs. VIRUS-VG aims to reconstruct full-length haplotypes together with their abundances from such contigs, represented as a genome variation graph.

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

5.29. Wengan

Making the path

KEYWORD: Genome assembly

FUNCTIONAL DESCRIPTION:WENGAN is a new genome assembler that unlike most of the current long-reads assemblers avoids entirely the all-vs-all read comparison. The key idea behind WENGAN is that long-read alignments can be inferred by building paths on a sequence graph. To achieve this, WENGAN builds a new sequence graph called the Synthetic Scaffolding Graph. The SSG is built from a spectrum of synthetic mate-pair libraries extracted from raw long-reads. Longer alignments are then built by performing a transitive reduction of the edges. Another distinct feature of WENGAN is that it performs self-validation by following the read information. WENGAN identifies miss-assemblies at differents steps of the assembly process.

- Participants: Alex Di Genova and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: https://github.com/adigenova/wengan

5.30. 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

<div align="center">

GENSCALE Project-Team

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6. New Software and Platforms

6.1. SVJedi

KEYWORDS: High throughput sequencing - Structural Variation - Genome analysis

FUNCTIONAL DESCRIPTION: SVJedi is a structural variation (SV) genotyper for long read data. Based on a representation of the different alleles, it estimates the genotype of each variant in a given individual sample based on allele-specific alignment counts. SVJedi takes as input a variant file (VCF), a reference genome (fasta) and a long read file (fasta/fastq) and outputs the initial variant file with an additional column containing genotyping information (VCF).

- Participants: Claire Lemaitre, Lolita Lecompte, Pierre Peterlongo and Dominique Lavenier
- Contact: Claire Lemaitre
- URL: https://github.com/llecompte/SVJedi

6.2. MinYS

MineYourSymbiont

KEYWORDS: High throughput sequencing - Genome assembly - Metagenomics

FUNCTIONAL DESCRIPTION: MinYS allows targeted assembly of a bacterial genome of interest in a metagenomic short read sequencing sample using a reference-guided pipeline. First, taking advantage of a potentially distant reference genome, a subset of the metagenomic reads is assembled into a set of backbone contigs. Then, this first draft assembly is completed using the whole metagenomic readset in a de novo manner. The resulting assembly is output as a genome graph, allowing to distinguish different strains with potential structural variants coexisting in the sample.

- Contact: Claire Lemaitre
- URL: https://github.com/cguyomar/MinYS

6.3. Simka

KEYWORDS: Comparative metagenomics - K-mer - Distance - Ecology

FUNCTIONAL DESCRIPTION: Simka is a comparative metagenomics method dedicated to NGS datasets. It computes a large collection of distances classically used in ecology to compare communities by approximating species counts by k-mer counts. The method scales to a large number of datasets thanks to an efficient and parallel kmer-counting strategy that processes all datasets simultaneoulsy. SimkaMin is distributed also with Simka. SimkaMin is a faster and more resource-frugal version of Simka. It outputs approximate (but very similar) results by subsampling the kmer space.

RELEASE FUNCTIONAL DESCRIPTION: Since release version 1.5.0, SimkaMin is distributed alongside Simka. SimkaMin is also a de novo comparative metagenomics tool. It is a faster and more resource-frugal version of Simka. It outputs approximate (but very similar) results as Simka by subsampling the kmer space. With this strategy, and with default parameters, SimkaMin is an order of magnitude faster, uses 10 times less memory and 70 times less disk than Simka.

- Participants: Claire Lemaitre, Dominique Lavenier, Gaëtan Benoit and Pierre Peterlongo
- Contact: Claire Lemaitre
- URL: https://gatb.inria.fr/software/simka/

6.4. 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.

RELEASE FUNCTIONAL DESCRIPTION: * Substantive improvements: better quality of results (accuracy and recall), better filtering of obtained results * Formal improvements: better organization of scripts, better presentation of results

- Participants: Pierre Peterlongo and Claire Lemaitre
- Contact: Pierre Peterlongo
- URL: https://github.com/GATB/DiscoSnp

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

5. New Software and Platforms

5.1. WellFARE

KEYWORDS: Bioinformatics - Statistics - Data visualization - Data modeling

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

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

NEWS OF THE YEAR: Publication in BMC Bioinformatics describing the new version of WellFARE
- Participants: Delphine Ropers, Hans Geiselmann, Hidde de Jong, Michel Page, Valentin Zulkower and Yannick Martin
- Partner: UGA
- Contact: Hidde de Jong
- Publication: Robust reconstruction of gene expression profiles from reporter gene data using linear inversion
- URL: https://github.com/ibis-inria/wellfare

5.2. WellInverter

KEYWORDS: Bioinformatics - Statistics - Data visualization - Data modeling

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

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

NEWS OF THE YEAR: Deployment of WellInverter on an Inria server and on the new cloud of the French Institute for Bioinformatics (see the web page for details). Publication in BMC Bioinformatics describing the new version of the application.
- Participants: Delphine Ropers, Hans Geiselmann, Hidde de Jong, Johannes Geiselmann, Michel Page, Valentin Zulkower and Yannick Martin
- Partner: UGA
- Contact: Hidde de Jong
- Publication: Robust reconstruction of gene expression profiles from reporter gene data using linear inversion
- URL: https://team.inria.fr/ibis/wellinverter/

5.3. GNA

Genetic Network Analyzer

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

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

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

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

NEWS OF THE YEAR: New mode of distribution from the IBIS web site. Tutorial on the use of the model formalism for analyzing synthetic genetic circuits.

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

LIFEWARE Project-Team

6. New Software and Platforms

6.1. BIOCHAM

The Biochemical Abstract Machine

KEYWORDS: Systems Biology - Bioinformatics

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

RELEASE FUNCTIONAL DESCRIPTION: – notebooks of Master classes – graphical user interface on top of Jupyter – synthesis of at most binary reactions with minimisation of the variables for negative values – detection of model reduction by subgraph epimorphism – option for partial tropical equilibrations

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

6.2. casq

CellDesigner as SBML-Qual

KEYWORDS: SBML - Logical Framework - Knowledge representation

FUNCTIONAL DESCRIPTION: CaSQ transforms a big knowledge map encoded as an SBGN-compliant SBML file in CellDesigner into an executable Logical Model in SBML-Qual

- Authors: Sylvain Soliman and Anna Niarakis
- Partner: Université d'Evry-Val d'Essonne
- Contact: Sylvain Soliman
- URL: https://gitlab.inria.fr/soliman/casq/

6.3. Platforms

6.3.1. Smart experimental platforms to automate microbiology experiments

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

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

5. New Software and Platforms

5.1. Obj.MPP

KEYWORDS: Object detection - Marked Point Process - Parametric model

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

- Author: Eric Debreuve
- Contact: Eric Debreuve
- Publications: Stochastic geometry for image analysis - Multiple objects detection in biological images using a marked point process framework - An efficient optimizer for simple point process models - Multiple Birth and Cut Algorithm for Multiple Object Detection
- URL: https://team.inria.fr/morpheme/obj-mpp-object-detection-using-a-marked-point-process/

5.2. ATOLS

Adaptative Threshold Operator based on Level Sets

KEYWORDS: Object detection - Level Set

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

- Authors: Kevin Giulietti and Guillaume Lavisse
- Contact: Xavier Descombes
- URL: https://team.inria.fr/morpheme/software/

5.3. Small particle detection

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

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

It is an simplified version of marked point process.

- Contact: Nicolas Cedilnik
- Publications: SPADE: A Small Particle Detection Method Using A Dictionary Of Shapes Within The Marked Point Process Framework - SPADE: A Small Particle Detection Method Using A Dictionary Of Shapes Within The Marked Point Process Framework
- URL: https://gitlab.inria.fr/ncedilni/spade

MOSAIC Project-Team

5. New Software and Platforms

5.1. cellcomplex

KEYWORDS: Polyhedral meshes - 3D

FUNCTIONAL DESCRIPTION: The cellcomplex library is a Python library that allows manipulating 2D or 3D multicellular complexes, with the study of plant tissues as a main application. It is mostly structured around a data structure that is used to represent such complexes as incidence graphs of dimension 2 or 3, and provides several key functionalities:

* The creation of structures from more basic representation (polygons of points for instance), from some geometrical primitives (2D or 3D) and the generation of synthetic regular or irregular grids, allowing notably the simulation of tissues.

* The computation of topological and geometrical properties on the multicellular complex structures, including notably useful computations on triangle meshes, a specific case of complexes with simplicial faces (areas, normals, triangle eccentricity, curvature estimator).

* The edition of structures by local topological operations, notably in th case of triangle meshes (edge flip, subdivision, vertex insertion) and multi-criteria geometrical optimization processes and isotropic remeshing.

* The import and export in various standard file formats for geometries (.obj, .ply, .msh) and notably in the standard formad defined by the community of plant tissue modelling (PLY, Saisnbury Computational Workshop 2015).

RELEASE FUNCTIONAL DESCRIPTION: * Major restructuration involving a change of namespace and a simplification of module architecture. * Inclusion of 3D visualization functionalities based on VTK.

- Participant: Guillaume Cerutti
- Contact: Guillaume Cerutti

5.2. draco_stem

DRACO-STEM : Dual Reconstruction by Adjacency Complex Optimization & SAM Tissue Enhanced Mesh

KEYWORDS: Meshing - Image segmentation - Computational biology - Optimization

FUNCTIONAL DESCRIPTION: Draco-stem provides a computational pipeline that allows going from multi-label segmented images of living tissue (typically resulting from a watershed segmentation of 3D microscopy image stacks) to topologically consistent, FEM-ready triangular meshes of all cell interfaces in the tissue.

It relies on an original topological optimization method that aims at reconstructing the simplicial complex of cellular adjacencies from the image, and on dualization and geometrical optimization to obtain a triangle mesh that satisfies simultaneously several quality criteria (triangle regularity, adequation to image, biological priors). The library provides implementations for 3D tissue reconstruction, single-layer 2.5D reconstruction and advanced 2D reconstruction.

RELEASE FUNCTIONAL DESCRIPTION: * Major refactoring, python3 compatibility * Addition of Draco2D functionalities

- Contact: Guillaume Cerutti
- Publication: DRACO-STEM: An Automatic Tool to Generate High-Quality 3D Meshes of Shoot Apical Meristem Tissue at Cell Resolution
- URL: https://gitlab.inria.fr/mosaic/draco_stem.git

5.3. Gnomon

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

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

FUNCTIONAL DESCRIPTION: Gnomon is a plugin-based computational platform for the analysis and simulation of morphogenesis. It relies on a scalable software architecture based on the dtk kernel developed by the group of software engineers (SED) from the Sophia-Antipolis Inria Center. The development of Gnomon aims at answering four main challenges:

* Provide an easily accessible computational tool for the exploration of morphogenesis, by focusing on the deployability of the software (using conda), on the ergonomics of the user interface and the availability of the documentation.

* Give access to powerful tools for the exploration of dynamical forms, through an interactive visualization framework allowing the exploration in space in time and the access to algorithmic resources developed by the team for image sequences of multicellular tissues or collections of branching forms.

* Ensure the interoperability of computational libraries within the platform and its extensibility by a generalized plugin-based architecture (facilitated by the dtk framework) for algorithms, visualizations and data structures, enabling the members of the team and future users to feed the platform with their own C++ and Python libraries.

* Bridge the gap between experimental data and computational simulations by offering the possibility to go from one to the other in the same platform in a nearly transparent way, thanks to a common dynamical system framework integrated to the core of the platform.

Gnomon project organization: * Project leader: Christophe Godin * Software development coordinator: Guillaume Cerutti * DTK coordinators: Julien Wintz, Thibaud Kloczko * Plugin coordinators: Jonathan Legrand, Romain Azais, Olivier Ali, Frédéric Boudon. * Diffusion coordinator: Teva Vernoux

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

RELEASE FUNCTIONAL DESCRIPTION: A major technical update has been carried out on the Gnomon platform with the switch of the platform core to dtk2, implying an upgrade of all involved Python code to python 3.6+. The newer version 0.13 displays a clearer and more customizable interface and all functionalities from the version 0.9. In terms of functionalities, a major effort has been put on recovering former applications of the team (LPy and PlantGL) and including them in a robust way in the scope of the platform. A release of the version 1.0 is planned for early 2020 including validated algorithms for the quantitative analysis of 3D images of tissue, a much more robust user interface and an extensive user and developer documentation made available online.

