informatics *mathematics*

Inria

RESEARCH CENTER

FIELD
Digital Health, Biology and Earth

Activity Report 2016

Section Software

Edition: 2017-08-25

MODELING AND CONTROL FOR LIFE SCIENCES

ABS Project-Team

5. New Software and Platforms

5.1. The Structural Bioinformatics Library

5.1.1. The SBL : overview

The SBL (http://sbl.inria.fr) is a generic C++/python library providing algorithms and applications to solve complex problems in computational structural biology (CSB). [20].

For Biologists, the key advantages are:

- comprehensive in silico environment providing software applications,
- answering complex bio-physical problems (modeling interfaces and contacts, modeling the flexibility of proteins, and modeling macro-molecular assemblies),
- in a robust, fast and reproducible way.

For Developers, the striking facts are:

- broad C++/python toolbox,
- with modular design and careful specifications,
- fostering the development of complex applications.

5.1.2. The SBL : rationale and design

Software development generally faces a dichotomy, with on the one hand generic libraries providing methods of ubiquitous interest, and on the other hand application driven libraries targeting specific application areas. Libraries in the former category typically provide state-of-the art low level algorithms carefully specified, at the detriment of high level applications. Libraries in the latter category are generally high level and user-friendly, but the lack of formalism often makes it difficult to couple them to low level algorithms with formal specifications. The SBL ambitions to reconcile both software development philosophies, based on an advanced design suited for all classes of users and developers.

In terms of high-level operations, the SBL provides various applications revolving around the problem of understanding the relationship between the structure and the function of macro-molecules and their complexes (see below). In terms of low-level operations, the design of the SBL is meant to accommodate both the variety of models coding the physical and chemical properties of macro-molecular systems (models based on unions of balls such as van der Walls models or solvent accessible models, or models based on conformations and conformational ensembles), as well as the variety of operations (geometric, topological, and combinatorial) undertaken on these models.

More precisely, the SBL consists of the following software components, detailed below:

- SBL-APPLICATIONS: high level applications solving specific applied problems.
- SBL-CORE: low-level generic C++ classes templated by traits classes specifying C++ concepts [0].
- SBL-MODELS: C++ *models* matching the C++ concepts required to instantiate classes from SBL-CORE.
- SBL-MODULES: C++ classes instantiating classes from the SBL-CORE with specific biophysical models from SBL-MODELS. A module may be seen as a black box transforming an input into an output. With modules, an application workflow consists of interconnected modules.

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[0]The design has been guided by that used in the Computational Geometry Algorithm Library (CGAL), see http://www.cgal.org

5.1.3. The SBL for end-users: SBL-APPLICATIONS

End users will find in the `SBL` portable applications running on all platforms (Linux, MacOS, Windows). These applications split into the following categories:

- **Space Filling Models:** applications dealing with molecular models defined by unions of balls.
- **Conformational Analysis:** applications dealing with molecular flexibility.
- **Large assemblies:** applications dealing with macro-molecular assemblies involving from tens to hundreds of macro-molecules.
- **Data Analysis:** applications providing novel data analysis - statistical analysis tools.
- **Data Management:** applications to handle input data and results, using standard tools revolving around the XML file format (in particular the XPath query language). These tools allow automating data storage, parsing and retrieval, so that upon running calculations with applications, statistical analysis and plots are a handful of python lines away.

5.1.4. The SBL for developers: SBL-CORE, SBL-MODELS and SBL-MODULES

The `SBL` makes it easy to develop novel high-level applications, by providing high level ready to use C++ classes instantiating various biophysical models.

In particular, modules allow the development of applications without the burden of instantiating low level classes. In fact, once modules are available, designing an application merely consists of connecting modules.

5.1.5. The SBL for low-level developers and contributors: SBL-CORE, and SBL-MODELS

Low level developments may use classes from / contribute classes to `SBL-CORE` and `SBL-MODELS`. In fact, such developments are equivalent to those based upon C++ libraries such as CGAL (http://www.cgal.org/) or boost C++ libraries (http://www.boost.org/). It should be noticed that the `SBL` heavily relies on these libraries. The `SBL-CORE` is organized into four sub-sections:

- CADS : Combinatorial Algorithms and Data Structures.
- GT : Computational geometry and computational topology.
- CSB : Computational Structural Biology.
- IO : Input / Output.

It should also be stressed that these packages implement algorithms not available elsewhere, or available in a non-generic guise. Due to the modular structure of the library, should valuable implementations be made available outside the `SBL` (e.g. in CGAL or boost), a substitution may occur.

5.1.6. Interoperability

The `SBL` is interoperable with existing molecular modeling systems, at several levels:

- At the library level, our state-of-the-art algorithms (e.g. the computation of molecular surfaces and volumes) can be integrated within existing software by instantiating the required classes from `SBL-CORE`, or using the adequate modules.
- At the application level, our applications can easily be integrated within processing pipelines, since the format used for input and output are standard ones. (For input, the PDB format can always be used. For output, our applications generate XML files.)
- Finally, for visualization purposes, our applications generate outputs for the two reference molecular modeling environments, namely Visual Molecular Dynamics (http://www.ks.uiuc.edu/Research/vmd/) and Pymol (http://www.pymol.org/).

5.1.7. Releases, distribution, and license

The `SBL` is released under a proprietary open source license, see http://sbl.inria.fr/license/.

The source code is distributed from http://sbl.inria.fr, using tarballs and a git repository. Bugzilla is used to handle user's feedback and bug tracking.

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

4. New Software and Platforms

4.1. GenRGenS

GENeration of Random GENomic Sequences
KEYWORDS: Bioinformatics - Genomic sequence
FUNCTIONAL DESCRIPTION

A software dedicated to the random generation of sequences. Supports different lasses of models, including weighted context-free grammars, Markov models, ProSITE patterns..

- Participants: Yann Ponty and Alain Denise
- Contact: Yann Ponty
- URL: https://www.lri.fr/~genrgens/

4.2. VARNA

Interactive drawing and editing of the RNA secondary structure
KEYWORDS: Bioinformatics - Structural Biology
SCIENTIFIC DESCRIPTION

VARNA is Java lightweight Applet dedicated to drawing the secondary structure of RNA. It is also a Swing component that can be very easily included in an existing Java code working with RNA secondary structure to provide a fast and interactive visualization.

Being free of fancy external library dependency and/or network access, the VARNA Applet can be used as a base for a standalone applet. It looks reasonably good and scales up or down nicely to adapt to the space available on a web page, thanks to the anti-aliasing drawing primitives of Swing.
FUNCTIONAL DESCRIPTION

Varna is a new tool for the automated drawing, visualization and annotation of the secondary structure of RNA, designed as a companion software for web servers and databases.

Varna implements four drawing algorithms, supports input/output using the classic formats dbn, ct, bpseq and RNAML and exports the drawing as five picture formats, either pixel-based (JPEG, PNG) or vector-based (SVG, EPS and XFIG).

It also allows manual modification and structural annotation of the resulting drawing using either an interactive point and click approach, within a web server or through command-line arguments.

- Participants: Alain Denise and Yann Ponty
- Partners: CNRS - Ecole Polytechnique - Université Paris-Sud
- Contact: Yann Ponty
- URL: http://varna.lri.fr/

BEAGLE Project-Team

5. New Software and Platforms

5.1. DeCoSTAR

KEYWORDS: Bioinformatics - Evolution

FUNCTIONAL DESCRIPTION Given a set of gene trees, a species tree and adjacency relations between extant genes, DeCoSTAR reconstructs adjacencies between ancestral genes

- Contact: Eric Tannier
- URL: http://pbil.univ-lyon1.fr/software/DeCoSTAR/

5.2. EvoEvo

Evolution of Evolution

KEYWORDS: Bioinformatics - Biology - Evolution

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

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

5.3. FluoBacTracker

KEYWORDS: Bioinformatics - Biology - Biomedical imaging

FUNCTIONAL DESCRIPTION FluoBacTracker is an ImageJ plugin designed to segment and track growing E. Coli cells from microscopy images and movies. FluoBacTracker is a software tool to : 1) Select regions of interest in each image (detect the colony) 2) Denoise and renormalize the images 3) Identify each cells in each image (segmentation) 4) Follow cells through the whole movie (tracking) 5) Detect divisions and construct cell lineage in the population FluoBacTracker is an open-source software (under a tailored license agrement), downloadable free of charge for academics.

- Participants: Magali Vangkeosay, David Parsons and Hugues Berry
- Partner: Université Descartes
- Contact: Hugues Berry
- URL: http://fluobactracker.inrialpes.fr

5.4. Tewep

Simulator of the dynamics of Transposable Elements Within Expanding Populations

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

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

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

5.5. aevol

Artificial Evolution

FUNCTIONAL DESCRIPTION Aevol is a digital genetics model: populations of digital organisms are subjected to a process of selection and variation, which creates a Darwinian dynamics. By modifying the characteristics of selection (e.g. population size, type of environment, environmental variations) or variation (e.g. mutation rates, chromosomal rearrangement rates, types of rearrangements, horizontal transfer), one can study experimentally the impact of these parameters on the structure of the evolved organisms. In particular, since Aevol integrates a precise and realistic model of the genome, it allows for the study of structural variations of the genome (e.g. number of genes, synteny, proportion of coding sequences). The simulation platform comes along with a set of tools for analysing phylogenies and measuring many characteristics of the organisms and populations along evolution. An extension of the model (R-Aevol), integrates an explicit model of the regulation of gene expression, thus allowing for the study of the evolution of gene regulation networks.

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

5.6. evowave

KEYWORDS: Data stream - Clustering - Evolution - Wireless network

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

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

BIGS Project-Team

6. New Software and Platforms

6.1. AGH

KEYWORDS: statistical analysis, ordered trees

SCIENTIFIC DESCRIPTION

The Matlab toolbox AGH provides methods for statistical analysis of ordered trees from their Harris paths in a user-friendly environment. More precisely it allows to easily compute estimators of the relative scale of trees which share the same shape. These estimators have been introduced for Galton-Watson trees conditioned on their number of nodes but may be computed for any ordered tree. The theoretical study of these estimators is presented in the associated paper [30] which should be consulted in parallel.

FUNCTIONAL DESCRIPTION

The Matlab toolbox AGH provides methods for statistical analysis of ordered trees from their Harris paths in a user-friendly environment.

- Participants: Romain Azaïs, Alexandre Genadot, Benoît Henry
- Contact: romain.azais@inria.fr
- URL: http://agh.gforge.inria.fr

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

6. New Software and Platforms

6.1. BCALM 2

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

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

FUNCTIONAL DESCRIPTION

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

- Participants: Rayan Chikhi, Antoine Limasset and Paul Medvedev

- Contact: Rayan Chikhi

- URL: https://github.com/GATB/bcalm

6.2. NORINE

Nonribosomal peptides resource
KEYWORDS: Bioinformatics - Biotechnology - Biology - Genomics - Graph algorithmics - Chemistry - Knowledge database - Drug development - Computational biology
SCIENTIFIC DESCRIPTION

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

FUNCTIONAL DESCRIPTION

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

- Participants: Maude Pupin, Areski Flissi, Valerie Leclere, Laurent Noe, Yoann Dufresne, Juraj Michalik and Stéphane Janot

- Partners: CNRS - Institut Charles Viollette - Université Lille 1 v

- Contact: Maude Pupin

- URL: http://bioinfo.lille.inria.fr/NRP

6.3. Olo

KEYWORDS: Bioinformatics - Indexation - Sequence alignment - Biological sequences - Approximate string matching

SCIENTIFIC DESCRIPTION

Approximate string matching of short sequences in a text often starts by a filtering step. That step relies on seed searching, which are shorter than the pattern. Usually in those seeds the number of errors is constrained, to allow more efficient computations. We designed the 01*0 seeds which offer a good trade-off between the number of false positives and filtering time.

FUNCTIONAL DESCRIPTION

We applied the 01*0 seeds to the similarity search of miRNA targets in a reference genome (Bwolo software) and to the similarity search between a pre-miRNA and mature miRNAs (Piccolo software).

- Participants: Sébastien Bini, Mikaël Salson, Hélène Touzet and Christophe Vroland
- Partners: CNRS - Université Lille 1
- Contact: Helene Touzet
- URL: http://bioinfo.lifl.fr/olo/

6.4. Vidjil

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

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

SCIENTIFIC DESCRIPTION

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

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

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

FUNCTIONAL DESCRIPTION

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

- Participants: Mathieu Giraud, Mikaël Salson, Marc Duez, Ryan Herbert, Tatiana Rocher and Florian Thonier
- Partners: CHRU Lille - CNRS - Inria - Université de Lille
- Contact: Mathieu Giraud
- URL: http://www.vidjil.org

CAPSID Project-Team

6. New Software and Platforms

6.1. Hex

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

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

FUNCTIONAL DESCRIPTION Hex is an interactive protein docking and molecular superposition program. Hex understands protein and DNA structures in PDB format, and it can also read small-molecule "SDF" files. Hex will run on most Windows-XP, Linux and Mac OS X PCs. The recent versions now include CUDA support for Nvidia GPUs. On a modern workstation, docking times range from a few minutes or less when the search is constrained to known binding sites, to about half an hour for a blind global search (or just a few seconds with CUDA). On multi-processor Linux systems, docking calculation times can be reduced in almost direct proportion to the number of CPUs and GPUs used. The calculations can be accelerated by using an optional disc cache (strongly recommended) of about 1 GB of disc space.

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

6.2. Kbdock

FUNCTIONAL DESCRIPTION Database 3D protein domain-domain interactions with a web interface

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

6.3. Kpax

KEYWORDS: Bioinformatics - Structural Biology

SCIENTIFIC DESCRIPTION To align and superpose the 3D structures of protein molecules.

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

6.4. Sam

Symmetry Assembler

FUNCTIONAL DESCRIPTION To predict the three-dimentional structures of symmetrical protein complexes using spherical polar Fourier representations

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

6.5. ECDomainMiner

KEYWORDS: Protein Domain Annotation

SCIENTIFIC DESCRIPTION

EC-DomainMiner is a recommender-based approach for associating EC (Enzyme Commission) numbers with Pfam domains.

FUNCTIONAL DESCRIPTION

EC-DomainMiner uses a statistical recommender-based approach to infer EC-Pfam relationships from EC-sequence relationships that have been annotated previously in the SIFTS and Uniprot databases.

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

6.6. Platforms

6.6.1. The MBI Platform

The MBI (Modeling Biomolecular Interactions) platform (http://bioinfo.loria.fr) was established to support collaborations between Inria Nancy – Grand Est and other research teams associated with the University of Lorraine. The platform is a research node of the Institut Français de Bioinformatique (IFB), which is the French national network of bioinformatics platforms (http://www.france-bioinformatique.fr).

- Contact: Marie-Dominique Devignes

DYLISS Project-Team

6. New Software and Platforms

6.1. AskOmics

KEYWORDS: RDF - SPARQL - Querying - Graph
FUNCTIONAL DESCRIPTION

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

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

6.2. PADMet

PortAble Database for Metabolism
KEYWORDS: Bioinformatics - Toolbox - Metabolic networks - Standardization
FUNCTIONAL DESCRIPTION

The PADMet package allows conciliating genomics and metabolic network information used to produce a genome-scale constraint-based metabolic model within a database that traces all the reconstruction process steps. It allows representing the metabolic model in the form of a Wiki containing all the used/traced information. Other standard outputs are made available with the package. The main concept underlying PADMet-Package is to provide solutions that ensure the consistency, the internal standardization and the reconciliation of the information used within any workflow that combines several tools involving metabolic networks reconstruction or analysis. The PADMet package is at the core of the AuReMe workflow, dedicated to the primary reconstruction of genome-scale metabolic networks from raw data. It allows the study of organisms for which few experimental data are available. Its main feature is to undergo the reconstruction of the metabolic network by combining several heterogeneous knowledge and data sources, including the information reported by several scaffold metabolic networks for cousin species.

- Partners: CNRS - Inria - Université de Rennes 1 - University of Chile.
- Contact: Meziane Aite
- https://gitlab.inria.fr/DYLISS/padmet-toolbox

6.3. PowerGrASP

Power Graph compression in ASP
KEYWORDS: Bioinformatics - Constraint-based Programming - Data visualization - Optimization - Decomposition - Graph - Graph visualization - Pattern extraction - Answer Set Programming - Formal concept analysis
FUNCTIONAL DESCRIPTION

Implementation of graph compression methods oriented toward visualization, and based on power graph analysis. The method relies of formal concept analysis and is implemented in the declarative langage Answer Set Programming. It is applied to regulatory networks currently produced in the domain of bioinformatics.

- Participants: Lucas Bourneuf, Jacques Nicolas
- Partners: Inria - Université de Rennes 1 - INRA.
- Contact: Lucas Bourneuf
- URL: http://github.com/aluriak/powergrasp

6.4. Platforms and toolboxes

A goal of the team is to facilitate interplays between tools for biological data analysis and integration. Our tools aim at guiding the user to progressively reduce the space of models (families of sequences of genes or proteins, families of keys actors involved in a system response, dynamical models) which are compatible with both knowledge and experimental observations.

Most of our tools are developed in collaboration with the GenOuest resource and data center hosted in the IRISA laboratory, including their computer facilities [more info]. It worths considering them into larger dedicated environments to benefit from the expertise of other research groups.

- The **BioShadock** repository allows one to share the different docker containers that we are developing [website].
- The **Inria chile Mobyle portal** gathers some of the tools that were developed in collaboration with Dyliss, such as meneco, shogen and lombarde [website].
- The **bioASP portal** gather most of ASP-based python packages that we are developping in collaboration with Potsdam university [website]
- The **GenOuest galaxy portal** now provides access to most tools for integrative biology and sequence annotation (access on demand).

6.4.1. AuReMe - Tracable reconstruction of metabolic networks

The toolbox **AuReMe** allows for the **Au**tomatic **Re**construction of **Me**tabolic networks based on the combination of multiple heterogeneous data and knowledge sources. Since 2016, the workflow has been made available as a Docker image to facilitate its distribution among the scientific community [web page].

- The **Model-management PADmet module** allows conciliating genomics and metabolic network information used to produce the metabolic model within a local database that traces all the reconstruction process steps and to connect software in the pipeline. This toolbox was completly redesigned in 2016. [package]
- The **meneco python package** allows filling the gaps of a metabolic network by using a qualitative approach to elaborate the biosynthetic capacities; the problem is viewed as a combinatorial optimization problem encoded in a Answer Set Programming Problem [87] [64]. [python package].
- The **shogen python package** allows aligning genome and metabolic network to identify genome units which contain a large density of genes coding for enzymes that regulate successive reactions of metabolic pathways; the problem is also encoded with an ASP program. [62]. [python package].
- The **Manual curation assistance PADmet module** allows for curating the reported metabolic networks and modify metadata [package].
- The **Wiki-export PADmet module** enables the export of the metabolic network and its functional genomic unit as a local wiki platform allowing the user-friendly investigation of the network together with the main steps used to reconstruct it. It was developed in 2016. [package].

6.4.2. Filtering interaction networks with graph-based optimization criteria

The goal is to offer a toolbox for the reconstruction of networks from genome, literature and large-scale observation data (expression data, metabolomics...) in order to elucidate the main regulators of an observed phenotype. Most of the optimization issues are addressed with Answer Set Programming.

- The **lombarde package** enables the filtering of transcription-factor/binding-site regulatory networks with mutual information reported by the response to environmental perturbations. The high level of false-positive interactions is filters according to graph-based criteria. Knowledge about regulatory modules such as operons or the output of the shogen package can be taken into account [48][13] [web server].

- The **KeyRegulatorFinder package** allows searching key regulators of lists of molecules (like metabolites, enzymes or genes) by taking advantage of knowledge databases in cell metabolism and signaling. The complete information is transcribed into a large-scale interaction graph which is filtered to report the most significant upstream regulators of the considered list of molecules [61] [package].

- The **powerGrasp python package** provides an implementation of graph compression methods oriented toward visualization, and based on power graph analysis. [package].

- The **iggy package** enables the repairing of an interaction graph with respect to expression data. It proposes a range of different operations for altering experimental data and/or a biological network in order to re-establish their mutual consistency, an indispensable prerequisite for automated prediction. For accomplishing repair and prediction, we take advantage of the distinguished modeling and reasoning capacities of Answer Set Programming. [5] [93] [Python package][web server].

6.4.3. Caspo - Studying synchronous boolean networks

The **caspo** pipeline is dedicated to automated reasoning on logical signaling networks. The main underlying issue is that inherent experimental noise is considered, so that many different logical networks can be compatible with a set of experimental observations.

Software provides an easy to use software for the study of synchronous logical (boolean) networks. In 2016, the tool was redesigned to enhance its functionalities and integrated in a docker container to facilitate its use on any platform [86] [28] [python package and docker container].

- The **caspo-learn module** performs an automated inference of logical networks from the observed response to different perturbations (phosphoproteomics datasets). It allows for identifying admissible large-scale logic models saving a lot of efforts and without any a priori bias. It is also included in the cellNopt package [0] [7] [94].

- The **caspo-classify, predict and visualize modules** allows for classifying a family of boolean networks with respect to their input–out- put predictions [7].