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

5.4. MorphoNet

KEYWORDS: 3D web - Morphogenesis - Big data - 3D reconstruction

FUNCTIONAL DESCRIPTION: MorphoNet is an open-source web-based morphological browser. It consists of a web application, exploiting the Unity3D gaming engine, which offers the user a comprehensive palette of interactions with the data, in order to explore the structure, the dynamics and the variability of biological systems. Users can also project quantitative and genetic properties onto the morphological scaffold, allowing for instance to easily explore the correlation between shape dynamics and gene expression patterns. On top of that, datasets and associated information can be shared with other selected users or with entire groups. This possibility of directly sharing results within and between research communities, together with the use of a unified, human readable format, makes MorphoNet a unique tool for multidisciplinary research. Its web-based, user-friendly and open-source structure is also ideal for science dissemination and teaching.

- Partner: CRBM - Centre de Recherche en Biologie cellulaire de Montpellier
- Contact: Emmanuel Faure
- URL: http://www.morphonet.org

5.5. TimageTK

Tissue Image ToolKit

KEYWORDS: 3D - Image segmentation - Fluorescence microscopy - Image registration - Image processing - Image filter

FUNCTIONAL DESCRIPTION: TimageTK (Tissue Image Toolkit) is a Python package dedicated to image processing of multicellular architectures such as plants or animals and is intended for biologists and modelers. It provides grayscale or labeled image filtering and mathematical morphology algorithms, as well as image registration and segmentation methods.

- Contact: Jonathan Legrand
- URL: https://mosaic.gitlabpages.inria.fr/timagetk/index.html

5.6. treex

KEYWORDS: Graph algorithmics - Data structures - Combinatorics - Machine learning

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

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

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

RELEASE FUNCTIONAL DESCRIPTION: In 2019, treex has been published in JOSS (Journal of Open Source Software). The subtree kernel has been released to accompany an article submitted to Journal of Machine Learning Research. In addition, the DAG class and the kernel class have been extensively redesigned to be more user-friendly.

- Participants: Romain Azais, Guillaume Cerutti, Didier Gemmerle and Florian Ingels
- Contact: Romain Azais
- Publication: treex: a Python package for manipulating rooted trees
- URL: https://gitlab.inria.fr/azais/treex

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

6. New Software and Platforms

6.1. magecal

KEYWORD: Genomics

SCIENTIFIC DESCRIPTION: Magecal independently runs training and prediction steps for Augustus, Conrad, GeneID, GeneMark, and Snap. The results are cleaned and integrated into a common format. Jigsaw is trained and used for model reconciliation. Consistency constraints are applied to ensure that phase and intron structure are biologically plausible.

FUNCTIONAL DESCRIPTION: Magecal predicts a set of protein coding genes in fungal genomic sequences, using different de novo prediction algorithms, and reconciling the predictions with the aid of comparative data. Magecal applies consistency constraints to guarantee that the predicted genes are biologically valid.

RELEASE FUNCTIONAL DESCRIPTION: Dockerization and compatibility with Alcyone

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

6.2. Declic

KEYWORDS: Data analysis - Machine learning - Taxonomies

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
- URL: https://gitlab.inria.fr/pleiade/declic

6.3. Magus

KEYWORDS: Bioinformatics - Genomic sequence - Knowledge database

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

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

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

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

6.4. Mimoza

KEYWORDS: Systems Biology - Bioinformatics - Biotechnology

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

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

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

6.5. 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

6.6. 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 James Sherman
- Contact: David James Sherman
- URL: https://team.inria.fr/pleiade/alcyone/

6.7. family-3d

KEYWORDS: Biodiversity - Point cloud - 3D modeling

SCIENTIFIC DESCRIPTION: The method statistically selects a subset of pairwise distances between proteins in the family, constructs a weighted graph, and lays it out using an adaptation of the three-dimensional extension of the Kamada-Kawai force-directed layout.

FUNCTIONAL DESCRIPTION: Family-3D lays out high-dimension protein family point clouds in 3D space. The resulting lower-dimension forms can be printed, so that they can be explored and compared manually. They can also be explored interactively or stereographically.

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

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

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

6.8. Yapotu

Yet Another Pipeline for OTU building

KEYWORDS: Taxonomies - Distance matrices - Clustering - Metagenomics

FUNCTIONAL DESCRIPTION: OTU building is one of the key operation in metabarcoding: how to delimit Operational Taxonomic Units in the "soup" where all amplicons of thousands of unicellular organisms have been lumped together (from visible plankton to nano- and picoplankton, for example). Yapotu is a software tool that enables approaches to unsupervised clustering on very large matrices of distances: each element is a distance between two reads produced by a sequencer. It permits one to select one method among several, like building MultiDimensional Scaling to produce an Euclidean image, and clustering within the point cloud, or building a graph where a node is a sequence and there is an edge if both sequences are at a distance smaller than a given threshold, and then after build connected components or communities on this graph. Other functions visualize the OTUs as clusters or subgraphs.

- Contact: Alain Franc
- URL: https://gitlab.inria.fr/afranc/diodon/tree/master/yapotu

6.9. Diodon

KEYWORDS: Dimensionality reduction - Data analysis

FUNCTIONAL DESCRIPTION: Most of dimension reduction methods inherited from Multivariate Data Analysis, and currently implemented as element in statistical learning for handling very large datasets (the dimension of spaces is the number of features) rely on a chain of pretreatments, a core with a SVD for low rank approximation of a given matrix, and a post-treatment for interpreting results. The costly part in computations is the SVD, which is in cubic complexity. Diodon is a list of functions and drivers which implement (i) pre-treatments, SVD and post-treatments on a large diversity of methods, (ii) random projection methods for running the SVD which permits to bypass the time limit in computing the SVD, and (iii) an implementation in C++ of the SVD with random projection at prescribed rank or precision, connected to MDS.

- Contact: Alain Franc
- URL: https://gitlab.inria.fr/afranc/diodon

SERPICO Project-Team

6. New Software and Platforms

6.1. 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. Colocalization amounts here to quantifying the interaction strength by the area/volume of the intersection between the two binary images viewed as random distributions of geometrical objects. Under mild assumptions, it turns out that the appropriately normalized Pearson correlation follows a standard normal distribution under the null hypothesis if the number of image pixels is large. Unlike previous methods, GcoPS handles 2D and 3D images, variable SNRs and any kind of cell shapes. It is able to co-localize large regions with small dots, as it is the case in TIRF-PALM experiments and to detect negative co-localization. The typical processing time is two milliseconds per image pair in 2D and a few seconds in 3D, with no dependence on the number of objects per image. In addition, the method provides maps to geo-co-localize molecule interactions in specific image regions.

- Participants: Thierry Pécot, Frédéric Lavancier, Charles Kervrann and Liu Zengzhen
- Partners: Université de Nantes - UMR 144 CNRS - Institut Curie - Hollings Cancer Center at the Medical University of South Carolina, Charleston SC, USA
- Contact: Charles Kervrann
- Publication: Testing independence between two random sets for the analysis of colocalization in bioimaging
- URL: http://icy.bioimageanalysis.org/plugin/GcoPS

6.2. THOTH

Testing HypOtheses for diffusion TricHotomy

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

FUNCTIONAL DESCRIPTION: The THOTH software classifies biomolecule trajectories of biomolecules (computed with tracking algorithms) into three groups of diffusion: (i) free diffusion, (ii) subdiffusion or (iii) superdiffusion. Brownian motion corresponds to the NULL hypothesis. THOTH is a nonparametric three-decision test whose alternatives are subdiffusion and superdiffusion. Single and multiple testing procedures control respectively the type I error and the false discovery rate. THOTH can be considered as an alternative to the Mean Square Displacement (MSD) method commonly used to address this issue. It gives more reliable results as confirmed by our Monte Carlo simulations and evaluations on real sequences of images depicting protein dynamics acquired with TIRF or SPT-PALM microscopy.

- Participants: Vincent Briane, Charles Kervrann and Myriam Vimond
- Partner: ENSAI
- Contact: Charles Kervrann
- Publication: Statistical analysis of particle trajectories in living cells
- URL: https://team.inria.fr/serpico/software/thot/

6.3. SparseVolution

Sparse Variation for 2D Image Decovolution

KEYWORDS: Fluorescence microscopy - Image processing - Deconvolution - Inverse problem

FUNCTIONAL DESCRIPTION: In order to improve the resolution of acquired fluorescence images, we introduced a method of image deconvolution by considering a family of convex regularizers. The considered regularizers are generalized from the concept of Sparse Variation which combines the L1 norm and the first (Total Variation) or second (Hessian Variation) derivatives to favor the colocalization of high-intensity pixels and high-magnitude gradient. The experiments showed that the proposed regularization approach produces competitive deconvolution results on fluorescence images, compared to those obtained with other approaches such as TV or the Schatten norm of Hessian matrix. The final algorithm has been dedicated to deconvolve very large 2D (e.g. 20 000 x 20 000) images or 3D images.

- Participants: Hoai Nam Nguyen, Charles Kervrann, Sylvain Prigent and Cesar Augusto Valades Cruz
- Partners: Innopsys - UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann

6.4. AiryscanJ

Reconstruction of AiryScan microscopy images

KEYWORDS: Image reconstruction - Fluorescence microscopy - Photonic imaging - Deconvolution - Image analysis

FUNCTIONAL DESCRIPTION: The AiryscanJ software enables to reconstruct a high resolution image from an array of multiple raw images acquired with the Airyscan technology (32 detectors). Airyscanning is a recent technique based on confocal laser scanning microscopy. The AiryscanJ software gathers four reconstruction methods (ISM, IFED, ISFED, ISM-Deconvolution) to compute a high resolution image: 1/ ISM amounts to summing the preliminarily registered raw images. 2/ IFED is the weighted difference between the inner detectors and the outer detector. 3/ ISFED is the weighted difference between the registered outer detectors and the original outer detectors. AiryscanJ automatically estimates the parameter controlling the IFED and ISFED algorithms. 4/ ISM-Deconvolution allows reconstructing a high resolution image by applying a deconvolution algorithm on the ISM image.

- Participants: Sylvain Prigent, Stephanie Dutertre and Charles Kervrann
- Partners: Université de Rennes 1 - CNRS
- Contact: Charles Kervrann
- URL: https://gitlab.inria.fr/serpico/airyscanj_bin

6.5. DeepFinder

Deep learning for macromolecule identification within 3D cellular cryo-electron tomograms

KEYWORDS: Image analysis - Deep learning - Cryo-electron microscopy - Object detection

FUNCTIONAL DESCRIPTION: DeepFinder is a computational approach that uses artificial neural networks to accurately and jointly localize multiple types and/or states of macromolecules in 3D cellular cryo-electron tomograms. DeepFinder leverages deep learning and outperforms the commonly-used template matching method on ideal data. On synthetic image data (SHREC 2019 challenge), DeepFinder is very fast and produces superior detection results when compared to other competitive deep learning methods, especially on small macromolecules. On experimental cryo-ET data depicting ribosomes, the detection results obtained by DeepFinder are consistent with expert annotations. We have got a high overlap of 86% and a similar structure resolution determined by subtomogram averaging.

- Participants: Emmanuel Moebel, Antonio Martinez and Charles Kervrann
- Partners: Max Planck Institute Martinsried - Fondation Fourmentin-Guilbert
- Contact: Charles Kervrann
- URL: https://gitlab.inria.fr/serpico/deep-finder

6.6. CPAnalysis

Change point detection algorithm for detecting switches of diffusion along 2D-3D single particle trajectories

KEYWORDS: Statistical modeling - Statistical physics - Fluorescence microscopy - Motion analysis

FUNCTIONAL DESCRIPTION: The change point detection algorithm is designed for detecting switches of diffusion along a given 2D-3D particle trajectory. We consider that the particle can switch between three main motion modes: 1/ Superdiffusion which occurs when the particle is transported via molecular motors along the cytoskeleton, 2/ Free diffusion (or Brownian motion) which arises when the particle evolves freely inside the cytosol, 3/ Subdiffusion observed when the particle is confined in a domain or evolves in a crowded area. The algorithm is a sequential nonparametric procedure based on a nonparametric three-decision test computed on local sliding windows along the trajectory.