- The **caspo-design module** designs experimental perturbations which would allow for an optimal discrimination of rival models in a family of boolean networks [95].

- The **caspo-control module** identifies key-players of a family of networks: it computes robust intervention strategies (i.e. inclusion minimal sets of knock-ins and knock-outs) that force a set of target species or compounds into a desired steady state [73].

- **caspo-timeseries module** have been designed by our colleagues from LRI as an extension of the caspo pipeline to take into account time-series observation datasets in the learning procedure [23] [python package and docker container].

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[0] http://www.cellnopt.org/

6.4.4. cadbiom - Building and analyzing the asynchronous dynamics of enriched logical networks

Based on Guarded transition semantic, the **cadbiom** software provides a formal framework to help the modeling of biological systems such as cell signaling network. It allows investigating synchronization events in biological networks. In 2016, the tool was integrated in a docker container in order to facilitate its use on any platform [49] [docker container][web server].

- **The cadbiom graphical interface** is useful to build and study moderate size models. It provides means for model exploration, simulation and checking. For large-scale models, the graphical interface allows to focus on specific nodes of interest.

- **The cadbiom API** allows to load a model (including large-scale ones), perform static analysis (exploration, frontier computation, statistics, and dependence graph computation) and check temporal properties on a finite horizon in the future or in the past.

- **Exploring large-scale knowledge repositories** A main feature of cadbiom is that automatic translation of the large-scale PID repository (about 10,000 curated interactions) have been automatically translated into the cadbiom formalism. Therefore, the API allows for computing the upstream regulators of any set of genes based on this large-scale repository.

6.4.5. Protomata - Expressive pattern discovery on protein sequences

Protomata is a machine learning suite for the inference of *automata* characterizing (functional) families of proteins from available sequences. Based on a new kind of alignment said partial and local, it learns precise characterizations of the families – beyond the scope of classical sequence patterns such as PSSM, Profile HMM, or Prosite Patterns – allowing to predict new family members with a high specificity.

Protomata gives access to the three main modules as stand-alone programs, which are also integrated in a single workflow *protomata-learner*:

- **Paloma** builds partial local multiple alignments;
- **Protobuild** infers automata from these alignements;
- **Protomatch and Protoalign** scan, parse and align new sequences based on the automata infered previously. This module was improved in 2016 by embedding new options to score the sequences with respect to all accepting paths (Forward score) in addition to the scoring module based on the best path (Viterbi score). More generally, we have worked on the efficiency of the automata's weighting scheme based on the state-of-the-art schemes used for profile HMMs.

The suite is completed by many tools to handle or visualize data and can be used online via a [web interface].

6.4.6. Logol - Complex pattern modelling and matching

The **Logol** toolbox is a swiss-army-knife for pattern matching on DNA/RNA/Protein sequences, using a high-level grammatical formalism to permit a large expressivity for patterns [54]. A Logol pattern consists in a complex combination of motifs (such as degenerated strings) and structures (such as imperfect stem-loop ou repeats). Compared to other specialized pattern matching tools, some of the Logol key features are the possibilities to divide a pattern description into several sub-patterns, to enable the use of ambiguous models or to permit the inclusion of negative conditions in a pattern definition. Possible fields of application are the detection of mutated binding sites [32] or stem-loop identification (e.g. in CRISPR [0] [10]) [web page].

- The **Graphical designer** allows a user to iteratively build a complex pattern based on basic graphical patterns. The associated grammar file is an export of the graphical designer. In 2015, the efficiency of the tool was improved by slight evolutions of the underlying grammar.

- The **LogolMatch** parser takes as input a biological (nucleic or amino acid) sequence and a grammar file (i.e. a pattern). It combines a grammar analyzer, a sequence analyzer and a prolog Library. It returns a file containing all the occurrences of the pattern in the sequence with their parsing details.

- Full genome analysis, and connection to biological databases have been made available recently.

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[0]http://crispi.genouest.org/

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

5. New Software and Platforms

5.1. AcypiCyc

FUNCTIONAL DESCRIPTION

Database of the metabolic network of *Acyrthosiphon pisum*.

- Participants: Patrice Baa Puyoule, Hubert Charles, Stefano Colella, Ludovic Cottret, Marie-France Sagot, Augusto Vellozo and Amélie Veron
- Contact: Hubert Charles
- URL: http://acypicyc.cycadsys.org/

5.2. AlViE

FUNCTIONAL DESCRIPTION

ALVIE is a post-mortem algorithm visualisation Java environment, which is based on the interesting event paradigm. The current distribution of ALVIE includes more than forty visualisations. Almost all visualisations include the representation of the corresponding algorithm C-like pseudo-code. The ALVIE distribution allows a programmer to develop new algorithms with their corresponding visualisation: the included Java class library, indeed, makes the creation of a visualisation quite an easy task (once the interesting events have been identified).

- Participants: Pierluigi Crescenzi, Giorgio Gambosi, Roberto Grossi, Carlo Nocentini, Tommaso Papini, Walter Verdese
- Contact: Pierluigi Crescenzi
- URL: http://javamm.sourceforge.net/piluc/software/alvie.html

5.3. Cassis

FUNCTIONAL DESCRIPTION

Algorithm for precisely detecting genomic rearrangement breakpoints.

- Participants: Christian Baudet, Christian Gautier, Claire Lemaitre, Marie-France Sagot, Eric Tannier
- Contact: Christian Baudet (not Inria), Claire Lemaitre (Inria GenScale), Marie-France Sagot (Inria ERABLE)
- URL: http://pbil.univ-lyon1.fr/software/Cassis/

5.4. Cidane

FUNCTIONAL DESCRIPTION

CIDANE is a novel framework for genome-based transcript reconstruction and quantification from RNA-seq reads.

- Participants: Stefan Canzar, Sandra Andreotti, David Weese, Kurt Reinert, Gunnar Klau
- Contact: Stefan Canzar (not Inria)
- URL: http://ccb.jhu.edu/software/cidane/

5.5. Coala

FUNCTIONAL DESCRIPTION

COALA stands for "CO-evolution Assessment by a Likelihood-free Approach". It is thus a likelihood-free method for the co-phylogeny reconstruction problem which is based on an Approximative Bayesian Computation (ABC).

- Participants: Christian Baudet, Pierluigi Crescenzi, Beatrice Donati, Christian Gautier, Catherine Matias, Marie-France Sagot, Blerina Sinaimeri
- Contact: Christian Baudet (not Inria), Marie-France Sagot and Blerina Sinaimeri
- URL: http://coala.gforge.inria.fr/

5.6. CophyTrees

FUNCTIONAL DESCRIPTION

COPHYTREES is a visualiser for host-parasite and gene-species trees evolution.

- Participants: Laurent Bulteau
- Contact: Laurent Bulteau (not Inria), Blerina Sinaimeri (for Inria ERABLE)
- URL: http://eucalypt.gforge.inria.fr/viewer.html

5.7. C3Part & Isofun

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. It is based on the notion of "common connected components" between graphs.

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

5.8. CycADS

FUNCTIONAL DESCRIPTION

Cyc annotation database system.

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

5.9. Dinghy

FUNCTIONAL DESCRIPTION

DINGHY is a visualisation program for network pathways of up to 150 reactions.

- Participants: Laurent Bulteau, Alice Julien-Laferrière, Delphine Parrot
- Contact: Laurent Bulteau (not Inria), Alice Julien-Laferrière, Delphine Parrot (not Inria), Marie-France Sagot (for Inria ERABLE)
- URL: http://dinghy.gforge.inria.fr/

5.10. Eucalypt

FUNCTIONAL DESCRIPTION

EUCALYPT stands for "EnUmerator of Co-evolutionary Associations in PoLYnomial-Time delay". It is an algorithm for enumerating all optimal (possibly time-unfeasible) mappings of a parasite tree unto a host tree.

- Participants: Christian Baudet, Pierluigi Crescenzi, Beatrice Donati, Marie-France Sagot, Blerina Sinaimeri
- Contact: Christian Baudet (not Inria), Beatrice Donati (not Inria), and Marie-France Sagot (Inria ERABLE)
- URL: http://eucalypt.gforge.inria.fr/index.html

5.11. Gobbolino & Touché

FUNCTIONAL DESCRIPTION

GOBBOLINO and TOUCHÉ were 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. Biologically, stories correspond to alternative metabolic pathways that may explain some stress that affected the metabolites corresponding to the black nodes by changing their concentration (measured by metabolomics experiments).

- Participants: Vicente Acuña, Etienne Birmelé, Ludovic Cottret, Pierluigi Crescenzi, Fabien Jourdan, Vincent Lacroix, Alberto Marchetti-Spaccamela, Andrea Marino, Paulo Vieira Milreu, Marie-France Sagot, Leen Stougie
- Contact: Paulo Vieira Milreu (not Inria), Marie-France Sagot (Inria ERABLE)
- URL: http://gforge.inria.fr/projects/gobbolino

5.12. HapCol

FUNCTIONAL DESCRIPTION

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

- Participants: Paola Bonizzoni, Riccardo Dondi, Gunnar Klau, Yuri Pirola, Nadia Pisanti, Simone Zaccaria
- Contact: Gunnar Klau, Nadia Pisanti, Paola Bonizzoni (not Inria)
- URL: http://hapcol.algolab.eu/

5.13. KisSNP & DiscoSNP

FUNCTIONAL DESCRIPTION

Algorithm for identifying SNPs without a reference genome by comparing raw reads. KISSNP has now given birth to DISCOSNP in a work involving V. Lacroix from ERABLE and the GenScale Inria Team at Rennes (contact: pierre.peterlongo@inria.fr).

- Participants: Vincent Lacroix, Pierre Peterlongo
- Contact: Pierre Peterlongo (EPI GenScale)
- URL: http://colibread.inria.fr/software/discosnp/

5.14. KisSplice

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.

- Participants: Lilia Brinza, Alice Julien-Laferrière, Janice Kielbassa, Vincent Lacroix, Leandro Ishi Soares de Lima, Camille Marchet, Vincent Miele, Gustavo Sacomoto
- Contact: Vincent Lacroix
- URL: http://kissplice.prabi.fr/

5.15. kissDE

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 NGS data pre-processing and gives as output a list of condition specific variants.

- Participants: Clara Benoit-Pilven, Lilia Brinza, Janice Kielbassa, Vincent Lacroix, Camille Marchet and Vincent Miele
- Contact: Vincent Lacroix
- URL: http://kissplice.prabi.fr/tools/kissDE/

5.16. KisSplice2RefTranscriptome

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 RNAseq data only, we obtain a list of condition-specific SNPs stratified by functional impact.

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

5.17. KisSplice2RefGenome

FUNCTIONAL DESCRIPTION

KISSPLICE (see above) identifies variations in RNAseq data, without a reference genome. In many applications however, a reference genome is available. KISSPLICE2REFGENOME enables to facilitate the interpretation of KISSPLICE's results after mapping them to a reference genome.

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

5.18. Lasagne

FUNCTIONAL DESCRIPTION

LASAGNE is a Java application which allows the user to compute distance measures on graphs by making a clever use either of the breadth-first search or of the Dijkstra algorithm. In particular, the current version of LASAGNE can compute the exact value of the diameter of a graph: the graph can be directed or undirected and it can be weighted or unweighted. Moreover, LASAGNE can compute an approximation of the distance distribution of an undirected unweighted graph. These two features are integrated within a graphical user interface along with other features, such as computing the maximum (strongly) connected component of a graph.

- Participants: Pierluigi Crescenzi, Roberto Grossi, Michel Habib, Claudio Imbrenda, Leonardo Lanzi, Andrea Marino
- Contact: Pierluigi Crescenzi
- URL: http://lasagne-unifi.sourceforge.net/

5.19. MeDuSa

FUNCTIONAL DESCRIPTION

MEDUSA (Multi-Draft based Scaffolder) is an algorithm for genome scaffolding. It exploits information obtained from a set of (draft or closed) genomes from related organisms to determine the correct order and orientation of the contigs.

- Participants: Emmanuelle Bosi, Sara Brunetti, Pierluigi Crescenzi, Beatrice Donati, Renato Fani, Marco Fondi, Marco Galardini, Pietro Lió, Marie-France Sagot,
- Contact: Pierluigi Crescenzi, Marco Fondi (not Inria)
- URL: http://combo.dbe.unifi.it/medusa

5.20. MetExplore

FUNCTIONAL DESCRIPTION

Web server to link metabolomic experiments and genome-scale metabolic networks.

- Participants: Michael Barrett, Hubert Charles, Ludovic Cottret, Fabien Jourdan, Marie-France Sagot, Florence Vinson, David Wildridge
- Contact: Fabien Jourdan (not Inria), Marie-France Sagot
- URL: http://metexplore.toulouse.inra.fr/metexplore/

5.21. Migal

FUNCTIONAL DESCRIPTION

Algorithm for comparing RNA structures.

- Participants: Julien Allali and Marie-France Sagot
- Contact: Marie-France Sagot
- URL: http://www-igm.univ-mlv.fr/~allali/logiciels/index.en.php

5.22. Mirinho

FUNCTIONAL DESCRIPTION

Predicts, at a genome-wide scale, microRNA candidates.

- Participants: Christian Gautier, Cyril Fournier, Christine Gaspin, Susan Higashi, Marie-France Sagot
- Contact: Susan Higashi (not Inria), Marie-France Sagot
- URL: http://mirinho.gforge.inria.fr/

5.23. Motus & MotusWEB

FUNCTIONAL DESCRIPTION

Algorithm for searching and inferring coloured motifs in metabolic networks (web-based version - offers different functionalities from the downloadable version).

- Participants: Ludovic Cottret, Fabien Jourdan, Vincent Lacroix, Odile Rogier and Marie-France Sagot
- Contact: Vincent Lacroix
- URL: http://doua.prabi.fr/software/motus and http://pbil.univ-lyon1.fr/software/motus_web/

5.24. MultiPus

FUNCTIONAL DESCRIPTION

MULTIPUS (for MULTIple species for the synthetic Production of Useful biochemical Substances) is an algorithm that, given a microbial consortium given 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: Laurent Bulteau, Alice Julien-Laferrière, Arnaud Mary, Alberto Marchetti-Spaccamela, Delphine Parrot, Marie-France Sagot, Leen Stougie and Susana Vinga
- Contact: Alice Julien-Laferrière, Arnaud Mary, Marie-France Sagot
- URL: http://multipus.gforge.inria.fr/

5.25. PepLine

FUNCTIONAL DESCRIPTION

Pipeline for the high-throughput analysis of proteomic data.

- Participants: Jérôme Garin, Alain Viari
- Contact: Alain Viari
- URL: Available upon request to the contact person

5.26. Pitufo and family

FUNCTIONAL DESCRIPTION

Algorithms to enumerate all minimal sets of precursors of target compounds in a metabolic network.

- Participants: Vicente Acuña Aguayo, Ludovic Cottret, Alberto Marchetti-Spaccamela, Fabio Henrique Viduani Martinez, Paulo Vieira Milreu, Marie-France Sagot, Leen Stougie
- Contact: Paulo Vieira Milreu (not Inria), Marie-France Sagot
- URL: https://sites.google.com/site/pitufosoftware/home

5.27. RepSeek

FUNCTIONAL DESCRIPTION

Finding approximate repeats in large DNA sequences.

- Participants: Guillaume Achaz, Eric Coissac, Alain Viari
- Contact: Guillaume Achaz (not Inria), Alain Viari
- URL: http://wwwabi.snv.jussieu.fr/public/RepSeek/

5.28. Rime

FUNCTIONAL DESCRIPTION

RIME detects long similar fragments occurring at least twice in a set of biological sequences.

- Participants: Maria Federico, Pierre Peterlongo, Nadia Pisanti, Marie-France Sagot
- Contact: Maria Federico (not Inria), Nadia Pisanti, Marie-France Sagot
- URL: https://code.google.com/p/repeat-identification-rime/

5.29. Sasita

FUNCTIONAL DESCRIPTION

SASITA is a software for the exhaustive enumeration of minimal stoichiometrically valid precursor sets in metabolic networks.

- Participants: Vicente Acuña, Ricardo Andrade, Alberto Marchetti-Spaccamela, Marie-France Sagot, Leen Stougie, Martin Wannagat
- Contact: Marie-France Sagot, Ricardo Andrade, Martin Wannagat
- URL: http://sasita.gforge.inria.fr/

5.30. Smile

FUNCTIONAL DESCRIPTION

Motif inference algorithm taking as input a set of biological sequences. A visualiser is currently being developed.

- Participants: Ricardo Andrade (visualiser), Mariana Ferrarini (visualiser), Laurent Marsan, Marie-France Sagot
- Contact: Ricardo Andrade, Marie-France Sagot
- URL: Soon available

5.31. Totoro & Kotoura

FUNCTIONAL DESCRIPTION

We proposed two methods to decipher the reaction changes during a metabolic transient state using measurements of metabolic concentrations. We called these *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.

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: Ricardo Andrade, Laurent Bulteau, Louis Duchemin, Alice Julien-Laferrière, Alberto Marchetti-Spaccamela, Arnaud Mary, Vincent Lacroix, Marie-France Sagot, Leen Stougie, Philippe Veber, Susana Vinga
- Contact: Alice Julien-Laferrière, Arnaud Mary, Ricardo Andrade, Marie-France Sagot
- URL: http://hyperstories.gforge.inria.fr/

5.32. WhatsHap and pWhatsHap

FUNCTIONAL DESCRIPTION

WHATSHAP is a DP approach for haplotype assembly from long reads that works until 20x coverage, solves the minimum error correction problem exactly. pWHATSHAP is a parallelisation of the core dynamic programming algorithm of WHATSHAP done by M. Aldinucci, A. Bracciali, T. Marschall, M. Patterson, N. Pisanti, and M. Torquati.

- Participants: Gunnar Klau, Tobias Marschall, Murray Patterson, Nadia Pisanti, Alexander Schönhuth, Leen Stougie, Leo van Iersel

- Contact: Alexander Schönhuth (not Inria), Gunnar Klau, Nadia Pisanti

- URL: https://bitbucket.org/whatshap/whatshap   and   https://bitbucket.org/whatshap/whatshap/branch/parallel

GENSCALE Project-Team

6. New Software and Platforms

6.1. AskOmics

KEYWORDS: RDF - SPARQL - Querying - Graph
FUNCTIONAL DESCRIPTION

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

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

6.2. BBhash

Basic binary representation of successive hash
KEYWORDS: C++ - Indexation - Data structures
FUNCTIONAL DESCRIPTION

BBHash is a simple library for building minimal perfect hash function. Given a set of N input keys, it will compute a bijective function that will associate to each key an integer between 1 and N. This then allows to create an indexed array that will hold some data for each key. It is designed to handle large scale datasets (hundred billion and more elements). The function itself is just a little bit larger than other state-of-the-art libraries, it takes approximately 3 bits / elements (compared to 2.62 bits/elem for the emphf lib), but construction is faster and does not require additional memory.

- Participants: Guillaume Rizk, Pierre Peterlongo, Rayan Chikhi and Antoine Limasset
- Contact: Guillaume Rizk
- URL: https://github.com/rizkg/BBHash

6.3. BCALM 2

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

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

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

- Participants: Rayan Chikhi, Antoine Limasset and Paul Medvedev
- Contact: Rayan Chikhi
- URL: https://github.com/GATB/bcalm

6.4. BGREAT

De bruijn graph read alignment tool
KEYWORDS: Short reads - Genome assembling
FUNCTIONAL DESCRIPTION

Mapping genomic extracts (reads) on genomic references is a central and necessary task in most genomic studies. But reference sequences are mainly extracted from assembly graphs through an inexact process that both creates chimeras and losses biological pieces of information. This motivates the need of mapping sequences on references represented by graphs. BGREAT is conceived to map reads on de Bruijn graph, a widely used graph in genome assembly.

- Participants: Pierre Peterlongo and Antoine Limasset
- Contact: Pierre Peterlongo
- URL: https://github.com/Malfoy/BGREAT

6.5. GATB-Core

Genome Assembly and Analysis Tool Box
KEYWORDS: Bioinformatics - NGS - Genomics - Genome assembling
FUNCTIONAL DESCRIPTION

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

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

6.6. GATB-Core Tutorial

Online GATB-Core tutorial
KEYWORD: Bioinformatics
FUNCTIONAL DESCRIPTION

"GATB-Core tutorial" is an interactive learning tool that aims at learning software development relying on the bioinformatics toolkit GATB-Core without the need of installing it, its dependencies and a C++ compiler. The tutorial relies on a client-server system. The client is simply a web browser running a full-featured C++ code editor. In turns, it is embedded in templates for the purpose of displaying various lessons. The server side is a Linux-based VM capable of compiling and running "online" any C++ code snippets using GATB-Core. That VM is deployed on Inria's Al|Go SaaS platform.

- Participant: Patrick Durand
- Contact: Patrick Durand
- URL: http://gatb-core.gforge.inria.fr/training/

6.7. MindTheGap

KEYWORDS: Bioinformatics - NGS - Genome assembling
FUNCTIONAL DESCRIPTION

MindTheGap performs detection and assembly of DNA insertion variants in NGS read datasets with respect to a reference genome. It is designed to call insertions of any size, whether they are novel or duplicated, homozygous or heterozygous in the donor genome. The main algorithmic improvement of version 2.0.0 is to detect additionnal variants, such as SNPs and deletions. This feature improves the sensitivity of the insertion detection algorithm for insertions that are located near these other variants. Additionnally, MindTheGap performs de novo assembly using the de Bruijn graph implementation of GATB. Hence, the computational resources required to run MindTheGap are significantly lower than that of other assemblers.