- Participants: Antoine Salomon, Vincent Briane, Myriam Vimond, Jean Salamero and Charles Kervrann
- Partners: ENSAI - UMR 144 CNRS - Institut Curie
- Contact: Charles Kervrann
- Publication: A sequential algorithm to detect diffusion switching along intracellular particle trajectories
- URL: https://team.inria.fr/serpico/software/cpanalysis/

6.7. FlowScope

Optical flow computation for 3D fluorescence microscopy

KEYWORDS: Motion analysis - Fluorescence microscopy - Image analysis - Data visualization

FUNCTIONAL DESCRIPTION: The FLOWSCOPE software is able to estimate 3D motion between two fluorescence microscopy volumes. The underlying variational method amounts to minimizing an energy functional made up of two terms: a data term and a regularization term. The data term is derived from the continuous form of Census signature and the smoothness of the flow field is imposed by a L2 regularization term. The method is implemented for a single core CPU. FLOWSCOPE outputs three separate files corresponding to the motion vector components. The flow fields can be visualized with an appropriate color code named 3PHS. The 3PHS map projects the flow field onto the three orthogonal planes selected by the user. The projections of the vector field is color coded in the Hue (direction) and the Saturation (amplitude) spaces.

- Participants: Patrick Bouthemy, Charles Kervrann, Sylvain Prigent, Leo Maury and Philippe Roudot
- Partner: Danuser lab, University of Texas Southwestern, Dallas, USA
- Contact: Sandeep Manandhar
- Publication: 3D Flow Field Estimation and Assessment for Live Cell Fluorescence Microscopy
- URL: https://gitlab.inria.fr/smanandh/flowscope

6.8. MWR

Missing Wedge Restoration (MWR) and Noise Removal in 3D Cryo-Tomography

KEYWORDS: Image analysis - Inverse problem - Cryo-electron microscopy - Monte-Carlo methods - Bayesian estimation

FUNCTIONAL DESCRIPTION: The Missing Wedge Restoration (MWR) software enables to reduce the high amount of noise and artifacts observed in 3D cellular cryo-tomograms, induced by the presence of a missing wedge (MW) in the spectral domain. MWR takes as input a 3D tomogram derived from limited-angle tomography, and gives as output a 3D denoised and artifact compensated volume. The artifact compensation is achieved by filling up the MW with meaningful information. A Minimum Mean Square Error (MMSE) estimator is computed by applying a dedicated Markov Chain Monte-Carlo (MCMC) sampling procedure based on the Metropolis-Hasting algorithm. MWR can be used to enhance visualization or as a pre-processing step for image analysis, including segmentation and classification of macromolecules.

- Participants: Emmanuel Moebel and Antonio Martinez
- Partners: Max Planck Institute Martinsried - Fondation Fourmentin-Guilbert
- Contact: Charles Kervrann
- Publication: A Monte Carlo framework for missing wedge restoration and noise removal in cryo-electron tomography
- URL: https://gitlab.inria.fr/serpico/mwr

6.9. Platforms

6.9.1. Mobyle@serpico platform and software distribution
Participants: Sylvain Prigent, Léo Maury, Charles Kervrann.

Figure 2. Mobyle@serpico web portal.

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

Free binaries: software packages have been compiled for the main operating systems (Linux, MacOS, Windows) using CMake (see http://www.cmake.org/). A few of them are freely available on the team website https://team.inria.fr/serpico/software/ under a proprietary license.

Mobyle@serpico web portal: An on-line version (http://mobyle-serpico.rennes.inria.fr) of the image processing algorithms has been developed 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[9], ATLAS[1], HULLKGROUND[48], KLTRACKER[52], MOTION2D[51], MS-DETECT[49], ND-SAFIR[4], OPTICALFLOW and FLUX ESTIMATION [9]. The web interface makes our image processing methods available for biologists at Mobyle@serpico 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 [4], HULLKGROUND [48], MOTION2D [51], ATLAS [1]. The C-CRAFT [9], QUANTEV and GCOPS [19] algorithms have been developed for the image processing ICY platform (http://icy.bioimageanalysis.org/).

Partners: CNRS-UMR 144 Institut Curie & France-BioImaging (UMS 3714 CEMIBIO).

6.9.2. *Bioimage-IT for bioimage management and processing*

Participants: Sylvain Prigent, Cesar Augusto Valades Cruz, Léo Maury, Jean Salamero, Charles Kervrann.

New image acquisition systems generate large number of images and large volume images. Such data sets are hard to store, to process and to analyze for one user in a workstation. Many solutions exist for data management (e.g. Omero, OpenImadis), image analysis (e.g. Fiji, Icy, CellProfiler) and statistics (e.g R). Each of them has its specificities and several bridges have been developed between pieces of software. Nevertheless, in many use-cases, we need to perform analysis using tools that are available in different pieces of software and different languages. It is then tedious to create a workflow that brings the data from one tool to another. It needs programing skills and most of the time, a dedicated script using a dedicated file system for processed data management is developed. The aim of BioImage-IT is to create a "bandmaster" application that allow any scientist to annotate, process, and analyze data using only one single high level application. This BioImage-IT application is based on 3 components:

- an image annotation method based on a JSON file system,
- an image processing and analysis tools integration method based on Docker and XML commands description,
- an application with a graphical interface to easily annotate data, run processing tools, and visualize data and results.

This software architecture has three main goals. First, data are annotated using a file system. This means that data are not dependent on any software like a SQL database, and each experiment can then be stored in a different directory and can be moved from one server to another or to any drive with a simple copy pasting operation. Second, the processing tools are used as binary packages managed by the Docker technology. Docker enables to gently handle dependencies and several versions of the same tool. Any existing tool can then be integrated in its native programming language. Third, using a single "bandmaster" application allows one to automatically generate metadata for any processed data, improving the traceability and the repeatability of any experimental result.

BioImage-IT (https://project.inria.fr/bioimageit) is developed in the context of the France-BioImaging research infrastructure in coordination with the IPDM-FBI (Image Processing and Data Management) node in order to provide a standardized image processing tool set and data management for the imaging facilities.

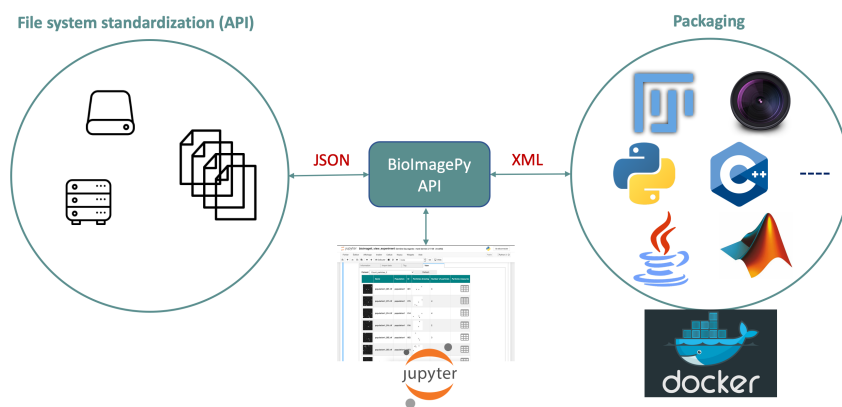**Partners:** CNRS-UMR 144 and U1143 INSERM/CNRS-UMR 3666, Institut Curie & France-BioImaging (UMS 3714 CEMIBIO).

Figure 3. Scheme of the BioImage-IT components interactions.

ARAMIS Project-Team

6. New Software and Platforms

6.1. Brain Networks Toolbox

KEYWORDS: Neuroimaging - Medical imaging

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

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

6.2. Deformetrica

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

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

Deformetrica comes with two applications:

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

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

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

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

6.3. Clinica

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

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

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

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

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

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

- Contact: Olivier Colliot

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

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

6.4. Platforms

6.4.1. *Platform Brain-computer interface*

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

ATHENA Project-Team

6. New Software and Platforms

6.1. Dmipy

Diffusion MRI Multi-Compartment Modeling and Microstructure Recovery Made Easy

KEYWORDS: Diffusion MRI - Multi-Compartment Modeling - Microstructure Recovery

FUNCTIONAL DESCRIPTION: Non-invasive estimation of brain microstructure features using diffusion MRI (dMRI) – known as Microstructure Imaging – has become an increasingly diverse and complicated field over the last decades. Multi-compartment (MC)-models, representing the measured diffusion signal as a linear combination of signal models of distinct tissue types, have been developed in many forms to estimate these features. However, a generalized implementation of MC-modeling as a whole, providing deeper insights in its capabilities, remains missing. To address this fact, we present Diffusion Microstructure Imaging in Python (Dmipy), an open-source toolbox implementing PGSE-based MC-modeling in its most general form. Dmipy allows on-the-fly implementation, signal modeling, and optimization of any user-defined MC-model, for any PGSE acquisition scheme. Dmipy follows a "building block"-based philosophy to Microstructure Imaging, meaning MC-models are modularly constructed to include any number and type of tissue models, allowing simultaneous representation of a tissue's diffusivity, orientation, volume fractions, axon orientation dispersion, and axon diameter distribution. In particular, Dmipy is geared toward facilitating reproducible, reliable MC-modeling pipelines, often allowing the whole process from model construction to parameter map recovery in fewer than 10 lines of code. To demonstrate Dmipy's ease of use and potential, we implement a wide range of well-known MC-models, including IVIM, AxCaliber, NODDI(x), Bingham-NODDI, the spherical mean-based SMT and MC-MDI, and spherical convolution-based single- and multi-tissue CSD. By allowing parameter cascading between MC-models, Dmipy also facilitates implementation of advanced approaches like CSD with voxel-varying kernels and single-shell 3-tissue CSD. By providing a well-tested, user-friendly toolbox that simplifies the interaction with the otherwise complicated field of dMRI-based Microstructure Imaging, Dmipy contributes to more reproducible, high-quality research.

- Authors: Rutger Fick, Demian Wassermann and Rachid Deriche
- Contact: Rachid Deriche

6.2. High Performance Diffusion MRI

KEYWORDS: Health - Neuroimaging - Medical imaging

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

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

6.3. OpenMEEG

KEYWORDS: Health - Neuroimaging - Medical imaging

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

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

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

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

- Participants: Alexandre Gramfort, Emmanuel Olivi, Geoffray Adde, Jan Kybic, Kai Dang, Maureen Clerc, Perrine Landreau, Renaud Keriven and Théodore Papadopoulo
- Contact: Théodore Papadopoulo
- Publications: inria-00467061v2 - inria-00584205v1 - hal-01278377v1
- URL: http://openmeeg.github.io/

6.4. OpenVIBE

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

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

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

6.5. BCI-VIZAPP

BCI visual applications

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

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

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

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

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

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

BIOVISION Project-Team

6. New Software and Platforms

6.1. Virtual Retina

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

KEYWORDS: Neurosciences - Simulation - Biology - Health

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

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

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

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 the 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 us to explore several aspects of retinal image processing such as understanding how to reproduce accurately the statistics of the spiking activity at the population level, or reconciling connectomics and simple computational rules for visual motion detection. This makes this tool a unique platform to better understand how the retina works.

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

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

6.3. Platforms

6.3.1. Macular

Macular https://team.inria.fr/biovision/macular-software/ is a platform for the numerical simulation of the retina and primary visual cortex. It aims to reproduce the response of the retina to visual or electrical stimulation – produced by retinal prostheses – under normal or pathological conditions. The objective is to develop a tool that can be used by neuroscience researchers to reproduce experimental results, but also to guide their experiments through hypotheses that can be tested in the simulator. This can save a considerable amount of experimental resources. Macular is based on the central idea that its use and its graphic interface can evolve according to the objective of the user. It can be used in several cases, such as the simulation of retinal waves, the simulation of retinal and cortical responses to electrosurgical stimulation, the study of the contribution of specific classes of retinal cells in the encoding of visual scenes. Macular's modular architecture makes it flexible and makes it easy to implement new features. It also includes a scripting option, which offers the user the ability to decode his own model, with a given set of equations, variables and parameters, without having to program a code. Finally, thanks to a highly parallelizable architecture, Macular makes it possible to simulate a large number of cells of different classes (see Fig. 1).
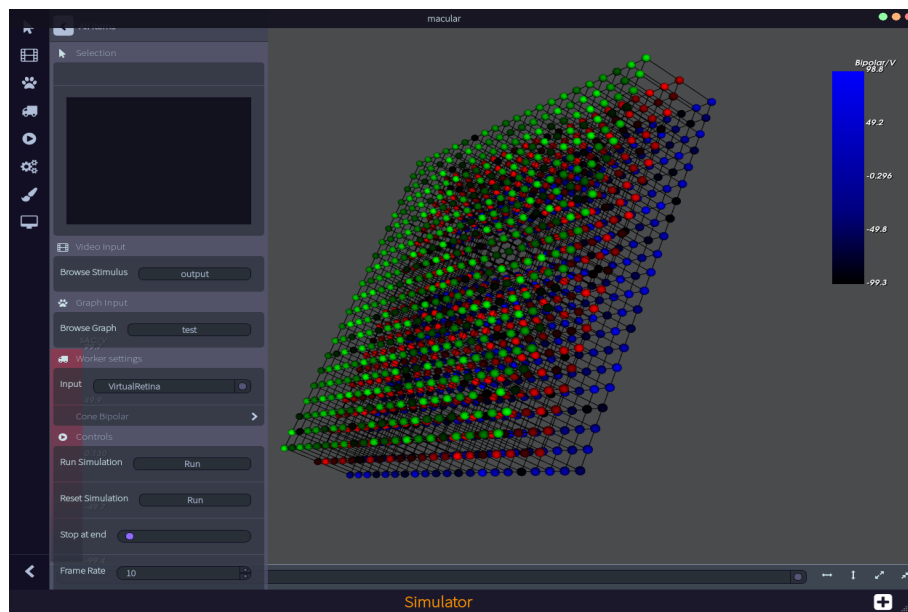

Figure 1. The Macular software. Here we see a three dimensional view of three retinal cells layers.