- Participants: Claire Lemaitre and Guillaume Rizk
- Contact: Claire Lemaitre
- URL: https://gatb.inria.fr/software/mind-the-gap/

6.8. PLAST

Local alignment tool
KEYWORDS: Bioinformatics - Genomic sequence - Genomics
FUNCTIONAL DESCRIPTION

PLAST is a parallel alignment search tool for comparing large protein banks.

Sequence similarity searching is an important and challenging task in molecular biology and next-generation sequencing should further strengthen the need for faster algorithms to process such huge amount of data. At the same time, the internal architecture of current microprocessors is tending towards more parallelism, leading to the use of chips with two, four and more cores integrated on the same die. The main purpose of this work was to design an effective algorithm to fit with the parallel capabilities of modern microprocessors. A parallel algorithm for comparing large genomic banks and targeting middle-range computers has been developed and implemented in PLAST software. The algorithm exploits two key parallel features of existing and future microprocessors: the SIMD programming model (SSE instruction set) and the multithreading concept (multicore). Compared to multithreaded BLAST software, tests performed on an 8-processor server have shown speedup ranging from 3 to 6 with a similar level of accuracy.

- Participants: Dominique Lavenier, Erwan Drezen and Van Hoa Nguyen
- Contact: Dominique Lavenier
- URL: https://team.inria.fr/genscale/high-throughput-sequence-analysis/plast-intensive-sequence-comparison/

6.9. 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.

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

6.10. short read connector

KEYWORDS: Bioinformatics - Genomics - Metagenomics
SCIENTIFIC DESCRIPTION

Short read connector enables the comparisons of two read sets B and Q. For each read from Q it provides either:

The number of occurrences of each k-mers of the read in the set B (SRC_counter) or A list of reads from B that share enough k-mers with the tested read from B (SRC_linker)
FUNCTIONAL DESCRIPTION

This tool uses a data structure (BBHASH) adapted to the indexing of big data. Short Read Connector works on reads, which are sequencing data from high-throughput sequencers. Once the data is indexed, short read connector makes it possible either to find the similar reads in a dataset or to simply retrieve the approximate number of these similar reads.

- Participants: Pierre Peterlongo, Camille Marchet and Antoine Limasset
- Partner: UPMC
- Contact: Pierre Peterlongo
- URL: https://github.com/pierrepeterlongo/short_read_connector

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

5. New Software and Platforms

5.1. Genetic Network Analyzer (GNA)

KEYWORDS: Bioinformatics - Gene regulatory networks - Qualitative simulation - Model checking
GENETIC NETWORK ANALYZER (GNA) is a tool for the qualitative modeling and simulation of gene regulatory networks developed in the IBIS project. 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. GNA is currently distributed by the company Genostar, but remains freely available for academic research purposes. The current version is GNA 8.7.2. In comparison with the previously distributed versions, GNA 8.7.2 has the following additional functionalities: (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.

- Participants: Hidde de Jong, Michel Page, François Rechenmann
- Partners: Genostar, Université Grenoble Alpes
- Contact: Hidde de Jong
- URL: http://www-helix.inrialpes.fr/gna

5.2. WellFARE

KEYWORDS: Bioinformatics - Statistics - Data visualization - Data modeling
WELLFARE is a Python library implementing linear inversion methods for the reconstruction of gene expression profiles from fluorescent or luminescent reporter gene data. 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.

- Participants: Johannes Geiselmann, Hidde de Jong, Yannick Martin, Michel Page, Delphine Ropers, Valentin Zulkower
- Partners: Université Grenoble Alpes
- Contact: Hidde de Jong
- URL: https://github.com/ibis-inria/wellfare

5.3. WellInverter

KEYWORDS: Bioinformatics - Statistics - Data visualization - Data modeling

WELLINVERTER is a web application that implements linear inversion methods for the reconstruction of gene expression profiles from fluorescent or luminescent reporter gene data. 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.

- Participants: Johannes Geiselmann, Hidde de Jong, Yannick Martin, Michel Page, Delphine Ropers, Valentin Zulkower
- Partners: Université Grenoble Alpes
- Contact: Hidde de Jong
- URL: https://team.inria.fr/ibis/wellinverter/

5.4. WellReader

WELLREADER is a program for the analysis of gene expression data obtained by means of fluorescent and luminescent reporter genes. WELLREADER reads data files in an XML format or in a format produced by microplate readers, and allows the user to detect outliers, perform background corrections and spline fits, compute promoter activities and protein concentrations, and compare expression profiles across different conditions. WELLREADER has been written in MATLAB and is available under an LGPL licence, both as source code (M files) and compiled code (platform-specific binary files).

- Participants: Johannes Geiselmann, Hidde de Jong, Michel Page, Delphine Ropers
- Partners: Université Grenoble Alpes
- Contact: Hidde de Jong
- URL: http://ibis.inrialpes.fr/article957.html

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 and analyzing biochemical reaction systems, performing static analyses, making simulations, specifying behaviors in temporal logic and searching parameter values in high dimension.

This year BIOCHAM has been completely rewritten with a modular architecture. The new version v4.0 will be released soon with new features for synthesizing biochemical reaction systems from input/output function specifications.

- Participants: François Fages, Guillaume Le Guludec, Thierry Martinez Sylvain Soliman
- Contact: François Fages
- URL: http://lifeware.inria.fr/biocham/

6.2. CellStar

KEYWORDS: Systems biology - Bioinformatics
FUNCTIONAL DESCRIPTION

In close collaboration with Kirill Batmanov, Cédric Lhoussaine and Cristian Versari (LIFL, CNRS/Lille Univ), with Szymon Stoma (Inria; now ETHZ), and with Pascal Hersen (MSC, CNRS/Paris7), we developed CellStar, a tool-chain for image processing and analysis dedicated to segmentation and tracking of yeast cells in brightfield time-lapse microscopy movies. To estimate algorithm quality we developed a benchmark made of manually-verified images illustrating various situations. On this benchmark, CellStar outperformed 5 other state-of-the-art tools. The tool-chain is implemented in Matlab and is provided together with the Python Yeast Image Toolkit benchmark tool.

- Participants: Pascal Hersen, Grégory Batt, Artémis Llamosi and Szymon Stoma
- Contact: Grégory Batt
- URL: http://cellstar-algorithm.org/

6.3. CLP2Zinc

KEYWORDS: Modeling language - Constraint programming - Search
FUNCTIONAL DESCRIPTION

CLP2Zinc is a rule-based modeling language for constraint programming. It extends the MiniZinc modeling language with Horn clauses which can be used to express search strategies as constraints in the model. This system was developed in the framework of the ANR Net-WMS-2 project and is a follow-up of the Rules2CP modeling language.

- Participants: Thierry Martinez, François Fages and Sylvain Soliman
- Contact: Thierry Martinez
- URL: http://lifeware.inria.fr/~tmartine/clp2zinc/

MORPHEME Project-Team

4. New Software and Platforms

4.1. SPADE: Small PArticle DEtection

FUNCTIONAL DESCRIPTION SPADE is an algorithm primarily designed to detect objects whose size is smaller than a few pixels (particles) on fluorescence microscopy images. It is a simplified version of a marked point process based on a shape dictionnary.

- Participants: N. Cedilnik, E. Debreuve, and X. Descombes
- Contact: Xavier Descombes

<div align="center">**PLEIADE Team**</div>

6. New Software and Platforms

6.1. Magus

KEYWORDS: Bioinformatics - Genomic sequence - Knowledge database
FUNCTIONAL DESCRIPTION

Comparative genomics requires efficient and scalable tools for managing knowledge about genomes, genes, and the high-dimensional relations between them.

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.
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.

- Participants: David Sherman, Pascal Durrens
- Partners: CNRS - INRA - Université de Bordeaux
- Contact: David James Sherman
- URL: http://magus.gforge.inria.fr

6.2. Mimoza

KEYWORDS: Systems Biology - Bioinformatics - Biotechnology
FUNCTIONAL DESCRIPTION

Mimoza uses metabolic model generalization and cartographic paradigms to allow human experts to explore a metabolic model in a hierarchical manner. 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 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. The resulting map can be explored on-line, or downloaded in a COMBINE archive.

- Participants: Anna Zhukova and David James Sherman
- Contact: David James Sherman
- URL: http://mimoza.bordeaux.inria.fr/

6.3. Pantograph

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

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

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

- Participants: Nicolas Loira, Anna Zhukova, David James Sherman and Pascal Durrens
- Partner: University of Chile
- Contact: Nicolas Loira
- URL: http://pathtastic.gforge.inria.fr/

6.4. BioRica

KEYWORDS: Systems Biology - Bioinformatics - Hierarchical models - Hybrid models - Stochastic models
FUNCTIONAL DESCRIPTION

BioRica is used to mathematically describe the behavior of complex biological systems.

It is a software platform that permits simulation of biological systems on the basis of their description. It allows one to reuse existing biological models and to combine them into more complex models.

- Partner: University of Chile
- Contact: David Sherman
- URL: http://biorica.gforge.inria.fr/

6.5. Declic

Metabarcoding relies on mapping large sets of reads on reliable databases, with taxonomically annotated sequences. Declic facilitates data analyses for metabarcoding.

FUNCTIONAL DESCRIPTION

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

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

- Partner: INRA
- Contact: Alain Franc

6.6. Platforms

6.6.1. Plafrim

Plafrim (http://plafrim.fr) is an essential instrument for PLEIADE. We use it for developing software data analysis methods and evaluating them at real world scale. The platform combines considerable computing power with excellent support, both in terms of the quality of the interactions with the local staff and of the ease of large-scale data transfer between Plafrim and PLEIADE's data storage infrastructure. Plafrim facilitates collaboration between team members who are not in the Bordeaux Sud-Ouest building, and furthermore allows us to share best practices and tools with other teams from the Center.

6.6.2. Inria forge and Inria continuous integration

The Inria forge (http://gforge.inria.fr) provides a secure collaboration platform for software project administration and source code management, and Inria's continuous integration platform (http://ci.inria.fr) provides a cloud-based service for automatic compilation and testing of software systems. PLEIADE uses these two services extensively for agile software development. The continuous integration platform allows us to verify the correct operation of our methods in different operating system and deployment environments.

6.6.3. Team Platform

PLEIADE maintains a dedicated computing platform for software development and experimentation by the team, comprised of a private cloud, storage, and a Project Atomic cluster for hosting Docker containers

SERPICO Project-Team

6. New Software and Platforms

6.1. TMA-Lib

KEYWORD: Biomedical imaging

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

- **Participants**: Hoai Nam Nguyen, Charles Kervrann.
- **Partner:** INNOPSYS Company.
- **Contact:** Charles Kervrann.
- **Languages:** C/C++, Matlab.

6.2. QuantEv

KEYWORD: Biomedical imaging

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

- **Participants**: Thierry Pécot, Charles Kervrann, Jean Salamero.
- **Contact:** Thierry Pécot, Charles Kervrann.
- **On-line demo:** http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::...
- **Languages:** C/C++ and JAVA (plug-in ICY: http://icy.bioimageanalysis.org).

6.3. C-CRAFT

KEYWORD: Biomedical imaging

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

- **Participants**: Thierry Pécot, Charles Kervrann, Patrick Bouthemy, Jean Salamero.
- **Contact:** Thierry Pécot, Charles Kervrann.
- **On-line demo:** http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::C-CRAFT
- **Languages:** C/C++ and JAVA (plug-in ICY: http://icy.bioimageanalysis.org/plugin/C-CRAFT).
- **Reference:** [12]

6.4. ATLAS

KEYWORD: Biomedical imaging

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

- **Participants**: Antoine Basset, Patrick Bouthemy, Thierry Pécot, Charles Kervrann.
- **Contact:** Thierry Pécot, Patrick Bouthemy, Charles Kervrann.
- **On-line demo:** http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::ATLAS
- **Language:** C/C++.
- **Reference:** [1]

6.5. Hullkground

KEYWORDS: Bioinformatics - Biomedical imaging

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

- **Participants:** Anatole Chessel, Jean Salamero, Charles Kervrann.
- **Contact:** Charles Kervrann.
- **APP deposit number:** IDDN.FR.001.400005.000.S.P.2009.000.21000
- **On-line demo:** http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::Hullkground
- **Free distribution:** http://serpico.rennes.inria.fr/doku.php?id=software:hullkground:hullkground
- **Language:** JAVA (plug-in IMAGEJ: http://rsbweb.nih.gov/ij/).

6.6. Motion2D

KEYWORDS: Image sequence - Motion model - 2D

FUNCTIONAL DESCRIPTION: The MOTION2D software is a multi-platform object-oriented library to estimate 2D parametric motion models in an image sequence. It can handle several types of motion models, namely, constant (translation), affine, and quadratic models. Moreover, it includes the possibility of accounting for a global variation of illumination and more recently for temporal image intensity decay (e.g. due to photo-bleaching decay in fluorescence microscopy). The use of such motion models has been proved adequate and efficient for solving problems such as optic flow computation, motion segmentation, detection of independent moving objects, object tracking, or camera motion estimation, and in numerous application domains (video surveillance, visual servoing for robots, video coding, video indexing), including biological imaging (image stack registration, motion compensation in videomicroscopy). Motion2D is an extended and optimized implementation of the robust, multi-resolution and incremental estimation method (exploiting only the spatio-temporal derivatives of the image intensity function). Real-time processing is achievable for motion models involving up to six parameters. Motion2D can be applied to the entire image or to any pre-defined window or region in the image.

- **Participants:** Patrick Bouthemy, Jean-Marc Odobez, Fabien Spindler.
- **Contact:** Patrick Bouthemy, Fabien Spindler.
- **APP deposit number:** FR.001.520021.001.S.A.1998.000.21000 / release 1.3.11, January 2005)
- **Free academic software distribution:** http://www.irisa.fr/vista/Motion2D
- **On-line demo:** http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::Motion2D
- **Languages:** C/C++ and JAVA (plug-in IMAGEJ: http://rsbweb.nih.gov/ij/).

6.7. ND-SAFIR

KEYWORDS: Biology - Health - Image analysis - Photonic imaging - Fluorescence microscopy - Biomedical imaging

SCIENTIFIC DESCRIPTION: The ND-SAFIR software removes additive Gaussian and non-Gaussian noise in still 2D or 3D images or in 2D or 3D image sequences (without any motion computation) [5]. The method is unsupervised and is based on a pointwise selection of small image patches of fixed size (a data-driven adapted way) in spatial or space-time neighbourhood of each pixel (or voxel). The main idea is to modify each pixel (or voxel) using the weighted sum of intensities within an adaptive 2D or 3D (or 2D or 3D + time) neighbourhood and to use image patches to take into account complex spatial interactions. The neighbourhood size is selected at each spatial or space-time position according to a bias-variance criterion. The algorithm requires no tuning of control parameters (already calibrated with statistical arguments) and no library of image patches. The method has been applied to real noisy images (old photographs, JPEG-coded images, videos, ...) and is exploited in different biomedical application domains (time-lapse fluorescence microscopy, video-microscopy, MRI imagery, X-ray imagery, ultrasound imagery, ...).

- **Participants:** Jérôme Boulanger, Charles Kervrann, Patrick Bouthemy, Jean Salamero.
- **Partners:** INRA, PiCT - CNRS - Institut Curie.
- **APP deposit number:** IDDN.FR.001.190033.002.S.A.2007.000.21000 / new release 3.0 in 2013)
- **Free academic software distribution:** Binaries of the software ND-SAFIR are freely and electronically distributed (http://serpico.rennes.inria.fr/doku.php?id=software:nd-safir:index).
- **On-line demo:** http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::NDSafir
- **Languages:** C/C++, MATLAB and JAVA (plug-in IMAGEJ: http://rsbweb.nih.gov/ij/). The C/C++ software has been developed under Linux using the CImg library and has been tested over several platforms such as Linux/Unix, Windows XP and Mac OS.
- **Commercial licence agreements:** Innopsys, Roper Scientfic, Photmetrics, Nikon Europe BV (2016).
- **Reference:** [5]

6.8. F2D-SAFIR

KEYWORD: Biomedical imaging

FUNCTIONAL DESCRIPTION: The F2D -SAFIR software removes mixed Gaussian-Poisson noise in large 2D images, typically $10^3 \times 10^3$ pixels, in a few seconds. The method is unsupervised and is a simplified version of the method related to the ND-SAFIR software. The software dedicated to microarrays image denoising, was licensed to the INNOPSYS company which develops scanners for disease diagnosis and multiple applications (gene expression, genotyping, aCGH, ChIP-chip, microRNA, ...).

- **Participant**: Charles Kervrann.
- **Partner:** INRA.
- **Contact:** Charles Kervrann.
- **APP deposit number:** IDDN.FR.001.190033.001.S.A.2007.000.21000
- **Language:** C/C++.

6.9. TubuleJ

KEYWORDS: Bioinformatics - Biomedical imaging

FUNCTIONAL DESCRIPTION: The TUBULEJ software written in java (plug-in ImageJ) is devoted to the analysis of microtubules and helical structures in 2D cryo electron microscope images. The software straightens curved microtubule images by estimating automatically point locations on the microtubule axis. The estimation of microtubule principal axis relies on microtubule cylindrical shape analyzed in the Fourier domain. A user-friendly interface enables to filter straight fiber images by selecting manually the layer lines of interest in the Fourier domain. This software can be used to generate a set of 2D projection views from a single microtubule projection view and a few parameters of this microtubule structure.

- **Participants:** Denis Chrétien, Charles Kervrann, Sophie Blestel.
- **Contact:** Denis Chrétien.
- **Partners:** University of Rennes 1, CNRS.
- **APP deposit number:** IDDN.FR.001.240023.000.S.P.2011.000.21000
- **On-line demo:** http://equipes.igdr.univ-rennes1.fr/en/tips/Software/TubuleJ/
- **Language:** JAVA (plug-in IMAGEJ: http://rsbweb.nih.gov/ij/).

6.10. Cryo-Seg

KEYWORDS: Bioinformatics - Biomedical imaging

FUNCTIONAL DESCRIPTION: The CRYO-SEG software has been developed to detect microtubule structures and helical structures in 2D cryo electron microscope images. Cryo electron tomography allows 3D observation of biological specimens in their hydrated state. Segmentation is formulated as Maximum A Posteriori estimation problem and exploits image patches to take into account spatial contexts (Markov Random Fields). Because of the contrast anisotropy in the specimen thickness direction, the whole tomogram is segmented section by section, with an automatic update of reference patches. This algorithm has been evaluated on synthetic data and on cryo electron tomograms of in vitro microtubules. On real data, this segmentation method extracts the most contrasted regions of microtubules, and 3D visualization is improved.

- **Participants:** Denis Chrétien, Charles Kervrann, Sophie Blestel.
- **Contact:** Denis Chrétien.
- **Partners:** University of Rennes 1, CNRS.
- **Languages:** C/C++ and JAVA (plug-in IMAGEJ: http://rsbweb.nih.gov/ij/).

6.11. Platforms

6.11.1. Mobyle@Serpico plateform and software distribution

The objective is to disseminate the distribution of SERPICO image processing software for biologists:

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

*Mobyle@*SERPICO *web portal*: An on-line version of the image processing algorithms has been developped using the Mobyle framework (Institut Pasteur, see http://mobyle.pasteur.fr/). The main role of this web portal (see Fig. 2) is to demonstrate the performance of the programs developed by the team: QUANTEV, C-CRAFT[12], ATLAS[1], HOTSPOTDETECTION[56], HULLKGROUND[45], KLTRACKER[55], MOTION2D[54], MS-DETECT[47], ND-SAFIR[5], OPTICALFLOW and FLUX ESTIMATION [12]. The web interface makes our image processing methods available for biologists at Mobyle@SERPICO (http://mobyle-serpico.rennes.inria.fr/cgi-bin/portal.py#welcome) without any installation or configuration on their own. The size of submitted images is limited to 200 MegaBytes per user and all the results are kept 15 days. The web portal and calculations run on a server with 2 CPU x 8 cores, 64 GigaBytes of RAM (500 MegaBytes for each user / Data is saved for 3 months).

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

IMAGEJ **plug-ins**: 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 [5], HULLKGROUND [45], MOTION2D [54], HOTSPOTDETECTION [56], STLAS [1]. The C-CRAFT algorithm [12] has been developped for the image processing ICY platform (http://icy.bioimageanalysis.org/).

Institut Curie CID iManage database: The microscopy facility of Institut Curie has co-developed a commercial database system (CID iManage/Strand Avadis company). The database can be searched via meta-data and includes menu selections that enable to run remote processing from a cluster. We have integrated ND-SAFIR and HULLKGROUND in the interface environment to allow the database users to process their images easily, and store associated results and parameters used.

- **Participants:** Thierry Pécot, Charles Kervrann, Charles Deltel (Inria Rennes SED).
- **Contact:** Thierry Pécot, Charles Kervrann.

6.11.2. IGRIDA-Serpico cluster

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

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

TAPDANCE Team (section vide)

VIRTUAL PLANTS Project-Team

5. New Software and Platforms

5.1. OpenAleaLab

KEYWORDS: Bioinformatics - Biology - Workflow - Modelling Environment
FUNCTIONAL DESCRIPTION

OpenAleaLab is an integrated modelling environment (IME) designed for scientists based on IPython and on OpenAlea components. This open source environment is extensible via plug-ins and allows user to work with a set of diverse modelling paradigms like imperative languages (Python, R), scientific workflows (visual programming) or rule-based language (L-System). This IME, built using PyQt, provides an IPython shell, a text editor, a project manager, a graphical package installer and a world, containing the objects and state variables shared by the different paradigms. The world can be graphically interpreted in 3D or 2D. Different paradigms and tools for plant modelling are available as plug-ins, such as a visual programming environment, a L-system language, a 3D viewer, and an R editor and interpreter. The plug-in system is based on setuptools entry-points and provide both functional and GUI components. This environment is designed to be easily extensible in order to include new plant modelling paradigms in the future or to be customized for other scientific domains. Several dedicated extensions (TissueLab, PlantLab) have been developed or are in development.

- Participants: Christophe Pradal, Christophe Godin.
- Contact: Christophe Pradal, Christophe Godin
- URL: http://virtualplants.github.io/

5.2. TissueLab

KEYWORDS: Bioinformatics - Biology - Modelling Environment
FUNCTIONAL DESCRIPTION

TissueLab is an OpenAleaLab extension dedicated to study plant morphogenesis at the scale of the tissues. This extension was built on the basis of several key concepts of OpenAleaLab (project, world, interactive panels, etc.) and using its plugin mechanism (dynamically discovered, modular, extensible, etc.). TissueLab provides a framework for the visualization, exploration, interaction, reconstruction, analysis and simulation of tissue development based on image sequences. It contains for instance the PyThor module, dedicated to 3D real-time interaction and modification of segmented images for the creation of ground truth segmentations.

- Participants: Sophie Ribes, Guillaume Baty, Guillaume Cerutti, Alizon Konig, Grégoire Malandain, Christophe Pradal, Christophe Godin.
- Contact: Christophe Godin
- URL: https://github.com/virtualplants/tissuelab

5.3. Draco-Stem

KEYWORDS: 3D Reconstruction - Triangular Mesh - Biomechanical Simulations
FUNCTIONAL DESCRIPTION

A computational tool called DRACO-STEM (Dual Reconstruction by Adjacency Complex Optimization - SAM Tissue Enhanced Mesh) has been made available, with the aim of bridging the gap between experimental data and tissue biomechanics models. It provides the necessary tools to generate a FEM-ready, topologically accurate, complete 3D triangular mesh of meristematic tissue, based on a segmented image obtained from a confocal microscopy acquisition. The produced meshes proved to be useable as an input for computational simulations of biomechanical and physiological cellular processes.

- Participants: Guillaume Cerutti, Christophe Godin, Olivier Ali
- Contact: Guillaume Cerutti
- URL: https://github.com/VirtualPlants/draco_stem/

5.4. ASTEC

KEYWORDS: Segmentation - Tracking - High resolution
FUNCTIONAL DESCRIPTION

A new algorithmic pipeline, ASTEC (Adaptative Segmentation and Tracking of Embryonic Cells), has been developed to segment and track cell shapes in 3D from movies with high spatio-temporal resolution of embryos where the membranes have been labeled (using dye or genetic markers for example). To segment the 3D embryo image at a given time-point, ASTEC takes advantage of the high spatial resolution of the movie in order to propagate the segmentation of the previous time points. This, coupled to biological knwoledge on the studied system, allows to constrain the segmentation and to track cells throughout time simulataneously. Moreover, the propagation allows to bound the potential mistakes of segmentation (e.g. a cells cannot disappear) which enables powerful post-correction based on the study of the resulting tracking.

- Participants: Léo Guignard, Emmanuel Faure, Grégoire Malandain, Patrick Lemaire, Christophe Godin
- Contact: Christophe Godin
- URL: https://gforge.inria.fr/projects/marsalt/

5.5. AutoWIG

KEYWORDS: Syntaxic Analysis
FUNCTIONAL DESCRIPTION

High-level programming languages, such as Python and R, are popular among scientists. They are concise, readable, lead to rapid development cycles, but suffer from performance drawback compared to compiled languages. However, these languages allow to interface C, C++ and Fortran code. In this way, most of the scientific packages incorporate compiled scientific libraries to both speed up the code and reuse legacy libraries. While several semi-automatic solutions and tools exist to wrap these compiled libraries, the process of wrapping a large library is cumbersome and time consuming. We developed AutoWIG [40], [47], a Python library that wraps automatically compiled libraries into high-level languages. Our approach consists in parsing C++ code using the LLVM/Clang technologies and generating the wrappers using the Mako templating engine. Our approach is automatic, extensible, and applies to very complex C++ libraries, composed of thousands of classes or incorporating modern meta-programming constructs. The usage and extension of AutoWIG have been illustrated on a set of statistical libraries (StructureAnalysis).

- Participants: Pierre Fernique, Christophe Pradal
- Contact: Pierre Fernique
- URL: https://github.com/VirtualPlants/AutoWIG

5.6. Phenomenal

KEYWORDS: Image Analysis, Phenotyping
FUNCTIONAL DESCRIPTION

Phenomenal [65] is a Python library dedicated to the analysis of high throughput phenotyping data and models. It has been developed in the frame of the Phenome high throughput phenotyping infrastructure. It is based on the OpenAlea platform [76], [77] that provides methods and softwares for the modelling of plants, together with a user-friendly interface for the design and execution of scientific workflows. OpenAlea is also part of the InfraPhenoGrid infrastructure that allows high throughput computation and recording of provenance during the execution [26].

- Participants: Simon Artzet, Jérôme Chopard, Tsu-Wei Chen, Nicolas Brichet, Christian Fournier, Christophe Pradal
- Contact: Christian Fournier, Christophe Pradal
- URL: https://gitlab.inria.fr/phenome/phenomenal

5.7. Platforms

5.7.1. Platform OpenAlea

OpenAlea is an open-software platform for interdisciplinary research in plant modeling and simulation. This scientific workflow platform is used for the integration and comparison of different models and tools provided by the research community. It is based on the Python (http://www.python.org) language that aims at being both a *glue* language for the different modules and an efficient modeling language for developing new models and tools. *OpenAlea* currently includes modules for plant simulation, analysis and modeling at different scales (*V-Plants* modules), for modeling ecophysiological processes (*Alinea* modules) such as radiative transfer, transpiration and photosynthesis (*RATP*, *Caribu*, *Adel*, *TopVine*, *Ecomeristem*) and for 3D visualization of plant architecture at different scales (*PlantGL*).

OpenAlea is the result of a collaborative effort associating 20 french research teams in plant modeling from Inria, CIRAD, INRA and ENS Lyon. The Virtual Plants team coordinates both development and modeling consortia, and is more particularly in charge of the development of the kernel and of some of the main data structures such as multi-scale tree graphs and statistical sequences.

OpenAlea is a fundamental tool to share models and methods in interdisciplinary research (comprising botany, ecophysiology, forestry, agronomy, applied mathematics and computer science approaches). Embedded in Python and its scientific libraries, the platform may be used as a flexible and useful toolbox by biologists and modelers for various purposes (research, teaching, rapid model prototyping, communication, etc.).

New methodological developments around scientific workflows in *OpenAlea* have been done recently.

5.7.2. Platform Sofa

Our team is increasingly using the platform SOFA developed at Inria by other teams, in conjunction with OpenAlea, to model biomechanics of plant tissues. SOFA (https://www.sofa-framework.org) is an Open Source framework primarily targeted at real-time simulation, with an emphasis on biological 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. It has been extensively used by our team in the recent years to conduct virtual mechanical experiments on plant tissues (see section 6.2.3).

ARAMIS Project-Team

6. New Software and Platforms

6.1. Clinica

KEYWORDS: Multimodal neuroimaging - anatomical MRI - diffusion MRI - functional MRI - PET - EEG/MEG

FUNCTIONAL DESCRIPTION

Clinica is a software platform for multimodal brain image analysis in clinical research studies. It aims at integrating a comprehensive set of processing tools for the main neuroimaging modalities: MRI (anatomical, functional, diffusion), PET and EEG/MEG. For each modality, it allows to easily extract various types of features (regional measures, parametric maps, surfaces, curves, networks) that can be 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 and in-house developments. It provides an integrated data management system to store raw and processing data.

- Participants: Olivier Colliot, Stanley Durrleman, Fabrizio De Vico Fallani, Michael Bacci, Alexandre Routier, Jorge Samper-Gonzalez, Junhao Wen, Jérémy Guillon, Sabrina Fontanella, Thomas Jacquemont
- Contact: Olivier Colliot

6.2. Brain Networks Toolbox

KEYWORDS: Neuroimaging - Medical imaging

FUNCTIONAL DESCRIPTION

Brain Networks Toolbox is a collection of Matlab routines developed to quantify topological metrics of complex brain networks.

- Participants: Mario Chavez and Fabrizio De Vico Fallani
- Contact: Mario Chavez
- URL: https://sites.google.com/site/fr2eborn/download

6.3. Deformetrica

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

SCIENTIFIC DESCRIPTION

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

Deformetrica comes with two applications:

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

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

FUNCTIONAL DESCRIPTION

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

Deformetrica comes with two applications:

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

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

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

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

6.4. SACHA

Segmentation Automatisée Compétitive de l'Hippocampe et de l'Amygdale
KEYWORDS: Neuroimaging - 3D - Hippocampus - Amygdala - Brain scan - Medical imaging
SCIENTIFIC DESCRIPTION

The current stable version is fully automatic and focused on cross-sectional segmentation. The software can be used both as a command-line program or through a graphical user interface (GUI). The core of the program is coded in C++. It has a dependency to the AIMS library and preprocessing steps rely on processes in Matlab from SPM. The GUI is coded in Python and is based on BrainVISA.
FUNCTIONAL DESCRIPTION

SACHA is a software for the fully automatic segmentation of the hippocampus and the amygdala from MRI 3D T1 brain scans. It has been validated in various populations including healthy controls and patients with Alzheimer's disease, epilepsy and depression. It has been successfully applied to over 3,000 subjects, both controls, from adolescents to elderly subjects, and patients with different types of pathologies.

- Participants: Marie Chupin and Ludovic Fillon
- Contact: Marie Chupin

6.5. WHASA

White matter Hyperintensity Automatic Segmentation Algorithm
KEYWORDS: Health - Neuroimaging - Biomedical imaging
SCIENTIFIC DESCRIPTION

The current stable version is fully automatic and focused on cross-sectional segmentation. The software can be used both as a Matlab command-line or through a graphical user interface (GUI). The core of the program is coded in Matlab. It has a dependency to the SPM environment. The GUI is coded in Python and is based on BrainVISA.
FUNCTIONAL DESCRIPTION

WHASA ("White matter Hyperintensity Automatic Segmentation Algorithm") is a software for the fully automatic segmentation of age-related white matter hyperintensities from MRI FLAIR and 3D T1 brain scans. It has been validated on a population showing a wide range of lesion load, and is being further evaluated on elderly subjects with few clinical abnormalisties and with different acquisition characteristics.

- Participants: Marie Chupin, Ludovic Fillon and Thomas Samaille
- Contact: Marie Chupin

6.6. QualiCATI

KEYWORDS: Health - Neuroimaging - Medical imaging

SCIENTIFIC DESCRIPTION

QualiCATI requires training for the visual parts, and is closely linked with a team of clinical research assistants. It has been used to analyse about 5000 subjects from about 15 multi centre research projects initiated before or after the CATI started. Other modules will be added in the future to embed new aspects of the MRI protocol proposed by the CATI. The Aramis team is in charge of the second and third modules and jointly in charge of the first module. The software is centered on a graphical user interface (GUI). The whole program is coded in Python within the pyPTK environment. It has dependencies to SPM and brainVISA environments as well as specific tools for DICOM management.

FUNCTIONAL DESCRIPTION

QualiCATI is a software designed for comprehensive quality control of multimodal MRI data acquisition in large multicentre clinical studies. The software is built as a platform receiving several modules, developed by several CATI engineers. The first module is dedicated to acquisition requirement checking and conversion to nifti format. The second module aims at making 3DT1 acquisition quality check more systematic, and relies both on visual inspection and quantitative indices. The third module allows a simultaneous evaluation of the clinical part of the CATI acquisition protocol. The fourth module embeds automatic indices to evaluate resting state fMRI acquisition. The fifth module is dedicated to first preprocessings and quality indices for dMRI. The sixth module is dedicated to qMRI, with visual and automated quality control together with preprocessings. The last module is dedicated to data and project management.

- Participants: Marie Chupin and Hugo Dary
- Contact: Marie Chupin

ASCLEPIOS Project-Team

5. New Software and Platforms

5.1. LSVF

KEYWORDS: Health - Brain - Medical Image Processing - Medical Imaging

FUNCTIONAL DESCRIPTION:

The Longitudinal Stationary Velocity Fields Framework is a set of tools based on the SVF parameterization of diffeomorphic deformations that allows a new type of longitudinal deformation-based morphometric analyses. The framework comprises tools to compute the deformation encoded by the exponential of an SVF, the log-demons registration software and the Pole ladder, an algorithm to parallel transport deformation trajectories. These tools can be organized in a Longitudinal Log-Demons Pipeline (LLDP), to estimate the longitudinal brain deformations from image data series, transport them in a common space and perform statistical groupwise analyses.

Sources are available under custom licence.

- Participants: Mehdi Hadj-Hamou, Marco Lorenzi and Xavier Pennec
- Contact: Xavier Pennec
- URL: http://team.inria.fr/asclepios/software/stationary-velocity-field-tools/
- URL: http://team.inria.fr/asclepios/software/lcclogdemons/

5.2. medInria

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

SCIENTIFIC DESCRIPTION

It aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010 and renewed in 2012. The Visages team leads this Inria national project and participates in the development of the common core architecture and features of the software as well as in the development of specific plugins for the team's algorithm.

FUNCTIONAL DESCRIPTION

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

- Participants: Jaime Garcia Guevara, Theodore Papadopoulo, Olivier Commowick, Rene-Paul Debroize, Guillaume Pasquier, Laurence Catanese, Olivier Commowick, Alexandre Abadie, Benoit Bleuze, Clement Philipot, Fatih Arslan, Florian Vichot, John Stark, Julien Wintz, Loïc Cadour, Maxime Sermesant, Michael Knopke, Nicolas Toussaint, Olivier Clatz, Pierre Fillard, Sergio Medina, Stephan Schmitt and Hakim Fadil
- Partners: HARVARD Medical School - IHU LIRYC - King's College London - UPF Barcelona - NIH
- Contact: Olivier Commowick
- URL: http://med.inria.fr

5.3. MUSIC

Multi-modality Platform for Specific Imaging in Cardiology

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

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: Loïc Cadour, Maxime Sermesant, Florian Vichot, Hakim Fadil, Florent Collot and Mathilde Merle
- Contact: Maxime Sermesant
- URL: https://team.inria.fr/asclepios/software/music/

5.4. SOFA

Simulation Open Framework Architecture

KEYWORDS: Physical simulation - Health - Biomechanics - GPU - Computer-assisted surgery

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.

A software consortium around SOFA is currently being set up to strengthen the perenial developement of the plateform https://www.sofa-framework.org/consortium/. The software is available under the LGPL licence.

- Participants: Chloé Audigier, Sophie Giffard-Roisin, Qiao Zheng, Roch-Philippe Molléro and Hervé Delingette
- Contact: Hervé Delingette
- URL: http://www.sofa-framework.org

5.5. VP2HF

Virtual Physiological Human for Heart Failure Platform

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

FUNCTIONAL DESCRIPTION

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

- Participants: Maxime Sermesant, Hakim Fadil and Loïc Cadour
- Contact: Maxime Sermesant
- URL: http://www.vp2hf.eu

ATHENA Project-Team

6. New Software and Platforms

6.1. Coadapt P300 Stimulator

KEYWORDS: Health - Brain-Computer Interface
FUNCTIONAL DESCRIPTION

In the domain of Brain Computer Interfaces, extracting relevant features requires a precise timing of all events occurring in the system. In particular, when dealing with evoked responses as in the P300 speller, the timing of the visual stimulations must be well controlled. To alleviate some timing issues with the P300 speller initially provided with OpenViBE, we have implemented an external visual stimulator that allows to flash the visual targets, in a time-robust manner. In 2016 a new generation of this software has been coded, which will be released publicly in 2017. It is being tested outside of Inria by a few beta-testers.

- Participants: Nathanaël Foy, Dieter Devlaminck, Loic Mahe, Maureen Clerc, Théodore Papadopoulo, Emmanuel Maby and Jérémie Mattout
- Partner: INSERM
- Contact: Maureen Clerc
- http://openvibe.inria.fr/coadapt-p300-stimulator-tutorial/

6.2. DIPY

Diffusion Imaging in Python
KEYWORDS: MRI - Medical imaging
FUNCTIONAL DESCRIPTION

Dipy is a free and open source software project focusing mainly on diffusion magnetic resonance imaging (dMRI) analysis. Nonetheless, as we solve problems in dMRI some of the solutions are applicable to the greater medical imaging and image processing communities. See for example our registration and denoising tutorials.

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

6.3. The White Matter Query Language

KEYWORDS: Neuroanatomy - Diffusion MRI - Automatic Segmentation - DSL
FUNCTIONAL DESCRIPTION The White Matter Query Language (WMQL) is a technique to formally describe white matter tracts and to automatically extract them from diffusion MRI volumes. This query language allows us to construct a dictionary of anatomical definitions describing white matter tracts. The definitions include adjacent gray and white matter regions, and rules for spatial relations. This enables the encoding of anatomical knowledge of the human brain white matter as well as the automated coherent labeling of white matter anatomy across subjects.

- Participants: Demian Wassermann
- Contact: Demian Wassermann
- URL:http://tract-querier.readthedocs.org/en/latest/

6.4. FindSources3D

KEYWORDS: Health - Neuroimaging - Visualization - Medical - Image - Processing

FUNCTIONAL DESCRIPTION

FindSources3D is a Matlab software program dedicated to the resolution of inverse source problems in electroencephalogrphy (EEG). From pointwise measurements of the electric potential, numerically obtained or taken by electrodes on the scalp, FindSources3D estimates pointwise dipolar current sources within the brain.

- Participants: Juliette Leblond, Maureen Clerc, Théodore Papadopoulo and Jean Paul Marmorat
- Contact: Juliette Leblond
- URL: http://www-sop.inria.fr/apics/FindSources3D/en/index.html

6.5. High Performance Diffusion MRI

KEYWORDS: Health - Neuroimaging - Medical imaging
FUNCTIONAL DESCRIPTION

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. These algorithms and software 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. This library has been transfered to the Company *Olea Medical*, where it will be at the heart of the new dMRI module to be included in the *Olea Sphere* platform.

- Participants: Aurobrata Ghosh, Théodore Papadopoulo, Rachid Deriche and Demian Wassermann
- Contact: Rachid Deriche

6.6. MedInria

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

It aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010 and renewed in 2012. The Visages team leads this Inria national project and participates in the development of the common core architecture and features of the software as well as in the development of specific plugins for the team's algorithm.

FUNCTIONAL DESCRIPTION

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

- Participants: Jaime Garcia Guevara, Théodore Papadopoulo, Olivier Commowick, Rene-Paul Debroize, Guillaume Pasquier, Laurence Catanese, Olivier Commowick, Alexandre Abadie, Benoit Bleuze, Clement Philipot, Fatih Arslan, Florian Vichot, John Stark, Julien Wintz, Loïc Cadour, Maxime Sermesant, Michael Knopke, Nicolas Toussaint, Olivier Clatz, Pierre Fillard, Sergio Medina, Stephan Schmitt and Hakim Fadil
- Partners: HARVARD Medical School - IHU - LIRYC - IHU - Strasbourg - NIH
- Contact: Olivier Commowick
- URL: http://med.inria.fr

6.7. OpenMEEG

KEYWORDS: Health - Neuroimaging - Medical imaging

FUNCTIONAL DESCRIPTION

OpenMEEG provides state-of-the art tools for processing EEG and MEG data. It incorporates a newly proposed, symmetric BEM for the forward problem, and a distributed source inverse problem, with three different types of regularizations, two of which are original, based on norms of the surface gradient of the source distribution. OpenMEEG is a free, open software written in C++, and can be accessed either through a command line interface or through a user-friendly interface. OpenMEEG is being used for functional neuroimaging, through third-party software (Brainstorm and Fieldtrip), as can be noticed by the citations to our articles [9] and [89].

- Participants: Théodore Papadopoulo, Maureen Clerc, Alexandre Gramfort, Emmanuel Olivi, Kai Dang, Geoffroy Adde, Perrine Landreau, Renaud Keriven and Jan Kybic
- Contact: Théodore Papadopoulo
- URL: http://openmeeg.github.io/

6.8. OpenVIBE

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

FUNCTIONAL DESCRIPTION

OpenViBE is a software platform for real-time neurosciences (that is, for real-time processing of brain signals). It can be used to acquire, filter, process, classify and visualize brain signals in real time from various signal sources. OpenViBE is free and open source software. It works on Windows and Linux operating systems.