CAMIN Project-Team

5. New Software and Platforms

5.1. RT_Stim

Real-Time simulation for functional electrical Stimulation

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

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

- Authors: Daniel Simon and Samy Lafnoune
- Contact: Daniel Simon
- URL: https://gforge.inria.fr/projects/rtstim/trunk

5.2. Platforms

5.2.1. Platform : IMUSEF Modular embedded architecture for real time control of a FES system

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

We have been working on the development of a new hardware and software architecture embedding a network of sensors and an electrical stimulator interfaced to a controller. The controller intends to be worn by the experiment participants.

A mini low-cost single board computer (Raspberry Pi3) was embedded in a 3D-printed case strapped around the waist of the subject. Using wireless inertial sensors connected as a WBAN, the sink node gets data from all the IMUs, therefore highly decreasing data flow when multiple IMUs are transmitting inside the network. To get rid of this limitation and guarantee an overall 100 Hz sampling rate no matter the number of IMUs, the wireless inertial sensors can be replaced by wired ones, low-cost with a high speed ARM Cortex-M0 based processor and a Kalman Filter directly providing quaternion estimation at 100 Hz for each IMU. The use of a multiplexer connected through an I2C interface (Inter Integrated Circuit) enabled to keep a 100 Hz rate using 4 IMUs.

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

This scalable architecture (fig. 3), developed as a modular system, allowed us to implement new commands laws for Real Time closed loop control as well as giving us the possibility to use various types of sensors and stimulators to meet the needs of specific applications. To achieve this and in order for the FES architecture to directly control different electrical stimulators, Application Programming Interfaces (APIs) were developed for 3 main commercial stimulators in the team. They each corresponds to a specific need and use case. The Vivaltis Phoenix Stimulator allows for low-weight embedding, wireless network control, but only 2 stimulation channels are available at the moment, while being scalable, it is mainly used for experiments on gait. The BerkelBike Stimulator v2.0 presents a cumbersome but extended control compromise with 8 independent stimulation channels, which is an ideal solution for FES-assisted cycling. And finally the Hasomed Rehastim v1.0 allowing fine control but isn't battery powered in its commercial version, used mainly for upper limb experiments.
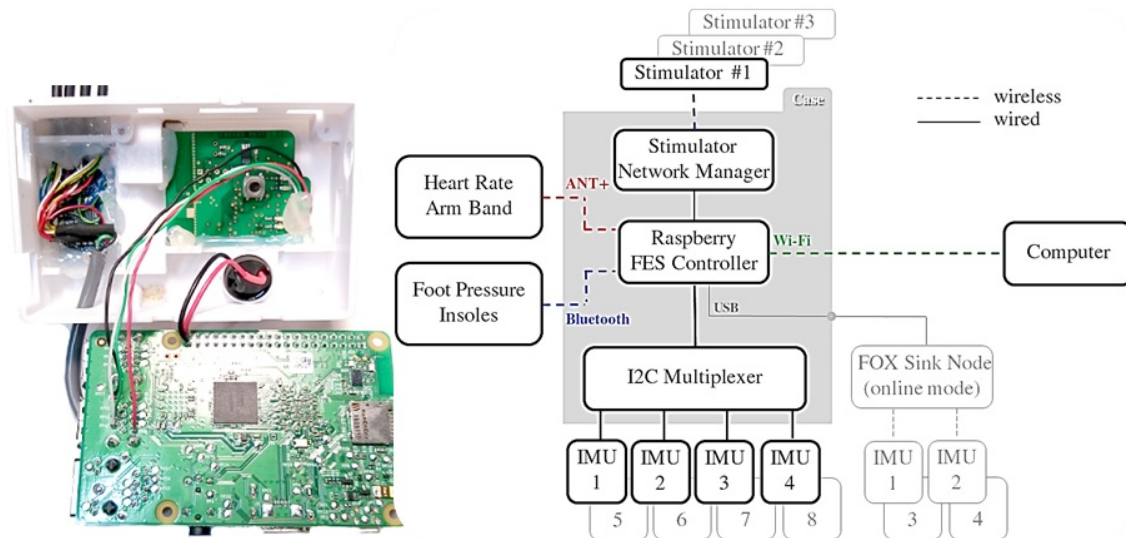
Figure 3. Experimental protocols have led to the development of a scalable hardware architecture decentralized on the subject.

This new architecture is currently used in clinical experiments and will continue to evolve with a goal of being easy to use, even by untrained clinicians (i.e. FES assisted cycling §6.8).

The software APP of this platform can be found at https://bil.inria.fr/fr/software/view/3520/tab as the *IMUSEF Project* with the Bil Id: Software_3520.

5.2.2. Platform : FESCYCLING FES-cycling platforms

Participants: Christine Azevedo Coste, Ronan Le Guillou, Martin Schmoll.

The embedded FES controller (IMUSEF) was reshaped for cycling application to improve modularity, performances and stability, using fully the capabilities of the Raspberry Pi 3B platform. These modifications now allow easier implementation, integration and usage of new control algorithms that could, in the future, be used for various end applications and contexts. Furthermore a Graphical User Interface (GUI) communicating with the embedded platform was developed, allowing on-the-fly modification of various parameters as well as safe control and monitoring of the running algorithms. An add-on relay box module allowing mechanical switching of the stimulating channels for more precise On/Off stimulation synchronization as well as more control and safety measures was also created. The two commercially available recumbent tricycles that we adapted for Spinal Cord Injured FES Cycling can be seen in Figure 4 .

5.2.3. Platform : MEDITAPARK Wearable Tremor monitoring system based on acceleration monitoring

Participants: Christine Azevedo Coste, Ronan Le Guillou, Marion Holvoet.

As part of a preliminary study on the effects of Mindfulness meditation on participants with Parkinson's Disease (PD) (§3), an application was developed to monitor at home tremor occurrence using a smartwatch Samsung Gear S3 and its newer model, the Samsung Galaxy Watch (Fig:5 a). A Python program has been developed to process and format data and present characteristics of the tremor under a user friendly and comprehensible format for clinicians. The goal of this system being to identify Parkinson's tremors
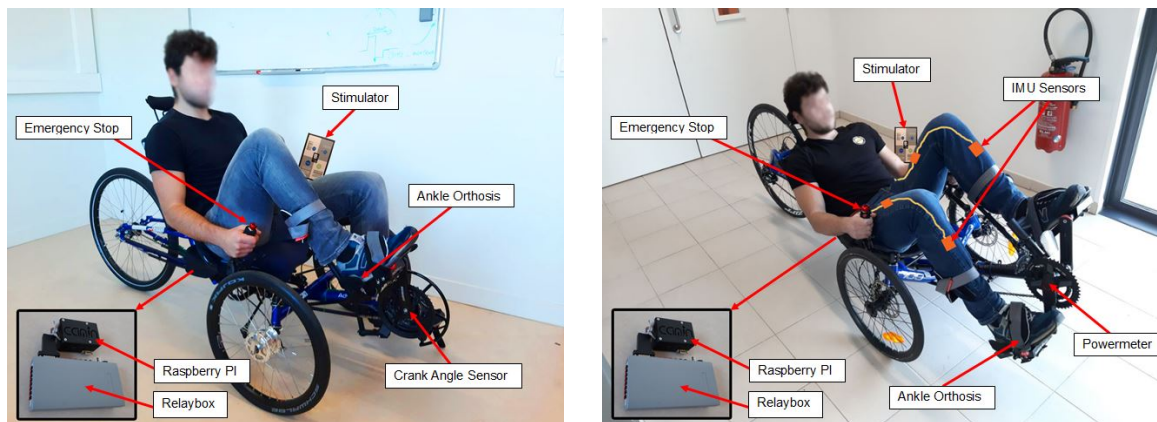
Figure 4. FES Cycling platforms developed in the CAMIN team. a) ICE Trike Adventure 26 setup adapted for Spinal Cord Injured FES Cycling b) CAT Trike 700 setup adapted for Spinal Cord Injured FES Cycling

characteristics qualitatively and quantitatively to highlight global tendencies and help objectively determine effectiveness of diverse treatments against PD tremors. This system was tested on long duration acquisitions (2 and 4 days) with 2 volunteers subject to PD tremors of moderate and high severity and proved to be able to highlight tremor tendencies and characteristics in real conditions. These acquisitions were done in order to experimentally validate the inner-workings of the developed system in real conditions and its capacity to detect PD tremors of moderate and high severity as well as to refine the classification and processing of the data. An example of 4 days acquisition is presented in Figure 5 b.

The created system allows qualification of tremors in punctual clinical check-ups in the Hospital as well as quantitative formatting of daily tendencies. This system should then allow to highlight the evolution of Parkinson's tremors characteristics throughout the MBSR (Mind-fullness Based Stress Reduction) meditation program which is yet to be undertaken. A protocol is still waiting for validation from the CPP to begin inclusions and conduct the MBSR meditation program, monitored with the developed system.

The software APP of this platform can be found at https://bil.inria.fr/fr/software/view/3565/tab as the *PARa-Keet Project* with the Bil Id: Software_3565.

5.2.4. Platform : AGILIS-EX software

Participants: Arthur Hiairrassary, Christine Azevedo Coste, David Guiraud.

The AGILIS-EX software was specially developed as part of the AGILIS project for exploratory clinical trials governed by the ID RCB research protocol: 2019-A02037-50. It allows the configuration and triggering of the stimulation generated by the STIMEP (neural stimulator) or the VIVALTIS (external stimulator) (Fig.6). The stimulation parameters are automatically selected according to predefined configurations (frequency, current and pulse-width) in order to obtain the functional movements of the hand desired by the subject (Fig.7). To detect and interpret patient voluntary movement or contraction to infer the activation or deactivation of the pre-programmed stimulation, it uses measurements from the DELSYS acquisition system (EMG, FSR, trigger).

This medical grade software is compliant with the IEC 62304 (class B).
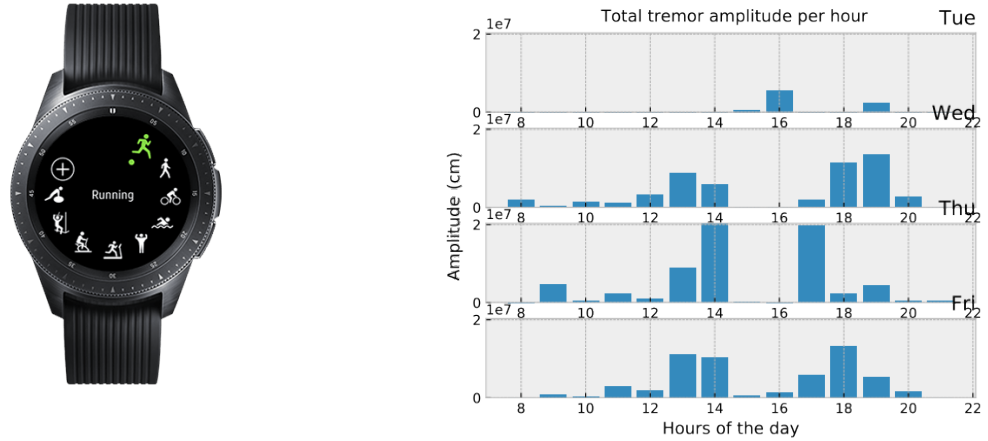
*Figure 5. Meditapark figures. a) Smart watch used as the embedded platform for this monitoring application :
Samsung Galaxy Watch b) Showcase of experimental data acquired in ecological conditions over 3.5 days
presenting a quantitative and objective evaluation of the Parkinson's tremors under a daily format condensed
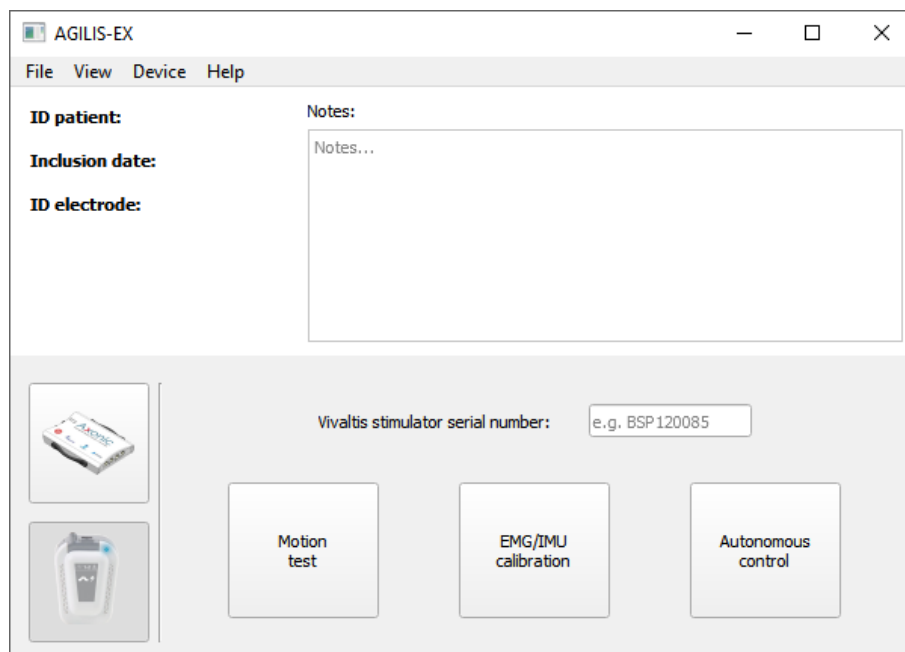hourly.*

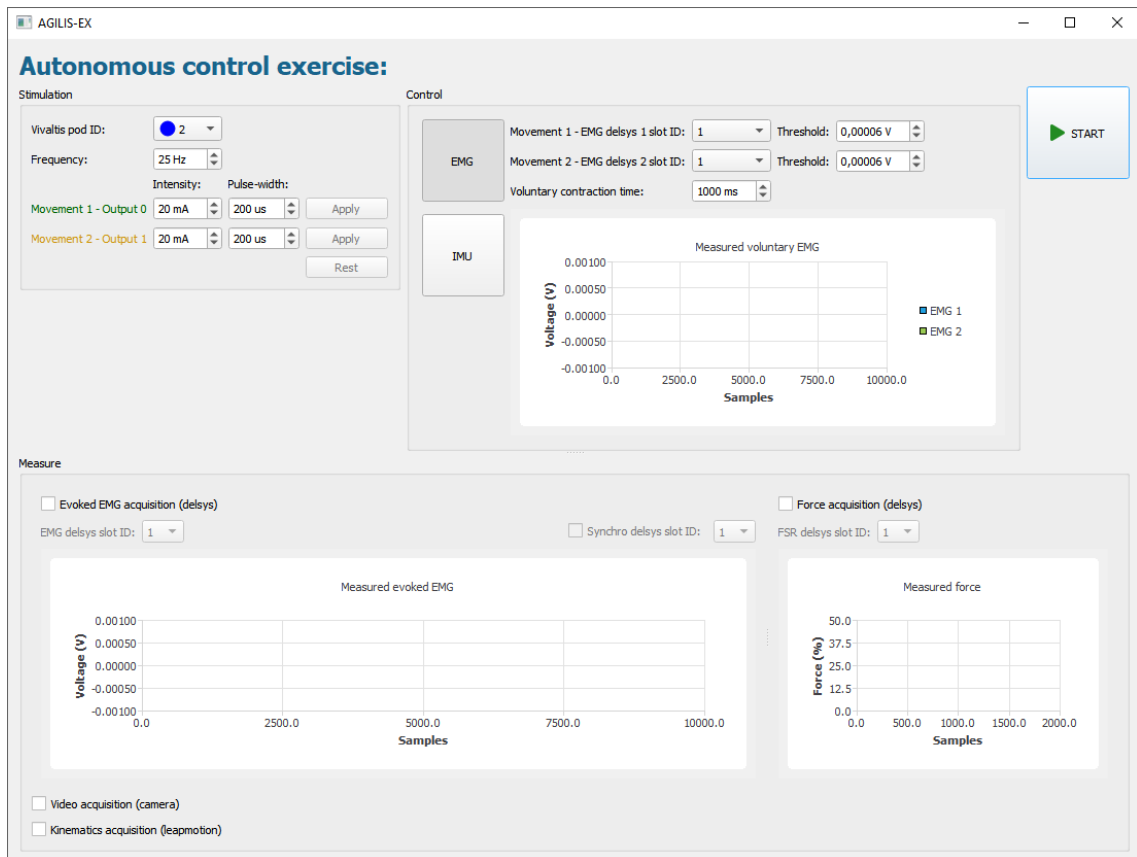*Figure 6. Main window of the AGILIS-EX software.*

Figure 7. Autonomous control exercise window used for external stimulation

EMPENN Project-Team

6. New Software and Platforms

6.1. Anima

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

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

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

6.2. autoMRI

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

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

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

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

6.3. MedInria

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

SCIENTIFIC DESCRIPTION: MedInria aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010, renewed in 2012. A fast-track ADT was awarded in 2017 to transition the software core to more recent dependencies and study the possibility of a consortium creation.The Empenn 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: https://med.inria.fr

6.4. QtShanoir

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

SCIENTIFIC DESCRIPTION: QtShanoir is based on Qt/C++ library. It interacts with the Shanoir server using SOAP web services. 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 : search, 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 share, archive, search and visualize neuroimaging data.

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

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

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

The clinical scores resulting from instrument-based assessments (e.g. neuropsychological tests) can also be entered and easily retrieved and exported in different formats (Excel, CSV, Xml). Scores and image acquisitions are bound together which makes relationship analysis possible. The instrument database is scalable 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 regard to security, the system requires authentication and user rights are tunable for each hosted study. The person responsible for the study can define which users are allowed to see, download or import data.

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

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

6.6. ShanoirUploader

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

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

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

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

6.7. Anima medInria plugins

KEYWORDS: IRM - Medical imaging - Diffusion imaging

FUNCTIONAL DESCRIPTION: Plugins for the medInria software based on the open source software Anima developed in the Visages / Empenn team. These plugins are interfaces between anima and medinria allowing to use Anima functionalities within the clinical user interface provided by medInria. The current functionalities included in the plugins are right now: image registration, denoising, quantitative image (relaxometry), and model estimation and visualization from diffusion imaging.

- Participants: Olivier Commowick, René-Paul Debroize and Guillaume Pasquier
- Contact: Olivier Commowick

6.8. Platforms

6.8.1. The Neurinfo Platform

Empenn 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, CNRS for the academic side, and the University Hospital of Rennes and the Cancer Institute "Eugene Marquis" for the clinical side, are partners of this neuroinformatics platform called Neurinfo (https://www.neurinfo.org).

Concerning the Neurinfo Platform, the activity domain is a continuum between methodological and techno-logical research built around specific clinical research projects. 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 proce-dures of brain lesions, neuro-oncology and radiotherapy planning. Beyond these central nervous system appli-cations, 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 collab-orations 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. A new 3T Siemens Prisma MRI scanner was installed at the Neuroinfo platform in February 2018. In 2014, an 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 High Performance Computing environment made of one large computing cluster and a data center that is shared and operated by the Inria center and IRISA (UMR CNRS 6074). The computation cluster (480 cores) and the data center (up to 150 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 60 sites). In 2019, an MRI and EEG-compatible fNIRS system was acquired through a co-funding from the INS2I institute of CNRS and FEDER. At the end of 2019, GIS IBISA awarded the Neurinfo platform with a complementary funding that will be dedicated to supplement the current system with additional sensors (from 8x8 optodes to 16x16 optodes).

EPIONE Project-Team

5. New Software and Platforms

5.1. CardiacSegmentationPropagation

KEYWORDS: 3D - Segmentation - Cardiac - MRI - Deep learning

FUNCTIONAL DESCRIPTION: Training of a deep learning model which is used for cardiac segmentation in short-axis MRI image stacks.

- Authors: Qiao Zheng, Hervé Delingette, Nicolas Duchateau and Nicholas Ayache
- Contact: Qiao Zheng
- Publication: 3D Consistent & Robust Segmentation of Cardiac Images by Deep Learning with Spatial Propagation

5.2. CardiacMotionFlow

KEYWORDS: 3D - Deep learning - Cardiac - Classification

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

- Contact: Qiao Zheng

5.3. MedInria

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

SCIENTIFIC DESCRIPTION: MedInria aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010, renewed in 2012. A fast-track ADT was awarded in 2017 to transition the software core to more recent dependencies and study the possibility of a consortium creation.The Empenn 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: https://med.inria.fr

5.4. GP-ProgressionModel

GP progression model

KEYWORDS: Data modeling - Data visualization - Data integration - Machine learning - Biostatistics - Statistical modeling - Medical applications - Evolution - Brain - Uncertainly - Uncertainty quantification - Alzheimer's disease - Probability - Stochastic models - Stochastic process - Trajectory Modeling - Marker selection - Health - Statistic analysis - Statistics - Bayesian estimation

FUNCTIONAL DESCRIPTION: Disease progression modeling (DPM) of Alzheimer's disease (AD) aims at revealing long term pathological trajectories from short term clinical data. Along with the ability of providing a data-driven description of the natural evolution of the pathology, DPM has the potential of representing a valuable clinical instrument for automatic diagnosis, by explicitly describing the biomarker transition from normal to pathological stages along the disease time axis.

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

This software is based on the publication:

Probabilistic disease progression modeling to characterize diagnostic uncertainty: Application to staging and prediction in Alzheimer's disease. Marco Lorenzi, Maurizio Filippone, Daniel C. Alexander, Sebastien Ourselin Neuroimage. 2019 Apr 15,190:56-68. doi: 10.1016/j.neuroimage.2017.08.059. Epub 2017 Oct 24. HAL Id : hal-01617750 https://hal.archives-ouvertes.fr/hal-01617750/

RELEASE FUNCTIONAL DESCRIPTION: - New interface and output - Completely based on pytorch

- Participant: Marco Lorenzi
- Contact: Marco Lorenzi
- Publication: Probabilistic disease progression modeling to characterize diagnostic uncertainty: application to staging and prediction in Alzheimer's disease
- URL: http://gpprogressionmodel.inria.fr

5.5. Music

Multi-modality Platform for Specific Imaging in Cardiology

KEYWORDS: Medical imaging - Cardiac Electrophysiology - Computer-assisted surgery - Cardiac - Health

FUNCTIONAL DESCRIPTION: MUSIC is a software developed by the Asclepios research project in close collaboration with the IHU LIRYC in order to propose functionalities dedicated to cardiac interventional planning and guidance. This includes specific tools (algorithms of segmentation, registration, etc.) as well as pipelines. The software is based on the MedInria platform.

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

5.6. SOFA

Simulation Open Framework Architecture

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

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

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

5.7. geomstats

Computations and statistics on manifolds with geometric structures

KEYWORD: Geometry

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

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

5.8. MC-VAE

Multi Channel Variational Autoencoder

KEYWORDS: Machine learning - Artificial intelligence - Medical applications - Dimensionality reduction - High Dimensional Data - Unsupervised learning - Heterogeneity

SCIENTIFIC DESCRIPTION: Interpretable modeling of heterogeneous data channels is essential in medical applications, for example when jointly analyzing clinical scores and medical images. Variational Autoencoders (VAE) are powerful generative models that learn representations of complex data. The flexibility of VAE may come at the expense of lack of interpretability in describing the joint relationship between heterogeneous data. To tackle this problem, in this work we extend the variational framework of VAE to bring parsimony and interpretability when jointly account for latent relationships across multiple channels. In the latent space, this is achieved by constraining the variational distribution of each channel to a common target prior. Parsimonious latent representations are enforced by variational dropout. Experiments on synthetic data show that our model correctly identifies the prescribed latent dimensions and data relationships across multiple testing scenarios. When applied to imaging and clinical data, our method allows to identify the joint effect of age and pathology in describing clinical condition in a large scale clinical cohort.