- Participants: Yann Renard, Anatole Lécuyer, Fabien Lotte, Bruno Renier, Vincent Delannoy, Laurent Bonnet, Baptiste Payan, Jozef Legeny, Jussi Tapio Lindgren, Alison Cellard, Loic Mahe, Guillaume Serriere, Marsel Mano, Maureen Clerc, Théodore Papadopoulo, Laurent Bougrain, Jeremy Frey and Nathanaël Foy
- Partners: CEA-List - GIPSA-Lab - INSERM
- Contact: Anatole Lécuyer
- URL: http://openvibe.inria.fr

BIOVISION Team

5. New Software and Platforms

5.1. Virtual Retina: A biological retina model with contrast gain control for large scale simulations

KEYWORDS: Neurosciences - Simulation - Biology - Health
SCIENTIFIC DESCRIPTION

The Virtual Retina software allows large-scale simulations of biologically-plausible retinas, with customizable parameters. Virtual Retina has been shown to reproduce a wide range of experimental data from salamander, cat and primate retinas [14], and has been used in several theoretical studies [65], [66], [67], [41], [17]. It has recently been shown to predict spikes in a mouse retina more accurately than linear-nonlinear (LN) models [79]. The underlying model includes a non-separable spatio-temporal linear model of filtering in the Outer Plexiform Layer, a shunting feedback at the level of bipolar cells, and a spike generation process using noisy leaky integrate-and-fire neurons to model RGCs. All parameters for the different stages of the model are customizable so that the visual field can be paved with different RGC types.

FUNCTIONAL DESCRIPTION.

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

- Participants: Bruno Cessac, Maria-Jose Escobar, Pierre Kornprobst, Selim Kraria, Daniela Pamplona, Selma Souihel, Thierry Vieville and Adrien Wohrer.
- Contact: Pierre Kornprobst
- URL: https://enas.inria.fr/virtual-retina.html

5.2. ENAS: Event Neural Assembly Simulation

KEYWORDS: Neurosciences - Health - Physiology
SCIENTIFIC DESCRIPTION

As one gains more intuitions and results on the importance of concerted activity in spike trains, models are developed to extract potential canonical principles underlying spike coding. These methods shed a new light on spike train dynamics. However, they require time and expertise to be implemented efficiently, making them hard to use in a daily basis by neuroscientists or modelers. To bridge this gap, we developed the license free multiplatform software ENAS (https://enas.inria.fr) integrating tools for individual and collective spike analysis and simulation, with some specificities devoted to the retina. The core of ENAS is the statistical analysis of population codes. One of its main strength is to provide statistical analysis of spike trains using Maximum Entropy-Gibbs distributions taking into account both spatial and temporal correlations as constraints, allowing to introduce causality and memory in statistics. It also generates simulated population raster from an user-specified Gibbs distribution.

We hope that ENAS will become a useful tool for neuroscientists to analyse spike trains and we hope to improve it thanks to user feedback. Our goal is to progressively enrich it with the latest research results, in order to facilitate transfer of new methods to the community.

FUNCTIONAL DESCRIPTION. ENAS is developed joinly by the Biovision, CORTEX/Mnemosyne, and DREAM Inria teams, under CeCILL-C licence, APP logiciel ENAS : IDDN.FR.OO1.190004.000.S.P.2014.000.31235. It can be freely loaded. ENAS has a friendly Graphical User Interface that avoids any scripting or writing code from user. Most methods have been implemented to run in parallel to reduce the time and memory consumption.

- Participants: Bruno Cessac, Pierre Kornprobst, Selim Kraria, Hassan Nasser, Thierry Vieville, Daniela Pamplona, Geoffrey Portelli, Selma Souihel.
- Contact: Bruno Cessac
- URL: https://enas.inria.fr

5.3. The Enas–Virtual Retina platform

In 2016 we merged Enas and Virtual Retina to produce the Enas platform https://enas.inria.fr. The initial version of Virtual retina has been extended to include lateral connections in the Inner Plexiform Layer. We can then simulate the response of the retina to visual stimuli (movies), including the effect of lateral connectivity, analyse the collective spike response to this stimulus using Gibbs distributions, and reproduce a similar raster using learning methods shaping the connectivity in the Inner Plexiform Layer.

This work has been presented in [27] and submitted to Frontiers in Neuroinformatics [3].

<p align="center" style="color:red">CAMIN Team</p>

6. New Software and Platforms

6.1. Software and platforms

6.1.1. HILECOP

Participants: Baptiste Colombani, David Andreu, Thierry Gil [LIRMM], Robin Passama [LIRMM].

High Level hardware Component Programming

FUNCTIONAL DESCRIPTION: Our SENIS (Stimulation Electrique Neurale dIStribuee) based FES architecture relies on distributed stimulation units (DSU) which are interconnected by means of a 2-wire based network. A DSU is a complex digital system since its embeds among others a dedicated processor (micro-machine with a specific reduced instruction set), a monitoring module and a 3-layer protocol stack. To face the complexity of the units digital part and to ease its prototyping on programmable digital devices (e.g. FPGA), we developed an approach for high level hardware component programming (HILECOP). To support the modularity and the reusability of sub-parts of complex hardware systems, the HILECOP methodology is based on components. An HILECOP component has: a Petri Net (PN) based behavior (fig.5), a set of functions whose execution is controlled by the PN, and a set of variables and signals. Its interface contains places and transitions from which its PN model can be inter-connected as well as signals it exports or imports. The interconnection of those components, from a behavioral point out view, consists in the interconnection of places and/or transitions according to well-defined mechanisms: interconnection by means of oriented arcs or by means of the "merging" operator (existing for both places and transitions).

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

Undergoing work concerns the integration, in the HILECOP tool, of the formalism evolutions that allow behavior agregation as well as exception handling, both for analysis and implementation sides.

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

6.1.2. PersoBalance: A Personalized Balance Assessment in Home Rehabilitation

Participants: Maxime Tournier, Alejandro Gonzalez, Philippe Fraisse, Mitsuhiro Hayashibe.

In 2014-2015, the team demonstrated the feasibility of a personalized balance assessment system using low-end sensors for home rehabilitation. The corresponding software (PersoBalance) performs an identification of inertial parameters for a subject using a depth camera and a connected balance board (in this case, a Nintendo Wii BalanceBoard) through a dedicated Kalman filter as the subject assumes various body postures. When the inertial parameters are estimated, the software is then able to compute a stability index for the subject based on criteria found in robotics and biomechanics literature. This year, in order to exploit the newer, more accurate and more robust sensors such as the Microsoft Kinect v2, a new version of the PersoBalance software was engineered. While the core method remainsthe same, several improvement have been made regarding efficiency, user interface and extensibility. The new system is faster, more accurate and robust. It automatically registers the balance board during identification, and features improved graphical feedback during both identification and stability estimation phases. New stability measures were added, and support for online inverse dynamics is on the way. Most of the new version uses a scripting language (Python) except for time-critical algorithm, making the software easily extensible without recompilation. It is supported by Inria ADT PersoBalance2. Currently the software is being adapted to embedded computers in order to provide monitoring data in the City4Age project.
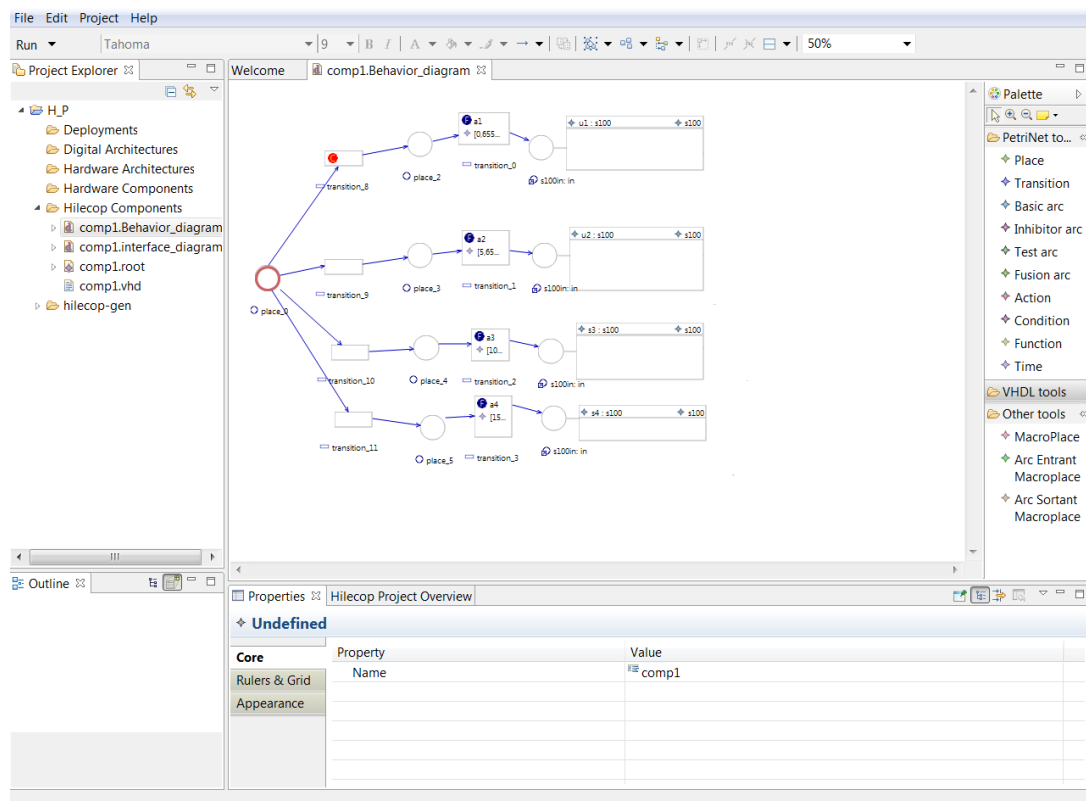
Figure 5. HILECOP screenshot

PersoBalance is registered with the Agency for the Protection of Programs (APP) and deposited at the BNF (Bibliotheque Nationale de France). Its registration number is Antepedia Deposit 20150710154654.

Figure 6. PersoBalance: Online stability estimation, from left to right: as a subject undergoes an unexpected external push, the system automatically estimates the ground reaction forces (pink arrow) and computes a stability index from the position of the ZRAM point relative to the support polygon (white/orange). The skeleton colour changes from green to red as the stability index decreases.

6.1.3. Sensbiotk

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

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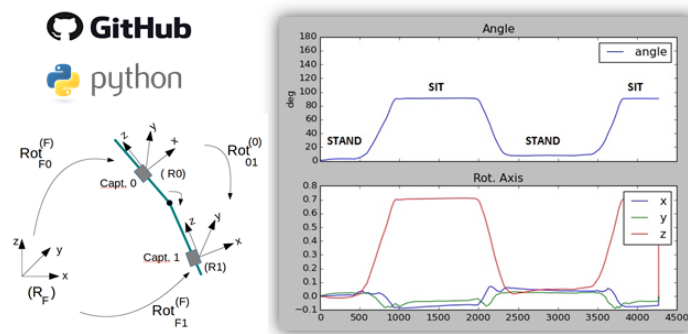
http://sensbio.github.io/sensbiotk/

Figure 7. Sensbiotk toolbox for the calibration, the acquisition, the analysis and visualization of motion capture Inertial Measurement Units (IMU)

6.1.4. MOS2SENS

Participants: Mélissa Dali, Olivier Rossel, David Guiraud.

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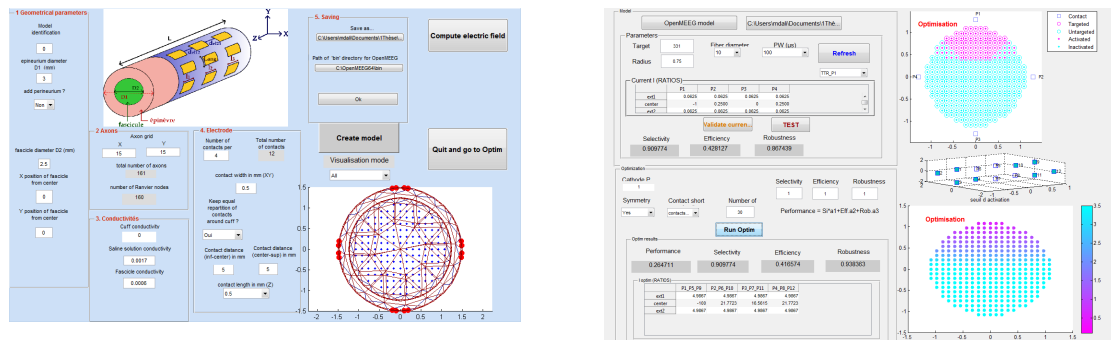

Figure 8. Graphical interface of software MOS2SENS, left: modeling multicontact CUFF electrode, right: optimization for spatial selectivity

6.1.5. STIMEP: An advanced real-time stimulation system based on a distributed architecture

Participants: Arthur Hiairrassary, David Andreu, David Guiraud, Olivier Rossel, Thomas Guiho.

The STIMEP has been developed within the EPIONE project (see section 9.3.1) which aims at assessing the use of invasive stimulation to relieve phantom pain. This innovative wearable stimulator allows to safely manipulate sensory afferent signals of an amputee through 4 TIME-4H intra fascicular electrodes, for a total of 56 channels.

The STIMEP is also designed to be controlled in real-time by a hand-prosthesis to generate feedback sensations; it permits as well a complex impedance follow-up.

The STIMEP is based on a distributed architecture and embeds:

- 1 x controller implemented on μC/OS-II RTOS exchanging data with a PC (USB) or an external device (SPI),
- 4 x neural stimulators with efficient modulation mechanisms to drive up to 4 multicontact electrodes simultaneously and independently,
- 6 x fully configurable procedures (formally modeled by Petri nets):
    – Contacts check, thresholds search, sensations characterization, therapy,
    – Real-time modulation of frequency, intensity and pulse-width,
    – Complex impedance measurement.
- 2 x smart and independent synchronization outputs,
- User and technical logs of relevant information.

The STIMEP is currently used in human trials and drives simultaneously 4 multicontact intrafascicular electrodes with real time control of the intensity, pulse-width and frequency of the stimulation to remove phantom pain and elicit very accurate sensation feedback.
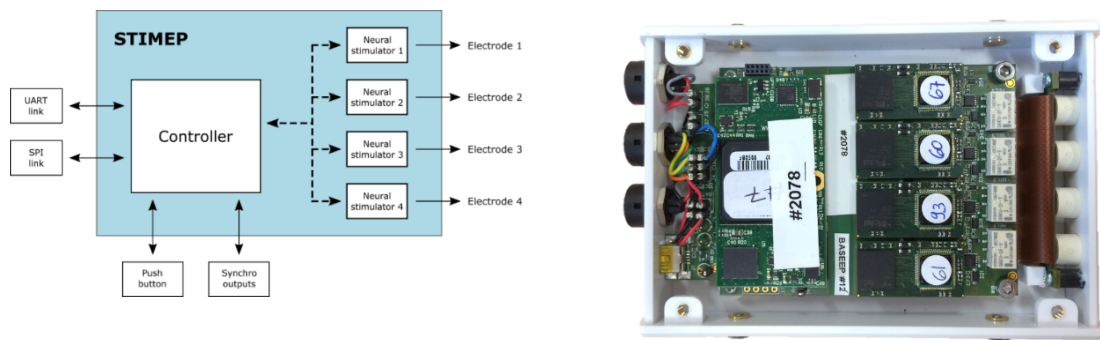
Figure 9. The STIMEP (STIMulator EPione)

GALEN Project-Team

6. New Software and Platforms

6.1. DISD

Dense Image and Surface Descriptors

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

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

6.2. DPMS

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

- Participant: Iasonas Kokkinos
- Contact: Iasonas Kokkinos
- URL: http://cvn.ecp.fr/personnel/iasonas/dpms.html

6.3. ECP

Part-Based Object Detection

FUNCTIONAL DESCRIPTION A DPM model gives rise to the energy function being optimized during inference and has to be learned offline beforehand. All functionality is accessible via a ROS interface. The work follows closely Felzenszwalb's "Object Detection with Discriminatively Trained Part Based Models", using the FFLD-library in the implementation and facilitating communication in a setup with NAO robots.

- Participants: Haithem Boussaid, Stefan Kinauer, Iasonas Kokkinos
- Contact: Stefan Kinauer
- URL: https://bitbucket.org/eu-reconfig/ecp

6.4. DROP

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

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

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

6.5. FastPD

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

- Contact: Nikolaos Paragyios
- URL: http://www.csd.uoc.gr/~komod/FastPD/

6.6. GraPeS

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

- Participant: Iasonas Kokkinos
- Contact: Iasonas Kokkinos
- URL: http://vision.mas.ecp.fr/Personnel/teboul/grapesPage/index.php

6.7. HOAP-SVM

High-Order Average Precision SVM
SCIENTIFIC DESCRIPTION

We consider the problem of using high-order information (for example, persons in the same image tend to perform the same action) to improve the accuracy of ranking (specifically, average precision). We develop two learning frameworks. The high-order binary SVM (HOB-SVM) optimizes a convex upper bound of the surrogate 0-1 loss function. The high-order average precision SVM (HOAP-SVM) optimizes a difference-of-convex upper bound on the average precision loss function. Authors of the research paper: Puneet K. Dokania, A. Behl, C. V. Jawahar and M. Pawan Kumar

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

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

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

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

6.8. LBSD

Learning-Based Symmetry Detection

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

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

6.9. TeXMeG

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

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

6.10. mrf-registration

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

- Participant: Nikos Paragios
- Contact: Nikos Paragios
- URL: http://www.mrf-registration.net/

6.11. Newton-MRF

FUNCTIONAL DESCRIPTION MAP inference in MRFs can be performed through the LP relaxation approach. This project was a study of the feasibility and benefit of Newton-type methods for solving the optimization problem that is obtained by smoothing the dual of the LP relaxation. The project TRN-MRF is a trust-region Newton method that can address inference in higher order MRFs, for cases in which decomposition according to individual cliques leads to practical convergence. The project QN-MRF works for problems that need decomposition according to larger sub-problems (like chains of higher order cliques) and it works as long as a node is shared by exactly two sub-problems.

- Participants: Hariprasad Kannan, Nikos Paragios, Nikos Komodakis
- Contact: Hariprasad Kannan
- URL: https://github.com/neostrider/TRN-MRF, https://github.com/neostrider/QN-MRF

6.12. Relative MMD

FUNCTIONAL DESCRIPTION This software can be used to compare two distributions to a reference distribution. Applications include model selection and exploratory data analysis.

- Participants: Eugene Belilovsky, Wacha Bounliphone, Matthew Blaschko (in collaboration with researchers at UCL and Deepmind)
- Contact: Eugene Belilovsky
- URL: https://github.com/eugenium/MMD

6.13. Deep Graph Structure Discovery

FUNCTIONAL DESCRIPTION Novel approach to graph structure discovery using neural network. This software provides a much faster approach to discover underlying conditional independence structure in small sample data.

- Participants: Eugene Belilovsky
- Contact: Eugene Belilovsky
- URL: https://github.com/eugenium/LearnGraphDiscovery

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

4. New Software and Platforms

4.1. New Software

4.1.1. *Julia library LSODA.jl*

LSODA.jl is a Julia package that interfaces to the liblsoda library, developed by Simon Frost (University of Cambridge), thereby providing a way to use the LSODA algorithm from Linda Petzold and Alan Hindmarsh from Julia.

4.1.2. *Julia library PDMP.jl*

PDMP.jl This is a joint work of Romain Veltz and Simon Frost.

PDMP.jl is a Julia package that allows simulation of Piecewise Deterministic Markov Processes (PDMP); this encompasses hybrid systems, comprising of continuous and discrete components, as well as processes with time-varying rates. It is based on an implementation of the True Jump Method for performing stochastic simulations of PDMP, and requires solving stiff ODEs in an efficient manner. Sundials.jl is used, but other solvers could be easily added.

MIMESIS Team

4. New Software and Platforms

4.1. Simulation Open Framework Architecture

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

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.

URL: http://www.sofa-framework.org

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MNEMOSYNE Project-Team

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6. New Software and Platforms

6.1. Positioning

Our previous works in the domain of well-defined distributed asynchronous adaptive computations [55], [52], [57] have already made us define a library (DANA [51]), closely related to both the notion of artificial neural networks and cellular automata. From a conceptual point of view, the computational paradigm supporting the library is grounded on the notion of a unit that is essentially a (vector of) potential that can vary along time under the influence of other units and learning. Those units can be organized into layers, maps and networks.

We will also have to interact with the High Performance Computing (HPC) community, since having large scale simulations at that mesoscopic level is an important challenge in our systemic view of computational neuroscience. Our approach implies to emulate the dynamics of thousands, or even millions, of integrated computational units, each of them playing the role of a whole elementary neural circuit (e.g. the microcolumn for the cortex). Mesoscopic models are considered in such an integrative approach, in order to exhibit global dynamical effect that would be hardly reachable by compartment models involving membrane equations or even spiking neuron networks.