FUNCTIONAL DESCRIPTION: This software implements the work published in the paper "Sparse Multi-Channel Variational Autoencoder for the Joint Analysis of Heterogeneous Data" presented at the conference ICML 2019 (Long Beach, California, USA).

The software extends classical variational autoencoders by identifying a joint latent code associated to heterogeneous data represented in different channels. The software is implemented in python and is based on pytorch. It can be applied to any kind of data arrays, and provides functions for optimisation, visualisation and writing of the modelling results.

RELEASE FUNCTIONAL DESCRIPTION: First release

NEWS OF THE YEAR: Method presented in the International Conference on Machine Learning (ICML 2019).

- Participants: Luigi Antelmi, Marco Lorenzi and Nicholas Ayache
- Partner: CoBteK
- Contact: Luigi Antelmi
- URL: https://gitlab.inria.fr/epione_ML/mcvae

5.9. SOFA-CardiacReduction

KEYWORDS: Simulation - 3D modeling - Model Order Reduction - Cardiac

SCIENTIFIC DESCRIPTION: Modification of a finite element deformation model : meshless approach and frame-based description, reduction in the number of affine degrees of freedom and integration points.

FUNCTIONAL DESCRIPTION: This SOFA plugin is intented to build a reduced model for deformable solids (especially cardiac simulations).

- Participants: Gaetan Desrues, Hervé Delingette and Maxime Sermesant
- Contact: Gaetan Desrues

MATHNEURO Project-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: Hugo Talbot
- URL: http://www.sofa-framework.org

6.2. SofaNeedleInsertion

Needle Insertion Plugin

KEYWORD: Simulation

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

- Contact: Hadrien Courtecuisse

6.3. SOFA Optimus

Optimization methods in SOFA: stochastic filtering and data assimilation.

KEYWORDS: Data assimilation - Kalman filter - Stochastic optimization

FUNCTIONAL DESCRIPTION: Optimus is a plugin to work with advanced methods of state estimation and parameter identification. It was created to provide a testing environment for data-driven physics-based modeling (typically finite elements). While currently the plugin implements only stochastic methods based on Kalman filtering, its architecture allows for the implementation of generic prediction–correction schemes where the model is employed as a predictor and correction is performed using given observation data.

- Contact: Stéphane Cotin
- URL: https://gitlab.inria.fr/mimesis/Optimus

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

6. New Software and Platforms

6.1. DANA

Distributed Asynchronous Numerical and Adaptive computing framework

KEYWORD: Neural networks

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

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

6.2. Virtual Enaction

KEYWORDS: Neurosciences - Simulation - Health

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

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

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

6.3. ReservoirPy

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

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

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

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

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

6.4. Platforms

6.4.1. Platform AIDE

Keywords : computational thinking initiation, learning analytics, machine learning

Functional description : This package provides source files to control a tapletop setup allowing to initiate learners to computational thinking using unplugged activities and connected objects, and collecting automatically learning activities including thanks to neuroinspired machine learning mechanisms, developed in collaboration with pobot and the Inria mission of science outreach and the LINE laboratory.

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

6. New Software and Platforms

6.1. OpenVIBE

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

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

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

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

6. New Software and Platforms

6.1. Platforms

6.1.1. *The Proximity Operator Repository*

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

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

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

6.1.2. *FIGARO*

Participants: Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with Claire Lefort, XLIM, Limoges).

link: https://imagejdocu.tudor.lu/plugin/analysis/figaro_psf_3d_optical_microscopy/start

The plugin FIGARO, for ImageJ software, helps tracking resolution of microscope systems by extracting dimensions and orientation of standardized microbeads images, acquired from test samples. In the development of optical microscopes for biomedical imaging, the evaluation of resolution is a fundamental parameter achieved by Point Spread Function (PSF) measurements. Sometimes, PSF measurement procedure is not easy or impossible in case of microspheres images presenting a high noise level. The current method proposed into the plugin FIGARO is based on a variational approach for PSF modeling through multivariate Gaussian fitting, adapted to images acquired in a high noise context [12].

6.1.3. *Kymatio*

Participant: Edouard Oyallon.

link: http://www.kymat.io

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

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

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

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

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

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

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

link: https://goo.gl/GpfCVZ

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

6.1.6. Graph-based text categorization

Participants: Fragkiskos Malliaros, Konstantinos Skianis and Michalis Vazirgiannis (École Polytechnique)
link: https://github.com/y3nk0/Graph-Based-TC/
Graph-based TC is a framework for text categorization that relies on a graph representation of documents. The framework uses various graph centrality criteria to determine the importance of a term within a document. It also makes use of word embeddings to further boost the performance of graph-based methods. It has been implemented in Python and has been built upon widely used modules, including `networkx`, `igraph`, `numpy` and `scikit-learn`.

6.1.7. KernelNE - Topical Node Embeddings

Participants: Abdulkadir Çelikkanat, Fragkiskos Malliaros
link: https://abdcelikkanat.github.io/projects/kernelNE/
KernelNE learns node representations on graphs based on a weighted matrix factorization model which encodes random walk-based information about the nodes, as described in [53].

6.1.8. EFGE - Exponential Family Graph Embeddings

Participants: Abdulkadir Çelikkanat, Fragkiskos Malliaros
link: https://abdcelikkanat.github.io/projects/EFGE/
EFGE learns node embeddings generalizing random walk-based network representation learning techniques to exponential family conditional distributions, as described in [54].

6.1.9. Semi-supervised Fake News Detection

Participants: Adrien Benamira, Benjamin Devillers, Etienne Lesot, Ayush K. Ray, Manal Saadi, and Fragkiskos Malliaros
link: https://github.com/bdvllrs/misinformation-detection-tensor-embeddings
We propose a graph-based semi-supervised fake news detection method, based on graph neural networks, as described in [34].

6.1.10. The PINK image library

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

6.1.11. The Vivabrain AngioTK toolkit

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

6.1.12. The PET/CT FIJI Viewer

Participant: Hugues Talbot
link: http://petctviewer.org/
Quantitive Positron Emission Tomography is a new area for which software is not readily availble. With our partners from Toulouse and Beth Israel hospitals, we have proposed a free open-source plugin allowing clinicians to view, interact and perform automated and interactive lesion segmentation in the context of PET/CT.

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

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. 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/

6.3. Scikit-learn

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

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

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

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

- Participants: Alexandre Gramfort, Bertrand Thirion, Fabian Pedregosa Izquierdo, Gaël Varoquaux, Loïc Estève, Michael Eickenberg and Olivier Grisel
- Partners: CEA - Logilab - Nuxeo - Saint Gobain - Tinyclues - Telecom Paris
- Contact: Olivier Grisel
- URL: http://scikit-learn.org

6.4. 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 - hal-01431618v3
- URL: http://github.com/arthurmensch/modl

6.5. MNE

MNE-Python

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

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

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

- Partners: HARVARD Medical School - New York University - University of Washington - CEA - Aalto university - Telecom Paris - Boston University - UC Berkeley
- Contact: Alexandre Gramfort
- URL: http://martinos.org/mne/

6.6. Dmipy

Diffusion MRI Multi-Compartment Modeling and Microstructure Recovery Made Easy

KEYWORDS: Diffusion MRI - Multi-Compartment Modeling - Microstructure Recovery

FUNCTIONAL DESCRIPTION: Non-invasive estimation of brain microstructure features using diffusion MRI (dMRI) – known as Microstructure Imaging – has become an increasingly diverse and complicated field over the last decades. Multi-compartment (MC)-models, representing the measured diffusion signal as a linear combination of signal models of distinct tissue types, have been developed in many forms to estimate these features. However, a generalized implementation of MC-modeling as a whole, providing deeper insights in its capabilities, remains missing. To address this fact, we present Diffusion Microstructure Imaging in Python (Dmipy), an open-source toolbox implementing PGSE-based MC-modeling in its most general form. Dmipy allows on-the-fly implementation, signal modeling, and optimization of any user-defined MC-model, for any PGSE acquisition scheme. Dmipy follows a "building block"-based philosophy to Microstructure Imaging, meaning MC-models are modularly constructed to include any number and type of tissue models, allowing simultaneous representation of a tissue's diffusivity, orientation, volume fractions, axon orientation dispersion, and axon diameter distribution. In particular, Dmipy is geared toward facilitating reproducible, reliable MC-modeling pipelines, often allowing the whole process from model construction to parameter map recovery in fewer than 10 lines of code. To demonstrate Dmipy's ease of use and potential, we implement a wide range of well-known MC-models, including IVIM, AxCaliber, NODDI(x), Bingham-NODDI, the spherical mean-based SMT and MC-MDI, and spherical convolution-based single- and multi-tissue CSD. By allowing parameter cascading between MC-models, Dmipy also facilitates implementation of advanced approaches like CSD with voxel-varying kernels and single-shell 3-tissue CSD. By providing a well-tested, user-friendly toolbox that simplifies the interaction with the otherwise complicated field of dMRI-based Microstructure Imaging, Dmipy contributes to more reproducible, high-quality research.

- Authors: Rutger Fick, Demian Wassermann and Rachid Deriche
- Contact: Rachid Deriche

6.7. PySAP

Python Sparse data Analysis Package

KEYWORDS: Image reconstruction - Image compression

FUNCTIONAL DESCRIPTION: The PySAP (Python Sparse data Analysis Package, https://github.com/CEA-COSMIC/pysap) open-source image processing software package has been developed for the 3 years between the Compressed Sensing group at Iniria-CEA Parietal team led by Philippe Ciuciu and the CosmoStat team (CEA/IRFU) led by Jean-Luc Statck. It has been developed for the COmpressed Sensing for Magnetic resonance Imaging and Cosmology (COSMIC) project. This package provides a set of flexible tools that can be applied to a variety of compressed sensing and image reconstruction problems in various research domains. In particular, PySAP offers fast wavelet transforms and a range of integrated optimisation algorithms. It also offers a variety of plugins for specific application domains: on top of Pysap-MRI and PySAP-astro plugins, several complementary modules are now in development for electron tomography and electron microscopy for CEA colleagues. In October 2019, PySAP has been released on PyPi (https://pypi.org/project/python-pySAP/, currently version 0.0.3) and in conda (https://anaconda.org/agrigis/python-pysap).

The Pysap-MRI has been advertised through a specific abstract accepted to the next workshop of ISMRM on Data Sampling & Image Reconstruction in late January 2020. It will be presented during a power pitch session together wih an hands-on demo session using JuPyter notebooks.

- Partner: CEA
- Contact: Philippe Ciuciu

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

5. New Software and Platforms

5.1. AGRIF

Adaptive Grid Refinement In Fortran

KEYWORD: Mesh refinement

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

NEWS OF THE YEAR: In 2019, a new contract has been signed with CMEMS (Copernicus Marine Environment Moniroting Service) in order to extent the multiresolution capabilities of the AGRIF and its integration into the NEMO ocean system.

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

5.2. BALAISE

Bilbliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement

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

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

- Contact: Arthur Vidard

5.3. NEMOVAR

Variational data assimilation for NEMO

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

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

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

5.4. Sensitivity

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

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

ANGE Project-Team

6. New Software and Platforms

6.1. Freshkiss

FREe Surface Hydrodynamics using KInetic SchemeS

KEYWORDS: Finite volume methods - Hydrostatic Navier-Stokes equations - Free surface flows

FUNCTIONAL DESCRIPTION: Freshkiss3D is a numerical code solving the 3D hydrostatic and incompressible Navier-Stokes equations with variable density.

- Participants: Fabien Souillé, 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 Chérel
- Contact: Vivien Mallet

6.6. Freshkiss3D

KEYWORDS: Python - Cython - Navier-Stokes

FUNCTIONAL DESCRIPTION: Tool for the numerical solution of free surface Navier-Stokes equations

- Participants: Cédric Doucet, Apolline El Baz and Jacques Sainte Marie
- Partner: UPMC
- Contact: Jacques Sainte Marie
- Publication: Numerical approximation of the 3d hydrostatic Navier-Stokes system with free surface

CASTOR Project-Team (section vide)

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

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. 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/

5.3. Compass

Computing Architecture to Speed up Simulation

KEYWORDS: Finite volume methods - Porous media - High performance computing

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

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

5.4. NS2DDV-M

2D Navier-Stokes equations with variable density

KEYWORDS: Partial differential equation - Finite volume methods - Finite element modelling

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

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

5.5. SimBiof

KEYWORDS: Bioinformatics - Chemistry

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

- Contact: Thierry Goudon

5.6. CELIA3D

KEYWORDS: Fluid mechanics - Multi-physics simulation

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

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

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

5. New Software and Platforms

5.1. 2DLayeredMotion

Estimation of 2D independent mesoscale layered atmospheric motion fields

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

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

5.2. 3DLayeredMotion

Estimation of 3D interconnected layered atmospheric motion fields

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

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

5.3. DenseMotion

Estimation of 2D dense motion fields

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

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

5.4. Low-Order-Motion

Estimation of low order representation of fluid motion

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

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

5.5. TYPHOON

KEYWORD: Fluid mechanics

FUNCTIONAL DESCRIPTION: Typhoon is a fluid motion estimator from image sequences. It is almost real-time dedicated to the measurement of LIDAR sequences, multi-scale, fast and precise to make a fine scale analysis of fluid flows with applications in the fields of energy, transport and environment.

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

5.6. H2OLab

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

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

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

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

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

5.7. PALMTREE

KEYWORD: Monte-Clarlo

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

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

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

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

5.8. GRT3D

Global Reactive Transport in 3D

KEYWORDS: Geochemistry - Dispersion - Scientific calculation - Simulation - Advection

SCIENTIFIC DESCRIPTION: Participants : Édouard Canot, Jocelyne Erhel [correspondant] .

Version: version 2.0, April 2014

APP: registered

Programming language: C

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

The software suite GRT3D has four executable modules:

SIA1D: Sequential Iterative Approach for 1D domains,

GDAE1D: Global DAE approach for 1D domains,

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

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

Current work: extension of the chemistry module and parallelization.

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

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

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

5. New Software and Platforms

5.1. SW2D

Shallow Water 2 Dimensions

KEYWORDS: Numerical simulations - Shallow water equations

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

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

RELEASE FUNCTIONAL DESCRIPTION: GUI, C++ translation

- Participant: Vincent Guinot
- Partner: Université de Montpellier
- Contact: Vincent Guinot

5.2. WindPoS-SDM-LAM

KEYWORDS: Numerical simulations - 3D - Fluid mechanics

FUNCTIONAL DESCRIPTION: Software platform for wind modeling.

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

5.3. SDM

Stochastic Downsaling Method

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

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

5.4. OceaPoS-SDM

KEYWORDS: 3D - Turbulence - Oceanography - Numerical simulations - Stochastic models - Marine Energies

FUNCTIONAL DESCRIPTION: Simulation platform for ocean turbulence and interaction with hydroturbines

- Partner: MERIC
- Contact: Mireille Bossy

<p style="text-align:center;color:red;font-weight:bold;">MAGIQUE-3D Project-Team</p>

6. New Software and Platforms

6.1. Elasticus

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

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

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

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

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

6.2. 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 2019, we have implemented the elasto-acoustic coupling and the poroelastic equations for the HDG formulation.

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

6.3. 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/

6.4. tmodeling-DG

Time-domain Wave-equation Modeling App

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

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

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

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

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

6.5. OpenWind

Open Wind Instrument Design

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

FUNCTIONAL DESCRIPTION: Computes resonating pipes' impedance using one-dimensional finite element method with tonholes and fingering chart.

RELEASE FUNCTIONAL DESCRIPTION: account for toneholes as a pipe network using transmission matrices for pipe junctions [Chaigne & Kergomard]

- Authors: Robin Tournemenne, Juliette Chabassier, Alexis Thibault, Augustin Ernoult and Guillaume Castera
- Contact: Juliette Chabassier
- Publication: hal-01963674v2
- URL: https://gitlab.inria.fr/openwind/release

6.6. ffwi

Frequency-domain Full Waveform Inversion

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

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

- Partner: TOTAL
- Contact: Florian Faucher

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

6. New Software and Platforms

6.1. CELIA3D

KEYWORDS: Fluid mechanics - Multi-physics simulation

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

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

6.2. DiSk++

Discontinuous Skeletal C++ Library

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

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

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

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

6.3. NEF-Draw

Numerical Experiments involving Fractures -Visualisation

KEYWORD: Fracture network

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

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

NEWS OF THE YEAR: Add vizualization of new quantities (a posteriori estimators, velocity fields,...). New features for user-friendly usage of NEF-Draw.

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

6.4. NEF-Flow

KEYWORDS: Hydrogeology - Numerical simulations - 3D

SCIENTIFIC DESCRIPTION: NEF-Flow is a Matlab software for the simulation of steady state single phase flow in Discrete Fracture Networks (DFNs) using the Mixed Hybrid Finite Element (MHFEM) method for conforming and non conforming discretizations. It includes: wells, sink/source terms boundary conditions, implementation of RT0 and P1 non conforming finite elements, data structures to save the information local to each fracture, a set of non regression tests to check the solution on the Inria continuous integration platform, wells and sink/sources boundary conditions in the function that check the solution.

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

NEWS OF THE YEAR: The last version includes new features (new APP v1.1): a full documentation of the code, new 2D test cases with analytical solutions to study the convergence of the non-conforming (Mortar) method, new organization of the non regression tests and automatic run on the Inria continuous integration platform, a refactoring of the solver parts, new developments of an iterative solver to solve flow in fractures networks (research work with Pr. Ludmil Zikatanov, PennState University), the computation of the velocity fields with P1 non conforming FE.

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

6.5. NEF++

KEYWORDS: Fracture network - Finite element modelling - High order methods

SCIENTIFIC DESCRIPTION: NEF++ is able to solve in a very efficient way flow in large scale fractures networks using the HHO method.

FUNCTIONAL DESCRIPTION: The software NEF++ allows to solve flow problems in fractured rocks. It is based on a hybrid high order (HHO) method. It is based on the C++17 standard. It relies on the Eigen library, which is a C++ template library for linear algebra and on the DiSk++ library for HHO https://bil.inria.fr/fr/software/view/3143/tab. The linear systems can be solved with direct solvers or with iterative solvers like the preconditioned conjugate gradient or multigrid solvers.

RELEASE FUNCTIONAL DESCRIPTION: Work in progress, no production release yet.

NEWS OF THE YEAR: NEF++ has been successfully tested on networks that contain up to 500,000 fractures. The following two direct solvers can be called: Pardiso from Intel MKL library or SuiteSparse. Both solvers support tasks parallelism, either using OpenMP or Intel TBB and support SIMD (Single Instruction, Multiple Data) vectorization. The input parameters are JSON files. The mesh data are in .vector files (see Appendix A, publication hal-00735675). The outputs are written in HDF5 files.

- Participants: Florent Hedin, Géraldine Pichot, Alexandre Ern and Nicolas Pignet
- Contact: Géraldine Pichot
- Publication: A hybrid high-order method for flow simulations in discrete fracture networks.
- URL: https://gitlab.inria.fr/nef/NEFpp

6.6. NEF-Flow-a-posteriori

KEYWORD: A posteriori error estimates

SCIENTIFIC DESCRIPTION: The a posteriori error estimates that are implemented are the ones described in the publication https://hal.archives-ouvertes.fr/hal-00019800/document.

FUNCTIONAL DESCRIPTION: Compute a posteriori estimators for diffusion problems.

NEWS OF THE YEAR: New software: implementation of the estimators, management of input files with Json.

- Participants: Géraldine Pichot and Martin Vohralík
- Contact: Géraldine Pichot
- Publication: A posteriori error estimates for lowest-order mixed finite element discretizations of convection-diffusion-reaction equations
- URL: https://gitlab.inria.fr/gpichot/nef-flow-a-posteriori

6.7. SBM

Skew Brownian Motion

KEYWORDS: Monte-Carlo methods - Skew Brownian Motion

FUNCTIONAL DESCRIPTION: SBM is a code allowing exact or approximated simulations of the Skew Brownian Motion. This code is used for the simulation, with a Monte-Carlo approach, of a 1D diffusion process with a discontinuous diffusion coefficient. Several benchmark tests are also implemented.

NEWS OF THE YEAR: - Refactoring and Cmake compilation - Automatic non regression tests on ci-inria.fr - Full documentation - Open source project on gitlab-inria

- Authors: Antoine Lejay and Géraldine Pichot
- Contact: Antoine Lejay
- Publication: Simulating diffusion processes in discontinuous media: Benchmark tests
- URL: https://gitlab.inria.fr/lejay/sbm

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

5. New Software and Platforms

5.1. 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 [15].

NEWS OF THE YEAR: In 2019 we started a refactoring of this software, together with an overhaul of the associated web service USAT-WEB.

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

5.2. 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 [21].

NEWS OF THE YEAR: In 2019 we started a complete overhaul of this software, together with a factorization of the underlying computation core (USAT).

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

5.3. LUM_OSM

Land Use Mix calculation from OpenStreepMap data

KEYWORD: Urban sprawl

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, Serge Fenet and Roger Pissard-Gibollet
- Partners: EPFL - Ecole Polytechnique Fédérale de Lausanne - LIRIS
- Contact: Peter Sturm
- URL: http://github.com/martibosch/landusemix

5.4. Comptabilité Ecologique

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

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

5.5. REDEM

REDuction Of EMission

KEYWORD: Climate change

FUNCTIONAL DESCRIPTION: REDEM soft is a tool designed for the benchmarking of national GHG emission reduction trajectories. The actual version of the software is implemented in Visual Basic under Microsoft Excel in order to facilitate handling and diffusion to climate/energy economists.

NEWS OF THE YEAR: In 2019, the database underlying REDEM was updated with recent national emission trajectory information.

- Participants: Constantin Ilasca, Hélène Benveniste, Olivier Boucher, Patrick Criqui and Roger Pissard-Gibollet
- Partners: EDDEN - IPSL
- Contact: Emmanuel Prados
- URL: http://redem.gforge.inria.fr/

5.6. REDEM web

REDEM Web

KEYWORDS: Benchmarking - Climate change - Global warming - Greenhouse gas emissions

FUNCTIONAL DESCRIPTION: Python Library of REDEM model and its web application.

- Participants: Constantin Ilasca, Emmanuel Prados, Hélène Benveniste, Nicolas Assouad, Olivier Boucher, Patrick Criqui and Roger Pissard-Gibollet
- Partners: UPMC - EDDEN
- Contact: Emmanuel Prados
- URL: http://redem.inria.fr/

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

6. New Software and Platforms

6.1. CLAC

Conservation Laws Approximation on many Cores

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

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

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

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

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

6.2. Selalib

SEmi-LAgrangian LIBrary

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

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

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

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

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

6.3. SCHNAPS

Solver for Conservative Hyperbolic Nonlinear Applications for PlasmaS

KEYWORDS: Discontinuous Galerkin - StarPU - Kinetic scheme

FUNCTIONAL DESCRIPTION: Generic systems of conservation laws. Specific models: fluids, Maxwell, Vlasov, acoustics (with kinetic representation). Multitasking with StarPU. Explicit solvers (RK2, RK3, RK4): accelerated with OpenCL Implicit solvers: through kinetic representations and palindromic time integration.

- Participants: Philippe Helluy, Matthieu Boileau and Bérenger Bramas
- Contact: Philippe Helluy
- URL: http://schnaps.gforge.inria.fr/

6.4. Slappy

KEYWORDS: Python - Opencl

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

- Contact: Emmanuel Franck

6.5. Patapon

Parallel Task in Python

KEYWORDS: Python - Parallel computing - High order time schemes

FUNCTIONAL DESCRIPTION: Patapon is a code in PyOpenCL which allows to solve PDE like MHD using the vectorial Lattice Boltzmann method on Cartesian grids.

- Participant: Philippe Helluy
- Contact: Philippe Helluy

6.6. tofu

Tomography for Fusion

KEYWORDS: 3D - Data visualization - Visualization - Magnetic fusion - Tomography - Diagnostics - Plasma physics - Ray-tracing - Python

FUNCTIONAL DESCRIPTION: tofu aims at providing the fusion and plasma community with an object-oriented, transparent and documented tool for designing tomography diagnostics, computing synthetic signal (direct problem) as well as tomographic inversions (inverse problem). It gives access to a full 3D description of the diagnostic geometry, thus reducing the impact of geometrical approximations on the direct and, most importantly, on the inverse problem.