The vast majority of high performance computing softwares for computational neuroscience addresses subneural or neural models [41], but coarser grained population models are also demanding for large scale simulations, with fully distributed computations, without global memory or time reference, as it is specified in (*cf.* § 3.2).

6.2. DANA

Distributed Asynchronous Numerical & Adaptive computing framework
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/

6.3. ENAS

Event Neural Assembly Simulation
Keywords: Neurosciences - Health - Physiology
Scientific Description

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

FUNCTIONAL DESCRIPTION

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

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

6.4. Virtual Enaction

KEYWORDS: Neurosciences - Simulation - Health

FUNCTIONAL DESCRIPTION

VirtualEnaction: A Platform for Systemic Neuroscience Simulation. The computational models studied in our team 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 have deployed an existing open-source video game middleware (Minecraft) in order to be able to shape the survival situation to be studied and we have begun to revisit some models in order to be able to integrate them as an effective brainy-bot. This was made as a platform associated to a scenario that is the closest possible to a survival situation (foraging, predator-prey relationship, partner approach to reproduction). We could integrate in the platform 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 was corresponding to the major anatomical regions studied in the team.

Nevertheless, we have seen recently that a major entertainment company (Microsoft) bought Minecraft to make similar (but larger) adaptations to what was being targeted by our VirtualEnaction project. We are currently studying the resulting product (the Malmö project) in order to adapt our strategy.

- Participants: André Garenne, Frédéric Alexandre, Nicolas Rougier and Thierry Viéville
- Contact: Frédéric Alexandre
- URL: http://virtualenaction.gforge.inria.fr/

NEUROSYS Project-Team

6. New Software and Platforms

6.1. AnaesthesiaSimulator

KEYWORDS: General anaesthesia - Spiking neural networks - Health
FUNCTIONAL DESCRIPTION

AnaesthesiaSimulator simulates the activity of networks of spiking neurons subject to specific receptor dynamics. The tool is a platform to test effects of anaesthetics on neural activity and is still in its first stage of development. The neural activity is planned to be visualized in a 2D and 3D-plot evolving in time. It is written in Python, open-source and involves heavily the simulation package BRIAN.

- Participants: Axel Hutt and Laure Buhry
- Partner: University of Auckland
- Contact: Axel Hutt
- URL: https://gforge.inria.fr/projects/anasim/

6.2. BrianModel

Library of Brian Neuron Models
KEYWORDS: Spiking neural networks - Neurosciences - Numerical simulations
FUNCTIONAL DESCRIPTION

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

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

6.3. MATCWT

continuous wavelet transform
KEYWORDS: Matlab - Visualization - Signal processing
FUNCTIONAL DESCRIPTION

This MATLAB script builds continuous wavelet transform (CWT) allowing to choose scales/frequencies and how to compute cone of influence (COI). It uses built-in MATLAB functions to calculate the transform (cwt.m and cwtft.m). This function returns scalogram, percentage energy for each coefficient of CWT. It also plots CWT (if such option is specified), all the values on the plot are linear ones. Plot function displays COI as hatched regions, to do so an additional function is required. Hatchfill function was used for that. I modifies this function slightly in order to control color of hatch lines and added to the repo for convenience. Otherwise, instead of using hatched regions, COI can be indicated by using MATLAB patch function with alpha set to a value less than 1.

- Contact: Mariia Fedotenkova
- URL: https://github.com/mfedoten/wavelets

6.4. MATSPECTRO

Spectrogram reassignment
KEYWORDS: Matlab - Visualization - Signal processing
FUNCTIONAL DESCRIPTION

This matlab function computes reassigned version of the conventional and multitaper spectrograms. The algorithm is based on Auger and Flandrin method, some parts are adopted from Fulop and Fitz. The idea is to first compute conventional spectrogram, then find optimal (in a sense of energy) time and frequency positions and reassigns values in the spectrogram to this new positions. The difference between conventional and multitaper spectrograms is that multitaper method computes additional spectrogram with each taper. Taper is a generic term for a window function but in this method tapers refer to Slepian sequences. As a result, generally multitaper spectrogram reveals less variance than conventional one.

- Contact: Mariia Fedotenkova
- URL: https://github.com/mfedoten/reasspectro

6.5. NFSimulator

NeuralFieldSimulator
KEYWORDS: Neurosciences - Simulation - Health
FUNCTIONAL DESCRIPTION

The NeuralFieldSimulator computes numerically activity in two-dimensional neural fields by solving integral-differential equations involving transmission delays and visualizes the spatio-temporal activity. The tool includes a GUI that allows the user to choose field parameters. It is written in Python, open-source and is aimed to be promoted to become a major graphical visualization tool in the domain of neural field theory. We aim to establish this simulation software as the first open-source standard simulator for the neural field research community.

- Contact: Axel Hutt
- URL: https://gforge.inria.fr/projects/nfsimulator/

6.6. OpenVIBE

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

OpenViBE is a software platform for real-time neurosciences (that is, for real-time processing of brain signals). It can be used to acquire, filter, process, classify and visualize brain signals in real time from various signal sources. OpenViBE is free and open source software. It works on Windows and Linux operating systems.

- Participants: Yann Renard, Anatole Lécuyer, Fabien Lotte, Bruno Renier, Vincent Delannoy, Laurent Bonnet, Baptiste Payan, Jozef Legény, Jussi Tapio Lindgren, Alison Cellard, Loïc Mahé, Guillaume Serriere, Marsel Mano, Maureen Clerc Gallagher, Théodore Papadopoulo, Laurent Bougrain, Jérémy Frey and Nathanaël Foy
- Partners: CEA-List - GIPSA-Lab - INSERM
- Contact: Anatole Lécuyer, Hybrid/Inria Rennes-Bretagne Atlantique
- URL: http://openvibe.inria.fr

6.7. Platforms

6.7.1. EEG experimental room

A room at Inria Nancy - Grand Est is now dedicated to electroencephalographic recordings. An umbrella agreement and several additional experiment descriptions have been approved by the Inria Operational Legal and Ethical Risk Assessment Committee (COERLE).

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

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

5. New Software and Platforms

5.1. 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/

5.2. 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: Gaël Varoquaux, Bertrand Thirion, Loïc Estève, Alexandre Abraham, Michael Eickenberg, Alexandre Gramfort, Fabian Pedregosa Izquierdo, Elvis Dohmatob and Virgile Fritsch
- Contact: Bertrand Thirion
- URL: http://nilearn.github.io/

5.3. PyHRF

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

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

- Participants: Thomas Vincent, Solveig Badillo, Lotfi Chaari, Christine Bakhous, Florence Forbes, Philippe Ciuciu, Laurent Risser, Thomas Perret and Aina Frau Pascual
- Partners: CEA - NeuroSpin
- Contact: Florence Forbes
- URL: http://pyhrf.org

5.4. Scikit-learn

KEYWORDS: Classification - Learning - Clustering - Regession - 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: Olivier Grisel, Gaël Varoquaux, Bertrand Thirion, Michael Eickenberg, Loïc Estève, Alexandre Gramfort, Arthur Mensch

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

- Contact: Olivier Grisel

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

SISTM Project-Team

6. New Software and Platforms

6.1. New software

6.1.1. *clogitLasso*

Lasso Estimation of Conditional Logistic Regression Models for Case-Crossover and Matched Case-Control Studies

- KEYWORDS: Classification , Statistics , Cluster , Machine learning , Regression
- FUNCTIONAL DESCRIPTION Fit a sequence of conditional logistic regression models with lasso, for small to large sized samples.
- Contact: Marius Kwémou
- URL: https://github.com/robingenuer/

6.1.2. *COVVSURF*

Combination of Clustering Of Variables and Variable Selection Using Random Forests

- KEYWORDS: Classification , Statistics , Cluster , Machine learning , Regression
- FUNCTIONAL DESCRIPTION This package implements a two stage strategy, where first we use ClustOfVar package to perform a clustering of variables and second we use VSURF package to select features (i.e. synthetic variables built in the first step).
- Contact: Robin Genuer
- URL: https://github.com/robingenuer/CoVVSURF

6.1.3. *NPflow*

Bayesian Nonparametrics for Automatic Gating of Flow-Cytometry Data

- KEYWORDS: Bayesian estimation , Bioinformatics , Biostatistics
- FUNCTIONAL DESCRIPTION Dirichlet process mixture of multivariate normal, skew normal or skew t-distributions modeling oriented towards flow-cytometry data pre-processing applications.
- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/NPflow/

6.1.4. *tcgsaseq*

Time-Course Gene Set Analysis for RNA-Seq Data

- KEYWORDS: Genomics , Biostatistics , Statistical modeling , RNA-seq , Gene Set Analysis
- FUNCTIONAL DESCRIPTION Gene set analysis of longitudinal RNA-seq data with variance component score test accounting for data heteroscedasticity through precision weights.
- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/tcgsaseq/

6.1.5. *CD4 Shiny*

Reference curves for CD4 response to antiretroviral therapy in HiV infected patients

- KEYWORDS: HIV infection, antiretroviral therapy, cd4 response, reference curves, quantile regression
- FUNCTIONAL DESCRIPTION References curves for CD4 response to antiretroviral therapy in HIV infected patients derived from large cohorts and estimated according to known factors associated with the response to antiretroviral therapy.
- Contact: Rodolphe Thiébaut
- URL: http://shiny.isped.u-bordeaux.fr/CD4refcurves/

6.2. Older software still maintained by SISTM

6.2.1. NIMROD

Normal approximation Inference in Models with Random effects based on Ordinary Differential equations

- KEYWORDS: Biostatistics - Optimization
- FUNCTIONAL DESCRIPTION We have written a specific program called NIMROD for estimating parameter of ODE based population models.
- Contact: Rodolphe Thiebaut
- URL: http://etudes.isped.u-bordeaux2.fr/BIOSTATISTIQUE/NIMROD/documentation/html/index.html

6.2.2. R2GUESS

Graphical processing Unit Evolutionary Stochastic Search

- KEYWORDS: Bioinformatics - Biostatistics
- 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
- URL: https://cran.r-project.org/web/packages/R2GUESS/index.html

6.2.3. 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. Under development, and soon to be available on the CRAN website, this package implements a Time-course Gene Set Analysis method and provides useful plotting functions facilitating the interpretation of the results.
- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/TcGSA/index.html

6.2.4. VSURF

Variable Selection Using Random Forests

- KEYWORD: Bioinformatics
- FUNCTIONAL DESCRIPTION An R package for Variable Selection Using Random Forests. Available on CRAN, this package performs an automatic (meaning completely data-driven) variable selection procedure. Originally designed to deal with high dimensional data, it can also be applied to standard datasets.
- Contact: Robin Genuer
- URL: https://cran.r-project.org/web/packages/VSURF/index.html

6.2.5. marqLevAlg

Function optimization (minimization or maximization)

- KEYWORDS: Optimization - Biostatistics
- FUNCTIONAL DESCRIPTION An R package for function optimization. Available on CRAN, this package performs a minimization of function based on the Marquardt-Levenberg algorithm. This package is really useful when the surface to optimize is non-strictly convex or far from a quadratic function. A new convergence criterion, the relative distance to maximum (RDM), allows the user to have a better confidence in the stopping points, other than basic algorithm stabilization.
- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/marqLevAlg/index.html

VISAGES 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: Olivier Commowick, Rene-Paul Debroize, Florent Leray and Renaud Hédouin
- Contact: Olivier Commowick
- APP number: IDDN.FR.001.460020.000.S.P.2015.000.31230
- URL: https://github.com/Inria-Visages/Anima-Public/wiki

6.2. MedInria

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

SCIENTIFIC DESCRIPTION: It aims at creating an easily extensible platform for the distribution of research algorithms developed at Inria for medical image processing. This project has been funded by the D2T (ADT MedInria-NT) in 2010 and renewed in 2012. The VisAGeS team leads this Inria national project and participates in the development of the common core architecture and features of the software as well as in the development of specific plugins for the team's algorithm.
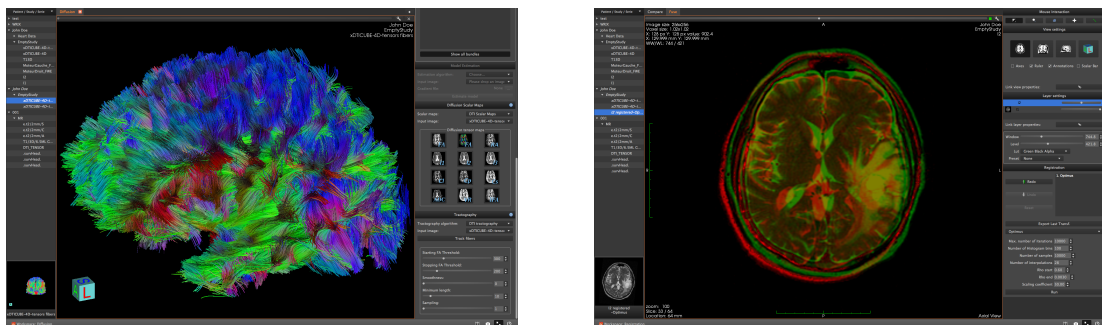

Figure 2. The medInria software platform: Tractography overlapped with 3D image (left), and Fused view of registered images (right).

FUNCTIONAL DESCRIPTION: MedInria is a free software platform dedicated to medical data visualization and processing as illustrated in Fig. 2 .

- Participants: Olivier Commowick and Rene-Paul Debroize
- Partners: HARVARD Medical School - IHU - LIRYC - IHU - Strasbourg - NIH
- Inria structures involved : ASCLEPIOS, ATHENA, PARIETAL, VISAGES
- Contact: Olivier Commowick
- URL: http://med.inria.fr
- APP number: IDDN.FR.001.130017.000.S.A.2012.000.31230

6.3. Shanoir

SHAring NeurOImaging Resources

KEYWORDS: Shanoir - Webservices - Data base - Biology - Health - DICOM - Neuroimaging - Medical imaging - PACS - Nifti - Data Sharing - Web Application

FUNCTIONAL DESCRIPTION: SHAring NeurOImaging Resources (Shanoir, Previously InriaNeuroTk) is an open source software platform designed to structure, manage, archive, visualize and share neuroimaging data with an emphasis on multi-centric collaborative research projects. It provides common features of neuroimaging data management systems along with research-oriented data organization and enhanced accessibility (see Fig. 3).

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

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

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

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

Shanoir serves neuroimaging researchers in organizing efficiently their studies while cooperating with other laboratories. By managing patient privacy, Shanoir allows the exploitation of clinical data in a research context. It is finally a handy solution to publish and share data with a broader community.
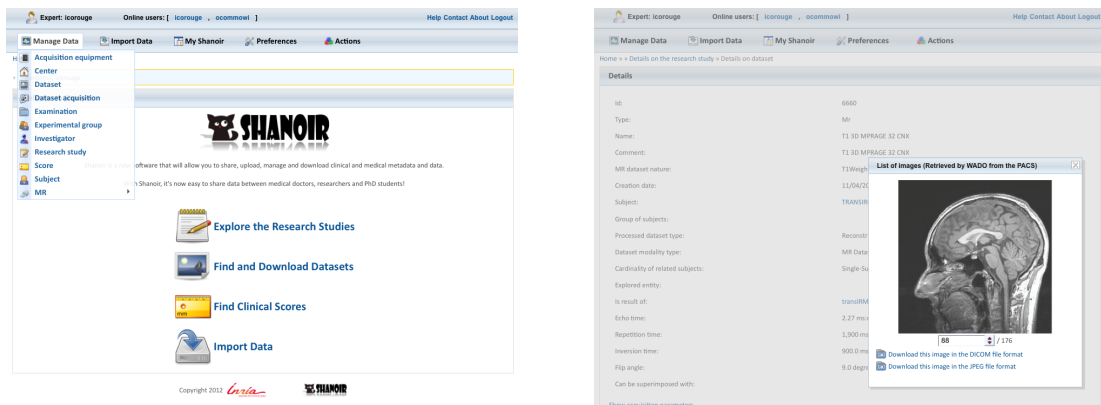
Figure 3. The SHANOIR software is a web application to share, archive, search and visualize neuroimaging data.

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

- Participants: Michael Kain, Christian Barillot, Anthony Baire, Mathieu Simon, Julien Louis, Isabelle Corouge, Élise Bannier, Aneta Morawin and Yao Chi
- Partners: CNRS - INSERM - Université de Rennes 1
- Contact: Christian Barillot
- URL: http://shanoir.gforge.inria.fr
- APP number: IDDN.FR.001.520021.003.S.A.2008.000.31230 (2014/08/20)

6.4. QtShanoir

KEYWORDS: Shanoir - Qt - Webservices - Soap - C++ - Health - DICOM - Plug-in - Medical imaging - Nifti
SCIENTIFIC DESCRIPTION: QtShanoir is based on Qt/C++ librairie. It interacts with the Shanoir server using SOAP web services provided. This application queries the server and displays hierarchical data extracted in tree view. Data could also be easily downloaded or uploaded on the server. In order to extend the Shanoir environment, QtShanoir is developed to contain two shared libraries:

- "GUI" that represents all user interfaces.
- "DAO" that takes in charge the data model. This library assures the connection to the server and provides all QtShanoir services : research, download and upload of Processed Dataset (NIfTI).

QtShanoir dynamic libraries are already reused and integrated in other projects: in the software medInria and in an under development command line program.
FUNCTIONAL DESCRIPTION: QtShanoir is a graphical client application of the medical imaging database Shanoir. This application provides various functionalities to satisfy researchers' needs. It allows users to:

- explore neuroimaging data derived from multicenter research trials. Through an intuitive user interface, users could easily visualize voluminous amount of structured data: studies, patients and datasets extracted from Shanoir
- download and to upload data from the server.

This application is available on Windows, UNIX, MacOs X. It is integrated as a plugin in medInria, a multi-plateform for medical image processing and visualization.

- Participants: Olivier Commowick and Florent Leray

- Contact: Christian Barillot

- URL: http://qtshanoir.gforge.inria.fr

- APP number: IDDN.FR.001.130017.000.S.A.2012.000.31230 (2012/02/08)

6.5. ShanoirUploader

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

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 as illustrated in Fig. 4 . 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.
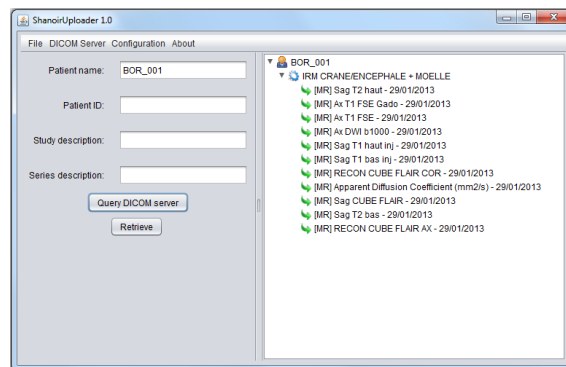

Figure 4. The ShanoirUploader software is a desktop application designed to interact with a PACS to query and retrieve the data stored on any PACS.

- Participants: Michael Kain, Inès Fakhfakh and Christian Barillot

- Contact: Christian Barillot

- URL: http://shanoir.gforge.inria.fr

- APP number: IDDN.FR.001.380026.000.S.P.2015.000.31230 (2015/09/11)

6.6. iShanoir

KEYWORDS: Shanoir - Biology - Health - Neuroimaging - Mobile application - Medical imaging - Biomedical imaging

FUNCTIONAL DESCRIPTION iShanoir is an iOS application, designed for iPhone and iPad. On base of this application a Shanoir server can be accessed as illustrated in Fig. 5 . For this the Shanoir SOAP web-services are called. iShanoir can be used to access and navigate in the data tree structure, stored on a Shanoir server. iShanoir displays as well additional meta data corresponding to the data entities in the tree structure. On base of these informations image files (NIfTI and DICOM) can be selected and downloaded on a local iPhone/iPad in a temporary cache. From this cache the files can be opened and displayed with a corresponding viewer, the user already has to have installed on his device.
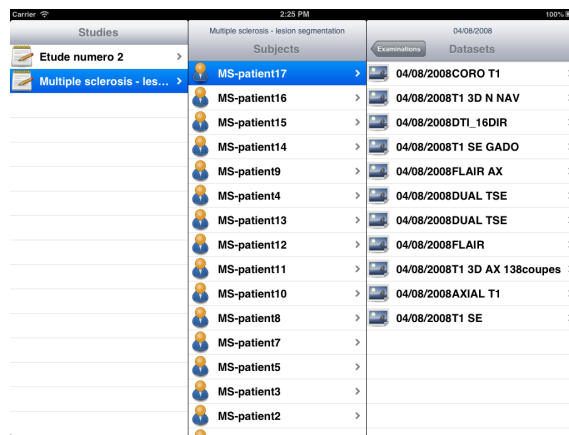

Figure 5. The iShanoir interface, showing the browsing tabs within the research studies stored in the Shanoir database.