RELEASE FUNCTIONAL DESCRIPTION: Python 2.7 is not supported anymore Python 3.6 and 3.7 are supported Several changes to try and make installation easier (on clusters, windows, mac....) and less verbose for users More explicit names for default saved configurations Major bug fix in one of the methods for computing synthetic signal Minor bug fixes in interactive figures Minor bug fixes in Plasma2D interpolation New configuration (ITER) available First version of a class handling 2D XRay bragg spectrometers First tools for magnetic field line tracing available on WEST Better documentation, more ressources More informative error messages extra tools for computing LOS length, closest point to magnetic axis... Better PEP8 compliance

- Partner: CEA
- Contact: Laura Mendoza
- URL: https://github.com/ToFuProject/tofu

BIOCORE Project-Team

6. New Software and Platforms

6.1. In@lgae

Numerical simulator of microalgae based processes

KEYWORDS: Simulation - Microalgae system - Productivity

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

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

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

6.2. Odin

Platform for advanced monitoring, control and optimisation of bioprocesses

KEYWORDS: Bioinformatics - Biotechnology - Monitoring - Automatic control

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

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

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

CARMEN Project-Team

6. New Software and Platforms

6.1. CEPS

Cardiac ElectroPhysiology Simulation

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

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

FUNCTIONAL DESCRIPTION: CEPS is a modular high-performance computing software for performing numerical simulations in cardiac electrophysiology. It is based on modules : - management of geometries represented by meshes in 3D, 2D or 1D (volumes, surfaces, trees), - model simulation of cellular electrophysiology, - calculating the tissue propagation of the action potentials in the cardiac geometries, - calculation of extracardiac potentials, - time approximation methods in order 2, 3 and 4 specific to electrocardiography.

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

6.2. OptimDBS

Optimizing the Deep Brain Stimulation

KEYWORDS: Image analysis - Deep brain stimulation - Statistical learning

FUNCTIONAL DESCRIPTION: Targeting software for deep brain stimulation

- Participants: Nejib Zemzemi, Louise-Amelie Schmitt, Emmanuel Cuny and Julien Engelhardt
- Partner: CHU de Bordeaux
- Contact: Nejib Zemzemi
- URL: https://gitlab.inria.fr/optimdbs/optimdbs-medinria/-/wikis/home

6.3. Platforms

6.3.1. CEMPACK

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

Propag-5.1   Applied modeling studies performed by the Carmen team in collaboration with IHU Liryc and foreign partners [7] [71], [60], [57], [53] rely on high-performance computations on the national supercomputers Irene, Occigen, and Turing. The Propag-5 code is optimized for these systems. It is the result of a decades-long development first at the *Université de Montréal* in Canada, then at Maastricht University in the Netherlands, and finally at the Institute of Computational Science of the *Università della Svizzera italiana* in Lugano, Switzerland. Since 2016 most of the development on Propag has been done by M. Potse at the Carmen team [72]. The code scales excellently to large core counts and, as it is controlled completely with command-line flags and configuration files, it can be used by non-programmers. It also features

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

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

Gepetto   The Gepetto suite, named after a famous model maker, transforms a surface mesh of the heart into a set of (semi-)structured meshes for use by the Propag software or others. It creates the different fiber orientations in the model, including the transmurally rotating ventricular fibers and the various bundle structures in the atria (figure 2), and creates layers with possibly different electrophysiological properties across the wall. A practically important function is that it automatically builds the matching heart and torso meshes that Propag uses to simulate potentials in the torso (at a resolution of 1 mm) after projecting simulation results from the heart model (at 0.1 to 0.2 mm) on the coarser torso mesh [68]. Like Propag, the Gepetto software results from a long-term development that started in Montreal, Canada, around 2002. The code for atrial fiber structure was developed by our team.

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

6.3.2. *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.

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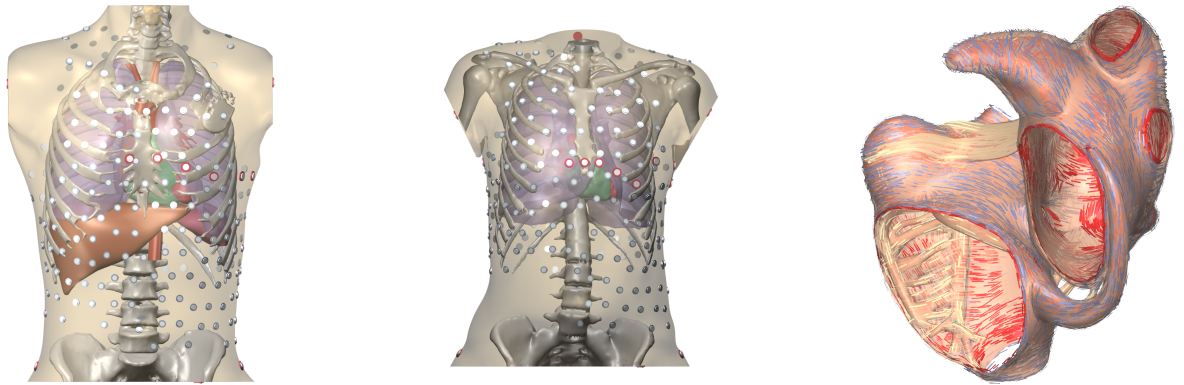
Figure 2. ***A and B:*** *Complete heart-torso geometries created with CEMPACK tools.* ***C:*** *Bundle structures and different layers of fiber orientation created by the Gepetto software.*

COMMEDIA Project-Team

6. New Software and Platforms

6.1. FELiScE

Finite Elements for Life SCiences and Engineering problems

KEYWORDS: Finite element modelling - Cardiac Electrophysiology - Cardiovascular and respiratory systems

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

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

6.2. FELiScE-NS

KEYWORDS: Incompressible flows - Thin-walled solids

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

- Participants: Benoit Fabreges, Miguel Ángel Fernández, Axel Fourmont, Jean-Frédéric Gerbeau and Marina Vidrascu
- Contact: Miguel Ángel Fernández

6.3. DCIMaL

KEYWORD: Cardiac Electrophysiology

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

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

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

M3DISIM Project-Team

5. New Software and Platforms

5.1. HeartLab

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

FUNCTIONAL DESCRIPTION: The heartLab software is a library designed to perform both simulation and estimation of the heart mechanical behavior (based on various types of measurements, e.g. images).

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

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

5.2. Verdandi

KEYWORDS: HPC - Model - Software Components - Partial differential equation

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

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

5.3. CardiacLab

KEYWORDS: Cardiovascular and respiratory systems - Matlab - Real time

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

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

5.4. MoReFEM

Modeling Research with the Finite Element Method

KEYWORDS: HPC - Multiphysics modelling - Data assimilation

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

- Participants: Philippe Moireau, Patrick Le Tallec, Antoine Olivier, Dominique Chapelle, Ustim Khristenko, François Kimmig, Gautier Bureau and Sébastien Gilles
- Contact: Sébastien Gilles
- URL: https://gitlab.inria.fr/MoReFEM

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

6. New Software and Platforms

6.1. TiQuant

Tissue Quantifier

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

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

- Author: Dirk Drasdo
- Contact: Dirk Drasdo

6.2. TiSim

Tissue Simulator

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

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

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

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

6.3. Platforms

6.3.1. TiSim

The deformable cell model [123], [52] has been integrated in addition to the center-based model in the software TiSim (Tissue Simulator), a follow-up of former CellSys [113]. Center-based models of cells represent forces between cells as forces between cell centers but lacks an explicit representation of cell shape. The deformable cell model represents cell shape explicitly. Applications are monolayers, multicellular spheroids and simulations of liver regeneration, whereby intracellular pathways can be integrated. The model shall be distributed as binary and will permit to use the deformable cell model to calibrate intercellular forces at high cell densities, where the two-body force models so far applied in center-based models fail.

6.3.2. TiQuant

This image processing and analysis software ([103]) now integrates a machine learning component. This is fundamental as it is more general and permits quicker adaptation to new images.

6. New Software and Platforms

6.1. August

Antibody Drug Uptake Simulator

KEYWORD: Mechanistic modeling

FUNCTIONAL DESCRIPTION: Numerical code to compute the uptake of an antibody drug at the scale of an histopathology blade. The computation domain (reconstructed from segmented images) is completely meshed and sub-divided accross computational nodes to distribute the load efficiently. The model (based on reaction-diffusion equations) is then solved in parallel using a domain decomposition method. C ++

- Contact: Olivier Saut

NUMED Project-Team

4. New Software and Platforms

4.1. Bingham flows

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

- Contact: Emmanuel Grenier

4.2. OptimChemo

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

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

4.3. SETIS

KEYWORDS: Health - DICOM - Medical imaging - Drug development

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

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

4.4. SIMPHYT

KEYWORDS: Bioinformatics - Cancer - Drug development

FUNCTIONAL DESCRIPTION: SimPHyt is an implementation in Python of the low grad glioma model. The aim is to predict the evolution of the glioma size of patients.

- Participant: Benjamin Ribba
- Contact: Benjamin Ribba

4.5. SITLOG

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

4.6. VAXSIMSTAB

KEYWORDS: Bioinformatics - Health - Drug development

FUNCTIONAL DESCRIPTION: VAXSIMSTAB is a modeler stability prediction of vaccine software.

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

REO Team (section vide)

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.

RELEASE FUNCTIONAL DESCRIPTION: This package has been updated so that the optimization is done in parallel and goes faster. This update has been done in collaboration Viviane Philipps and Cecile Proust-Lima from Inserm BPH

- Partner: INSERM
- 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.

RELEASE FUNCTIONAL DESCRIPTION: * add RFimplem parameter which allows to choose between randomForest, ranger and Rborist to compute random forests predictors. This can be a vector of length 3 to chose a different implementation for each step of VSURF() * update of the parallel and clusterType parameters to also give the possibility to choose which step to perform in parallel with a clusterType per step * add progress bars and information of the progress of the algorithm, and also an estimated computational time for each step

- 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/package=NPflow

6.4. COVVSURF

Combination of Clustering Of Variables and Variable Selection Using Random Forests

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

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

6.5. clogitLasso

KEYWORDS: Biostatistics - Bioinformatics - Machine learning - Regression

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

RELEASE FUNCTIONAL DESCRIPTION: Optimisation

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

6.6. TcGSA

Time-course Gene Set Analysis

KEYWORDS: Bioinformatics - Genomics

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

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

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/package=tcgsaseq

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/package=cytometree

6.10. CRTgeeDR

KEYWORDS: Missing data - Statistics - Regression

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

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

6.11. ludic

KEYWORDS: Probability - Biostatistics

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

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

6.12. CoDaPCA

KEYWORDS: Unsupervised learning - PCA

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

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

6.13. Left-censored Lasso

KEYWORDS: Biostatistics - Machine learning

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

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

- Contact: Marta Avalos Fernandez

6.14. dd-sPLS

Data-Driven Sparse PLS

KEYWORDS: Marker selection - Classification - Regression - Missing data - Multi-Block - High Dimensional Data - PLS - SVD

SCIENTIFIC DESCRIPTION: Allows to build Multi-Data-Driven Sparse PLS models. Multi-blocks with high-dimensional settings are particularly sensible to this. Whatsmore it deals with missing samples (entire lines missing per block) thanks to the Koh-Lanta algorithm. SVD decompositions permit to offer a fast and controlled method.

FUNCTIONAL DESCRIPTION: That software solves the missing samples problem selecting interesting variables under multi-block supervised settings.

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

6.15. kernscr

KEYWORDS: Genomics - Biostatistics

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

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

6.16. phenotypr

KEYWORDS: Phenotyping - Automatic labelling - Automatic Learning

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

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

6.17. R2GUESS

Graphical processing Unit Evolutionary Stochastic Search

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

- Contact: Rodolphe Thiebaut

XPOP Project-Team

6. New Software and Platforms

6.1. mlxR

KEYWORDS: Simulation - Data visualization - Clinical trial simulator

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

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

6.2. Rsmlx

R speaks Monolix

KEYWORDS: Data modeling - Nonlinear mixed effects models - Statistical modeling

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

- Partner: Lixoft
- Contact: Marc Lavielle
- URL: http://rsmlx.webpopix.org/

6.3. SPIX

KEYWORDS: Data modeling - Mass spectrometry - Chemistry

FUNCTIONAL DESCRIPTION: SPIX allows you to - automatically identify, on the basis of statistical approaches, small but significant differences in spectra measured under different conditions, - model the kinetics of entities that evolve over time

- Authors: Marc Lavielle and Yao Xu
- Partner: Laboratoire de Chimie Moléculaire - Ecole Polytechnique
- Contact: Marc Lavielle
- URL: http://spix.webpopix.org/