- Participants: Michael Kain and Christian Barillot
- Contact: Christian Barillot
- URL: http://shanoir.gforge.inria.fr

6.7. autoMRI

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

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

FUNCTIONAL DESCRIPTION: 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).
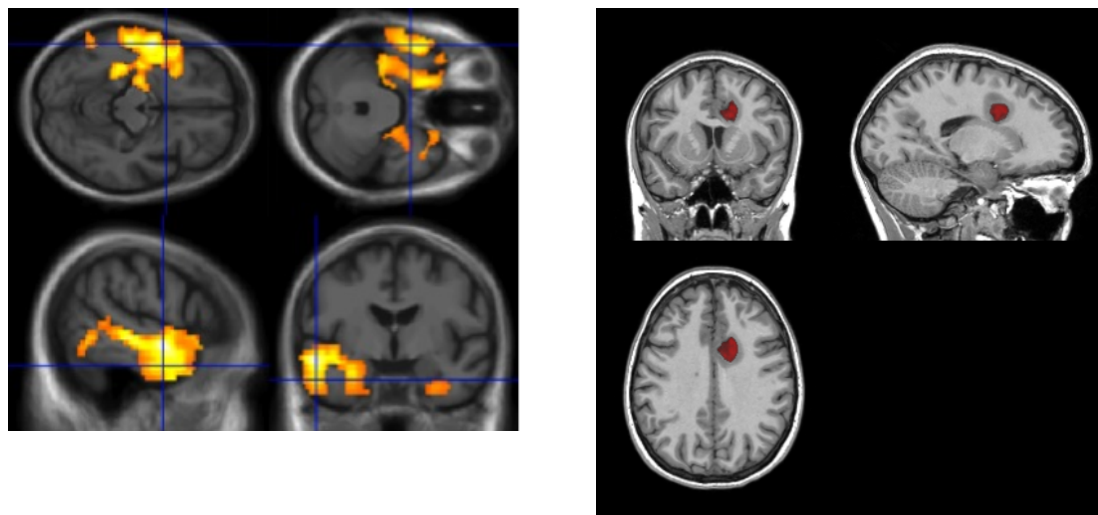

Figure 6. Illustrations of results obtained with autoMRI: Conjunction map showing areas of hypoperfusion and hypometabolism in semantic dementia (left) and detection of relaxometry defect in an MS patient (right).

- Participants: Isabelle Corouge, Quentin Duché, Cédric Meurée, Pierre Maurel and Élise Bannier.
- Contact: Isabelle Corouge
- URL: http://www.irisa.fr/visages/
- APP number: Part in IDDN.FR.001.130017.000.S.A.2012.000.31230

6.8. Integration of EEG and fMRI

KEYWORDS: medical imaging - EEG - fMRI

FUNCTIONAL DESCRIPTION: Related to the project Hemisfer there have been development of new functions, scripts and demos for the acquisition and processing of the EEG and fMRI data in Real-time. These include:

- Functions for fMRI header info reader, volume reader, motion correction, slice time correction nifty output conversion, real time fMRI initialization, real time fMRI processing, z-score calculation, volume smoother, alignment, etc., functions for real time EEG data acquisition, filtering, power calculation and display.
- Scripts for various protocols used in offline fMRI experiments, real time processing loop for EEG and fMRI.
- Demo for real time acquisition of the EEG and fMRI data, demo for real time processing efficiency of the fMRI data, demo for the real time processing of EEG data, real time z-Score for fMRI data.
- Several small aux functions for I/O interfaces (e.g. com, serial)

In the current stage the prototype also relies on various other free toolboxes (e.g. SPM, pnet).

- Participants: Marsel Mano, Lorraine Perronnet, Anatole Lecyuer, Christian Barillot.
- Contact: Marsel Mano
- International Patent Number: PCT/EP2016/1652279

6.9. Platforms

6.9.1. The Neurinfo Platform

VisAGeS is the founding actor of an experimental research platform which was installed in August 2009 at the University Hospital of Rennes. The University of Rennes 1, Inria, Inserm for the academic side, and the University Hospital of Rennes and the Cancer Institute "Eugene Marquis" for the clinical side, are partners of this neuroinformatics platform called Neurinfo [0]. This platform has been supported under the "Contrat de Projets Etat-Région" (Christian Barillot is the PI) and has received a total amount of 4.01 M€ for the period 2007–2014. European (FEDER), National (through Ministry of research, Inria, Inserm and ANR) and local councils (Brittany Region, Ille et Vilaine, and Rennes Metropole) have joined their effort to support this operation for a total amount of 4 010 k€ (600 k€ for the infrastructures, 2 850 k€ for the equipments and 560 k€ for the functioning). This application was set up through the Regional PIMATGI initiative coordinated by INSERM in Brittany (C. Roux). The overall PIMATGI initiative served for the financing of three distinct, but complementary, platforms: Neurinfo, TheraFONC as a technical platform dedicated to therapy guided by functional imaging especially in the oncology domain (Inserm U650 - LaTIM, Dir. Ch. Roux, Brest), and TherA-Image as a platform dedicated to image guided mini-invasive surgery and therapy especially in the domain of cardio-vascular diseases (U642 -LTSI, Dir. L. Senhadji, Rennes).

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

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

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

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

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[0]http://www.neurinfo.org

6. New Software and Platforms

6.1. mlxR

A R package for the simulation and visualization of longitudinal data. 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.

6.2. FactoMineR

A R package dedicated to principal component methods (PCA, Correspondence Analysis for contingency tables, Multiple Correspondence Analysis for categorical data, MFA for multi-blocks data). Google users group and you-tube videos available.

6.3. missMDA

A R package to perform principal component methods (PCA, MCA, MFA) with missing values and to impute continuous, categorical and mixed data. Multiple imputation is available.

6.4. denoiseR

A R package that approximates a low-rank matrix from noisy data (Gaussian and Poisson Noise). Singular values shrinkage methods are implemented.

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AIRSEA Project-Team

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6. New Software and Platforms

6.1. AGRIF

Adaptive Grid Refinement In Fortran

FUNCTIONAL 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.

- Participants: Laurent Debreu, Marc Honnorat and Cyril Mazauric
- Contact: Laurent Debreu
- URL: http://www-ljk.imag.fr/MOISE/AGRIF

6.2. 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

6.3. DiceDesign

Designs of Computer Experiments
FUNCTIONAL DESCRIPTION

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

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

6.4. DiceEval

Construction and Evaluation of Metamodels
FUNCTIONAL DESCRIPTION

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

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

6.5. 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 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

6.6. 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. Freshkiss3D (FREe Surface Hydrodynamics using KInetic SchemeS)

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

- Participants: Nora Aïssiouene, Marie-Odile Bristeau, David Froger, Jacques Sainte-Marie, Fabien Souillé
- Formerly: Emmanuel Audusse, Anne-Céline Boulanger, Alain Dervieux, Raouf Hamouda, Bijan Mohammadi
- Partners: CEREMA – UPMC
- Contact: Jacques Sainte-Marie

A review of last developments is given in § 7.5.1 . See [20] for recent numerical results obtained thanks to the Freshkiss3D software.

6.2. TSUNAMATHS

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, Raouf Hamouda, Jacques Sainte-Marie
- Contact: Jacques Sainte-Marie
- URL: http://ange.raoufhamouda.com/tsunami/en_motivation.htm

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

4. New Software and Platforms

4.1. Equinox

FUNCTIONAL DESCRIPTION

EQUINOX is a code dedicated to the numerical reconstruction of the equilibrium of the plasma in a Tokamak. The problem solved consists in the identification of the plasma current density, a non-linear source in the 2D Grad-Shafranov equation which governs the axisymmetric equilibrium of a plasma in a Tokamak. The experimental measurements that enable this identification are the magnetics on the vacuum vessel, but also polarimetric and interferometric measures on several chords, as well as motional Stark effect measurements. The reconstruction can be obtained in real-time and the numerical method implemented involves a finite element method, a fixed-point algorithm and a least-square optimization procedure. A deposit with APP (Agence pour la protection des programmes) has been done in 2016.

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

4.2. VacTH

FUNCTIONAL DESCRIPTION

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

- Contact: Blaise Faugeras

4.3. CEDRES++

FUNCTIONAL DESCRIPTION

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

Under this assumption of axisymmetric configuration, the equilibrium in the whole space reduces to solving a 2D problem in which the magnetic field in the plasma is described by the well known Grad Shafranov equation. The unknown of this problem is the poloidal magnetic flux. The P_1 finite element code CEDRES++ solves this free boundary equilibrium problem in direct and inverse mode and in static and evolutive formulations. The direct problem consists in the computation of the magnetic configuration and of the plasma boundary, given a plasma current density profile and the total current in each poloidal field coils (PF coils) for the static case and the voltages applied to PF supplies in the evolutive one. The aim of the inverse problem is to find currents in the PF coils in order to best fit a given plasma shape. The code is one of the free boundary codes avalaible in the european Eurofusion - WPCD (WorkPackage Code Development for integrated modelling) platform.

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

4.4. FEEQS.M

Finite Element Equilibrium Solver in MATLAB
FUNCTIONAL DESCRIPTION

FEEQS.M (Finite Element Equilibrium Solver in Matlab) is a MATLAB implementation of the numerical methods in [Heumann2015] to solve equilibrium problems for toroidal plasmas. Direct and inverse problems for both the static and transient formulations of plasma equilibrium can be solved. FEEQS.M exploits MATLAB's evolved sparse matrix methods and uses heavily the vectorization programming paradigm, which results in running times comparable to C/C++ implementations. FEEQS.M complements the production code CEDRES++ in being considered as fast prototyping test bed for computational methods for equilibrium problems. This includes aspects of numerics such as improved robustness of the Newton iterations or optimization algorithms for inverse problems (see [4]). The recent developments include:

- the comparison of FEM-BEM coupling (with B. Faugeras),
- overlapping mesh methods for free-boundary equilibrium,
- direct and inverse modes for simulations and optimal control approach to breakdown (with Eric Nardon, CEA Cadarache)
- Participant: Holger Heumann
- Contact: Holger Heumann
- URL: https://scm.gforge.inria.fr/svn/holgerheumann/Matlab/FEEQS.M

4.5. Fluidbox

FUNCTIONAL DESCRIPTION

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

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

4.6. Jorek-Django

FUNCTIONAL DESCRIPTION

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

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

4.7. FBGKI

Full Braginskii
FUNCTIONAL DESCRIPTION

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

- Contact: Sebastian Minjeaud

4.8. PlaTo

A platform for Tokamak simulation
FUNCTIONAL DESCRIPTION

PlaTo (A platform for Tokamak simulation) is a suite of data and software dedicated to the geometry and physics of Tokamaks. Plato offers interfaces for reading and handling distributed unstructured meshes, numerical templates for parallel discretizations, interfaces for distributed matrices and linear and non-linear equation solvers. Plato provides meshes and solutions corresponding to equilibrium solutions that can be used as initial data for more complex computations as well as tools for visualization using Visit or Paraview. Plato is no more developed and is in the process of being merged with Jorek-Django

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

CLIME Project-Team

6. New Software and Platforms

6.1. Heimdali

- Participants: Isabelle Herlin, Dominique Bereziat and David Froger
- Contact: Isabelle Herlin

SCIENTIFIC DESCRIPTION

The main components of Heimdali concern:

- the pre/post processing of image sequences,
- the image assimilation with numerical models,
- the visualization of image sequences.

FUNCTIONAL DESCRIPTION

The initial aim of the image processing library Heimdali was to replace an internal Inria library (named Inrimage) by a library based on standard and open source tools, and mostly dedicated to satellite acquisitions.

The leading idea of the library is to allow the following issues:
- making easier the sharing and development of image assimilation softwares. For that purpose, the installation is easily achieved with the package manager Conda.
- developing generic tools for image processing and assimilation based on ITK (Insight Segmentation and Registration Toolkit http://www.itk.org). In reverse provide tools to ITK and contribute to the ITK community. Our software corresponds to issues related to satellite acquisitions but could be of interest for processing medical image sequences.

6.2. Image Forecast

- Authors: Isabelle Herlin and Yann Lepoittevin
- Contact: Isabelle Herlin

SCIENTIFIC DESCRIPTION

From a given number of images, Image Forecast synthetizes the future images at a given and short temporal horizon.

FUNCTIONAL DESCRIPTION

Image forecast includes two components:

- it estimates the dynamics from an image sequence. Various options are available in the software: stationarity, Lagrangian conservation, description of structures. The result is the motion field explaining the temporal evolution of image data.
- the estimated dynamics is applied for forecasting future images at short temporal horizon.

6.3. Polyphemus

- Participants: Sylvain Doré (CEREA, École des Pont ParisTech) and Vivien Mallet
- Contact: Vivien Mallet
- URL: http://cerea.enpc.fr/polyphemus/

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.

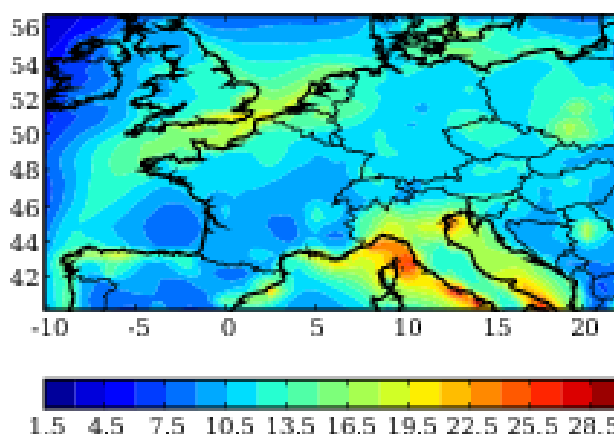Fig. 1 depicts a typical result produced by Polyphemus.

Figure 1. Map of the relative standard deviation (or spread, %) of an ensemble built with Polyphemus (ozone simulations, $\mu g\ m^{-3}$). The standard deviations are averaged over the summer of 2001. They provide an estimation of the simulation uncertainties.

Clime is involved in the overall design of the system and in the development of advanced methods in model coupling, data assimilation and uncertainty quantification (through model drivers and post-processing).

6.4. SoundCity - Ambiciti

- Authors: Pierre-Guillaume Raverdy (SED), Fadwa Rebhi (Mimove), Cong Kinh Nguyen (Mimove), Rajiv Bhatia (TheCivicEngine), Vivien Mallet and Valerie Issarny (Mimove)
- Contact: Valerie Issarny (Mimove)

FUNCTIONAL DESCRIPTION

Ambiciti measures the actual noise levels to which you are exposed. It can monitor noise levels throughout the day and inform you about your instantaneous, hourly and daily exposures.
Ambiciti also computes the air quality index in your region or at the exact location where you stand. You can also access to forecasts.

Ambiciti includes a lot of features:

- Measuring noise level, anytime on demand or automatically during the day,

- Air quality indexes, in the past, present and future hours or days,

- Pollution levels for nitrogen dioxide, fine particulate matter and ozone,

- Statistics on exposure to pollutions, hourly, daily, during daytime and nighttime,

- Maps with your noise measurements,

- Hourly air quality maps, at street resolution in Paris, San Francisco, Oakland, Richmond (California), at present time,

- The recommendation of pedestrian routes which minimize the exposure to noise pollution or to air pollution,

- The ability to take pictures with pollution levels on top.

6.5. Urban noise analysis

- Authors: Vivien Mallet, Raphael Ventura and Guillaume Cherel

- Contact: Vivien Mallet

FUNCTIONAL DESCRIPTION

This software merges noise simulations and mobile observations. It can extract a given region of a noise map and filter out the buildings. It extends a previous software for data assimilation of air pollution observations at city scale. This prior software computes the so-called best linear unbiased estimator (BLUE), with a special background error covariance model that depends on the city geometry. The extension for noise introduces special treatments for the errors in mobile observations, and includes more statistical verifications.

The software also comes with a Python module for the management of a large database of mobile noise measurements, especially with many filters relying the observations metadata.

The software finally includes the automatic generation of a report based on intensive measurements in a city district. This report targets participants of crowdsensing experiments.

6.6. Verdandi

- Participants: Vivien Mallet, Gautier Bureau (Medisim), Dominique Chapelle (Medisim), Sébastien Gilles (Medisim) and Philippe Moireau (Medisim)

- Contact: Vivien Mallet

- URL: http://verdandi.gforge.inria.fr/

FUNCTIONAL DESCRIPTION

Verdandi is a free and open-source (LGPL) library for data assimilation. It includes various 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.

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

5. New Software and Platforms

5.1. APPartFlow

FUNCTIONAL DESCRIPTION

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

- Contact: Thierry Goudon

5.2. Compass

FUNCTIONAL DESCRIPTION

Compass is a parallel code for the discretization of polyphasic flows by Finite Volumes methods. The code is mainly devoted to applications in porous media. It works on quite general polyhedral meshes.

- Participants: Thierry Goudon, Roland Masson, Cindy Guichard, Chang Yang and Robert Eymard
- Contact: Roland Masson
- URL: http://math.unice.fr/~massonr/ComPASSHighEnergyGeothermy.html

5.3. NS2DDV

FUNCTIONAL DESCRIPTION

It is devoted to the simulation of non-homogeneous viscous flows, in two-dimensional geometries. The code is based on an original hybrid Finite Volume/Finite Element scheme, it works on unstructured meshes and can include mesh refinements strategies.

- Contact: Creusé Emmanuel
- URL: math.univ-lille1.fr/~simpaf/SITE-NS2DDV/home.html

5.4. SimBiof

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

FLUMINANCE Project-Team

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: Etienne Memin
- Contact: Etienne Memin
- 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: Etienne Memin
- 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: Etienne Memin
- Contact: Etienne Memin
- 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: Etienne Memin and Anne Cuzol
- Contact: Etienne Memin
- URL: http://fluid.irisa.fr

5.5. TYPHOON

GPU implementation of wavelet based motion estimator for Lidar data. This code is developed in coproperty between Inria and Chico.
FUNCTIONAL DESCRIPTION Typhoon is a motion estimation software specialized in fluid motion estimation. It is based on a dense optical flow technique associated to a multiscale wavelet representation of the estimated motion.

- Participants: Pierre Derian, Christopher Mauzey and Etienne Memin
- Partner: CSU Chico
- Contact: Etienne Memin
- URL: http://phys.csuchico.edu/lidar/typhoon/

5.6. GRT3D

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.

- Participants: Yvan Crenner, Jocelyne Erhel
- Partner: ANDRA
- Contact: Jocelyne Erhel
- URL: http://www.irisa.fr/sage/recherche/chemistry.html

5.7. H2OLab

KEYWORDS: Simulation - Multiscale - Uncertainly - Heterogeneity - Hydrogeology - Groundwater - Contamination - Energy
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: Jean-Raynald De Dreuzy, Jocelyne Erhel
- Partners: Université de Rennes 1 - CNRS - Université de Lyon - Université de Poitiers
- Contact: Jocelyne Erhel
- URL: http://h2olab.inria.fr/

5.8. PALMTREE

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.

- Participants: Lionel Lenotre
- Contact: Jocelyne Erhel

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

6. New Software and Platforms

6.1. TsunamiLab

Participant: Antoine Rousseau.

Tsunami-Lab is an educational platform enabling simulation and visualization of tsunami effects in real time, with several historical scenarios and the possibility to build your own one. The target of this project is to provide students as well as general audience with an educational tool, intended to reduce tsunamis impact in Chile and help sparing human lives.

Tsunami-Lab was initated by José Galaz, engineer in mathematics and civil ingeneering, when he was working at the National Research Center for Integrated Gestion of Natural Hazards (CIGIDEN). The app is born with the match of a need - teach general audience more efficient methods to decrease tsunamis impact and spare human lives - and the use of new technologies. Later, a collaboration came up between CIGIDEN, Inria Chile and Inria (team LEMON) in order to optimize this project development.
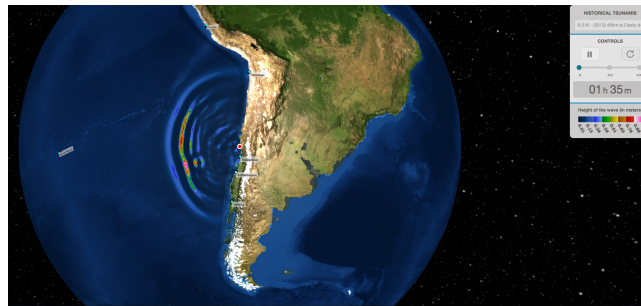

Figure 2. Propagation of a tsunami wave created by the a 8.3M earthquake in Chile (2015) using the TsunamiLab platform.

- Participant: Antoine Rousseau
- Contact: José Galaz, jdgalazm@gmail.com
- URL: https://tsunamilab.inria.fr/

6.2. SW2D

Participants: Carole Delenne, Vincent Guinot.

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

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

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

- three different closure relationships between the averaged flow variables and porosity-based fluxes

- 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.
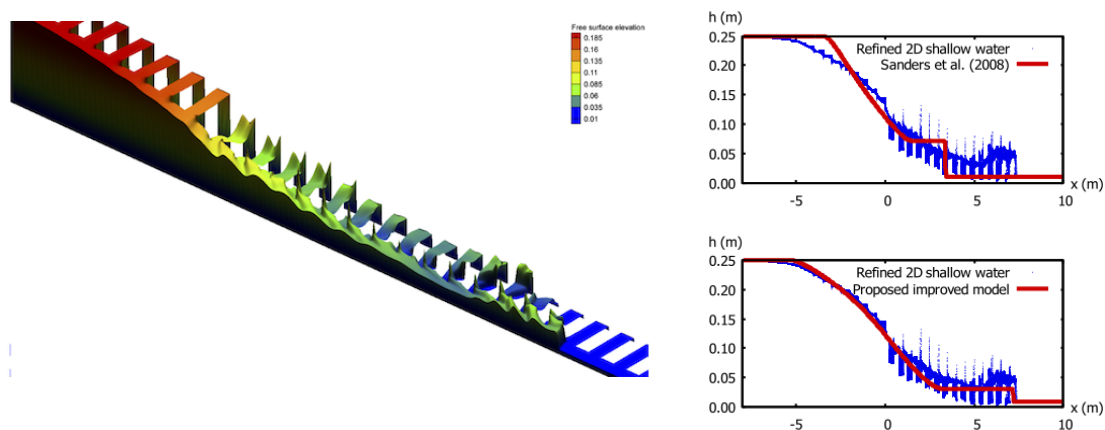

Figure 3. Propagation of a flood wave into a channel with lateral storage. Refined 2D simulation using the SW2D computational code

- Contact: Vincent Guinot
- URL: http://vincentguinot.free.fr

6.3. WindPoS

Participant: Antoine Rousseau.

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).
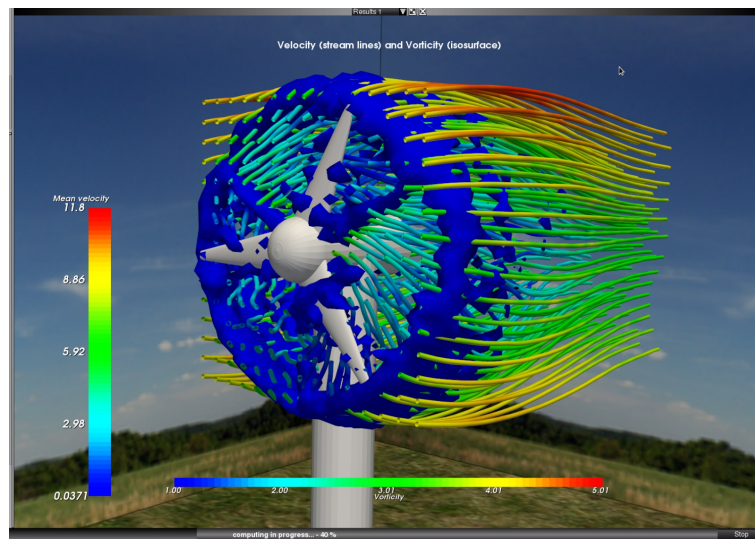
Figure 4. Velocity streamlines and vorticity around a wind mill (artistic view). WINDPOS Project.

In 2013, WindPoS became the kernel of the wind farm modeling of the Fundacion Inria Chile. In France, its development is going on through the collaborative Modéol project on the evaluation of wind potential.

This is a joint work with Mireille Bossy from the team TOSCA.

- Contact: Mireille Bossy, mireille.bossy@inria.fr
- URL: http://windpos.inria.fr

MAGIQUE-3D Project-Team

5. New Software and Platforms

5.1. Elasticus

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 DIVA 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. Contrary to DIVA which only computes approximate solutions with P1, P2 and P3 elements, Elasticus manages arbitrary orders for the spatial discretization with DG method.

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

5.2. Hou10ni

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).

- Participants: Julien Diaz, Marie Bonnasse-Gahot and Lionel Boillot
- Contact: Julien Diaz

5.3. Montjoie

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, elasto-dynamic 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. For time-domain simulations, a wide range of ODE (Ordinary Differential Equation) solvers have been implemented : high-order explicit or implicit time schemes. Several applications are currently available : wave equation, elastodynamics, aero-acoustics, Maxwell's equations.

- Participants: Marc Duruflé, Juliette Chabassier, Mamadou N'Diaye and Michaël Leguèbe
- Contact: Marc Duruflé
- URL: http://montjoie.gforge.inria.fr/

5.4. TMBM-DG

Time-Marching Based Methods-Discontinuous Galerkin

SCIENTIFIC DESCRIPTION TMBM-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 TMBM-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.

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

<div style="text-align:center; color:red;">

SERENA Team

</div>

5. New Software and Platforms

5.1. GEOFRACFLOW

GEOFRACFLOW

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

- Participants: Géraldine Pichot, Jocelyne Erhel, and Jean-Raynald De Dreuzy
- Contact: Géraldine Pichot
- URL: https://bil.inria.fr/fr/software/view/2653/tab

5.2. SBM

Skew Brownian Motion

SCIENTIFIC 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.

- Participants: Antoine Lejay, Géraldine Pichot
- Contact: Antoine Lejay
- URL: https://gforge.inria.fr/projects/sbm

5.3. Sklml

The OCaml parallel skeleton system

SCIENTIFIC DESCRIPTION Writing parallel programs is not easy, and debugging them is usually a nightmare. To cope with these difficulties, the skeleton programming approach uses a set of predefined patterns for parallel computations. The skeletons are higher-order functional templates that describe the program underlying parallelism. Sklml is a new framework for parallel programming that embeds an innovative compositional skeleton algebra into the OCaml language. Thanks to its skeleton algebra, Sklml provides two evaluation regimes to programs: a regular sequential evaluation (merely used for prototyping and debugging) and a parallel evaluation obtained via a recompilation of the same source program in parallel mode. Sklml was specifically designed to prove that the sequential and parallel evaluation regimes coincide.

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

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

STEEP Project-Team

6. New Software and Platforms

6.1. 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

6.2. InterfacesTRANUS

FUNCTIONAL DESCRIPTION

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

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

6.3. LUM_OSM

Land Use Mix calculation from OpenStreepMap data
FUNCTIONAL DESCRIPTION

The software uses Mapzen Metro Extracts to retrieve the OpenStreetMap data of a given region in the PostgreSQL format. Afterwards, a continuous representation of residential and activity land uses is created. Finally, a GIS output containing the degree of land use mixture is calculated by means of using the land uses maps. The implemented approach is documented in [9].

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

6.4. QGIS_Tranus_Reports

FUNCTIONAL DESCRIPTION

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

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

6.5. REDEM

REDuction Of EMission

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.

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

6.6. REDEM web

REDEM Web is a reimplementation of the REDEM soft as a web application. The main library which contains the code corresponding to REDEM model is written in Python and the web part uses Javascript.

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

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

6.7. Wassily

SCIENTIFIC DESCRIPTION

The software is structured in three different modules:

- the database module stores all the input-output data coming from Eurostat, OCDE, Insee or other sources.
- the computation module performs the input-output calculations
- the visualization module displays the results in a synthetic manner.

The database module is based on the SQlite format and makes use of SQL to manipulate the various tables involved in the process. The goal of this module is to provide a normalized data interface for the computation module, from various types of input-output data which are often stored as Excel sheet on web sites.

FUNCTIONAL DESCRIPTION

The purpose of this software ans website is to automatize most of the work of standard input-output analysis and to visualize the resultes in a user-friendly way in order to efficently adress related key environmental questions.

- Participants: Julien Alapetite and Jean-Yves Courtonne
- Contact: Jean-Yves Courtonne

TONUS Team

5. New Software and Platforms

5.1. SCHNAPS - KIRSCH

Participants: Emmanuel Franck, Pierre Gerhard, Philippe Helluy, Michel Massaro, Malcolm Roberts, David Coulette, Laura Mendoza, Bruno Weber.

SCHNAPS: Solveur pour les lois de Conservation Hyperboliques Non-linéaires Appliqué aux PlasmaS
SCIENTIFIC DESCRIPTION

The 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 or Xeon Phi). When designing new algorithms, it is important to adapt them to this kind of architecture. Practically, we use the MPI library for managing the coarse grain parallelism, while the OpenCL library 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. OpenCL programs are quite complicated to construct. For instance it is difficult to distribute efficiently the computation or memory operations on the different available accelerators. StarPU http://starpu.gforge.inria.fr/ is a runtime system developed at Inria Bordeaux that simplifies the distribution of tasks on heterogeneous compute units. We have started to use this software tool in SCHNAPS.

Because of the envisaged applications, which may be either academic or commercial, it is necessary to conceive a modular framework. The kernel 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. With our partner AxesSim, we also develop a C++ specific version of SCHNAPS for electromagnetic applications.
Since the middle of the year a specific version of SCHNAPS (called KIRSCH for Kinetic Representation of SChnaps) has been developed to handle Lattice Boltzwell schemes for MHD and fluid simulations.

FUNCTIONAL DESCRIPTION

SCHNAPS and KIRSCH are a generic Discontinuous Galerkin solver and an implicit Lattice Boltzmann solver, written in C, based on the OpenCL, MPI and StarPU frameworks.

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

5.2. Selalib

Participants: Sever Adrian Hirstoaga, Michel Mehrenberger, Pierre Navaro, Laurent Navoret, Thi Trang Nhung Pham, Christophe Steiner.

KEYWORDS: Plasma physics - Semi-Lagrangian method - PIC - Parallel computing - Plasma turbulence
SCIENTIFIC DESCRIPTION

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

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

FUNCTIONAL DESCRIPTION

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

- Partners: Max Planck Institute - Garching - IRMA, Université de Strasbourg - IRMAR, Université Rennes 1 - LJLL, Université Paris 6
- Contact: Michel Mehrenberger
- URL: http://selalib.gforge.inria.fr/

5.3. Django

Participants: Emmanuel Franck [correspondent], Boniface Nkonga, Ahmed Ratnani.

- Scientific description:
  The JOREK code is one of the most important MHD codes in Europe. This code written 15 years ago allows to simulate the MHD instabilities which appear in the Tokamak. Using this code the physicists have obtained some important results. However to run larger and more complex test cases it is necessary to extend the numerical methods used.
  In 2014, the DJANGO code has been created, the aim of this code is twofold: have a numerical library to implement, test and validate new numerical methods for MHD, fluid mechanics and Electromagnetic equations in the finite element context and prepare the future new JOREK code. This code is a 2D-3D code based on implicit time schemes and IsoGeometric (B-Splines, Bezier curves) for the spatial discretization.

- Functional description:
  DJANGO is a finite element implicit solver written in Fortran 2008 with a Basic MPI framework.

- Authors:
  Ahmed Ratnani (Max Planck Institut of Plasma Physic, Garching, Germany), Boniface Nkonga (University of Nice and Inria Sophia-Antipolis, France), Emmanuel Franck (Inria Nancy Grand Est, TONUS Team)

- Contributors:
  Mustafa Gaja, Jalal Lakhlili, Matthias Hoelzl and Eric Sonnendrücker (Max Planck Institut of Plasma Physic, Garching, Germany), Ayoub Iaagoubi (ADT Inria Nice), Hervé Guillard (University of Nice and Inria Sophia-Antipolis, France), Virginie Grandgirard, Guillaume Latu (CEA Cadarache, France)

- Year 2016:
  Between the years 2015 and 2016 the code has been partially rewritten using Fortran 2008 to prepare the implementation of new methods (compatible finite element spaces, 3D B-Splines meshes). The different models, hyperbolic, parabolic and elliptic introduced in the previous version of the code have been rewritten and validated. Actually, we will begin to introduce the Maxwell equations for the coupling with kinetic equations and the nonlinear fluid models (first step for the MHD simulations). A large effort of optimization and parallelization in the matrices assembly has been made and new preconditioning for elliptic models has been introduced.

  - Partners: Max Planck Institute - Garching - IRMA, Université de Strasbourg - Inria Nice Sofia- Antipolis
  - Contact: Emmanuel Franck

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.

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

6.2. Odin

Platform for advanced monitoring, control and optimisation of bioprocesses
KEYWORDS: Bioinformatics - Biotechnology
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: Melaine Gautier, Florian Guenn, Fabien Dilet, Olivier Calabro, Romain Primet, Serigne Sow, Olivier Bernard, Mathieu Lacage and Francesco Novellis
- Contact: Olivier Bernard
- URL: https://team.inria.fr/biocore/software/odin/

CARMEN Project-Team

6. New Software and Platforms

6.1. CEPS: a Cardiac ElectroPhysiology Simulator

The Carmen team develops a software library to perform high-performance numerical simulations in cardiac electrophysiology using unstructured three-dimensional grids. The software, called CEPS (*Cardiac Electrophysiology Simulation*) is developed as a common tool for researchers in the Carmen team and for our partners and colleagues in scientific computing and biomedical engineering. The goal of CEPS is to facilitate the development of new numerical methods and new physical models.

Compared to other existing software, 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. The largest part of CEPS was developed by the Junior Engineer M. Juhoor, supervised by N. Zemzemi, during the CEPS ADT (*Action de Développement Technologique*).

To enforce a sound development process, some engineering and validation tools are used:

- Git hosted at the Inria GForge (ceps) to manage versions;
- Cmake for the building process
- Jenkins, hosted at the Inria continuous integration service, which runs a test suite of about 200 tests after every commit.

Main users and developers of CEPS are the PhD students of Carmen, i.e.

- A. Gérard, who uses CEPS for patient-specific modeling, has implemented a bilayer model using coupled nodes.
- Charlie Douanla-Lountsi currently works on high-order temporal integration methods, for later integration in CEPS.
- P. E. Bécue is developing a code to run microscopic-scale models (section 3.4) and wrote a coupled node assembler to support this work.

Since January 2015, M. Fuentes from the *Service d'Experimentation et de Développement* (SED), is responsible for developing new features in CEPS, improve robustness, efficiency, and documentation. M. Juhoor, who has previously worked on CEPS, and works on the IDAM project, brings us from time to time his expertise. Actions done in 2016 include:

- support for P2 Lagrange finite Elements
- node partitioning using the PTScotch partitioner
- input files and VtkReader (M. Juhoor)
- code refactoring
- documentation writing

6.2. IDAM

The goal of the IDAM project is to define a collection of plugins in the MUSIC software in order to create realistic meshes for the CEPS code. MUSIC is a multimodal platform for cardiac imaging developed by the imaging team at IHU LIRYC (https://bil.inria.fr/fr/software/view/1885/tab). Information comes from magnetic resonance imaging and cardiac tomography performed in the clinic and in the LIRYC laboratories. Building complete cardiac models directly from imaging data requires expert knowledge and is time-consuming and error-prone: specific expertise and multiple software tools are often needed to process data stemming from medical imaging into realistic meshes and parameter distributions.

IDAM aims to streamline the workflow of a complete cardiac simulation: anatomical mesh generation from patient-specific data, description of simulation parameters, and eventually analysis of simulation results obtained by simulation packages like CEPS (https://bil.inria.fr/fr/software/view/2630/tab). IDAM integrates tools from other Inria teams by using specialized libraries, for example MMG (https://bil.inria.fr/fr/software/view/2824/tab) for high-quality mesh generation.
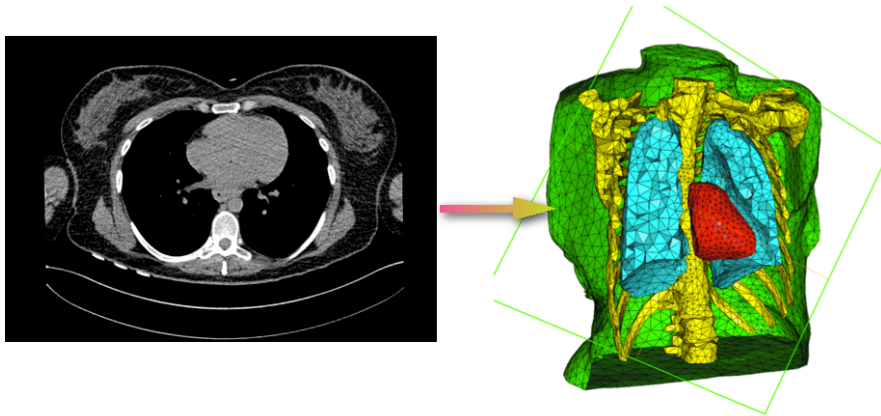

Figure 1. Mesh of a human torso and one of the X-ray computed-tomography slices on which it was based.

6.3. Platforms

6.3.1. *Propag-5*

Applied modeling studies performed by the Carmen team, especially M. Potse and M. Kania, in collaboration with IHU Liryc and foreign partners [39], [43], [18], [20], [14] [45], rely to a great extent on high-performance computations on the national supercomputers Curie, Occigen, and Turing. While the newly developed CEPS code is not ready to run efficiently on these systems we rely on an older code named Propag-5. This code 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. Relatively small contributions to this code have been made by the Carmen team.

The predecessor of Propag-5, named Propag-4, was developed by M. Potse at the *Université de Montréal* [8]. It was based on earlier model code developed there by the team of Prof. R. Gulrajani [50], [53], and was parallellized with OpenMP to utilize the shared-memory SGI supercomputers available there at the time. Propag-4 was the first code ever able to run a bidomain reaction-diffusion model of the entire human ventricles; a problem 30 times larger than what had been reported before [8].

In order to utilize the more recent distributed-memory architectures Propag-4 was transformed into the hybrid MPI-OpenMP code Propag-5 at the Institute of Computational Science in Lugano by D. Krause and M. Potse [49]. The resulting code has been used for numerous applied studies. An important limitation of the Propag code is that it relies on a semi-structured mesh with a uniform resolution. On the other hand, the code scales excellently to large core counts and, as it is controlled completely with command-line flags and configuration files, it can be used by non-programmers. It also features

- a plugin system for membrane models,
- a completely parallel workflow, including the initial anatomy input and mesh partitioning, which allows it to work with meshes of more than 10^9 nodes,

- a flexible output scheme allowing hundreds of different state variables and transient variables to be output to file, when desired, using any spatial and temporal subsampling,
- a configurable, LUSTRE-aware parallel output system in which groups of processes write HDF5/netCDF files, and
- CWEB documentation of the entire code base.

The code has been stable and reliable for several years, and only minor changes are being made currently. It can be considered the workhorse for our HPC work until CEPS takes over.

6.3.2. Gepetto

Gepetto, named after a famous model maker, is a sofware suite that 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 [52]. 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.
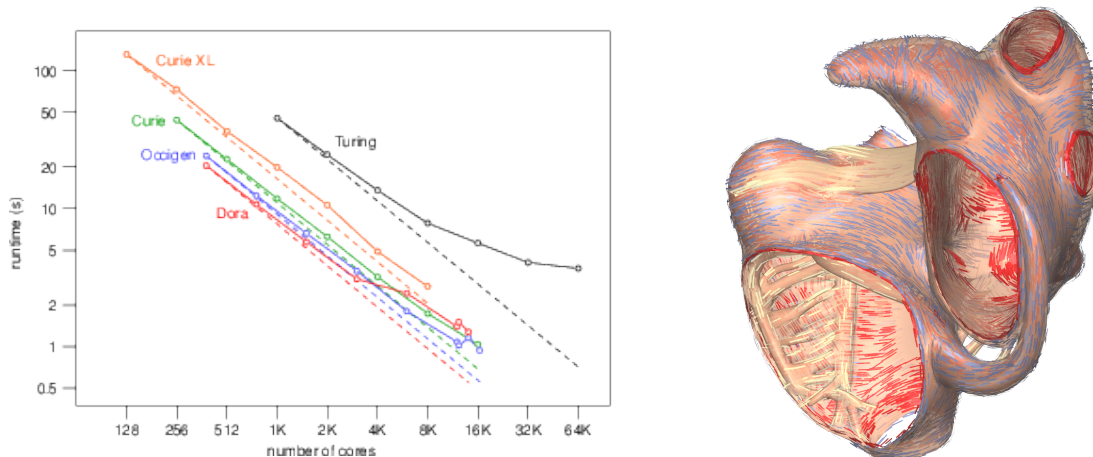

*Figure 2. **Left:** Strong scaling of the Propag-5 code on a monodomain reaction-diffusion equation for four systems: The Bull clusters Curie (small nodes and large nodes, XL) and Occigen, The Cray XC30 "Piz Dora" at the Swiss supercomputing center CSCS and the IBM BlueGene/Q "Turing". The graph shows the runtime needed for 10 ms of propagated activity using an explicit (forward) Euler integration. Dashed lines indicate the ideal scaling line with respect to the lowest number of cores measured. **Right:** Bundle structures and different layers of fiber orientation created by the Gepetto software.*

6.3.3. 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. The team also contributes a series of plugins for MUSIC through the IDAM project (section 6.2).

DRACULA Project-Team

5. New Software and Platforms

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

<p style="text-align:center">**M3DISIM Project-Team**</p>

6. New Software and Platforms

6.1. FELiScE-branch HappyHeart

Finite Elements for Life SCiences and Engineering problems

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

SCIENTIFIC DESCRIPTION

FELISCE – standing for "Finite Elements for LIfe SCiences and Engineering" – is a new finite element code. 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 cardiovascular models considered in the teams M3DISIM and REO – namely, involving fluid and solid mechanics, electrophysiology, and the various associated coupling phenomena.

FUNCTIONAL DESCRIPTION

In FELISCE we have prepared a branch called HappyHeart, which aims at providing a user-friendly interface able to deal efficiently with complex cardiovascular simulations. Started in 2013, the code is already quite large (about 55,000 lines of code in almost 700 different files) and its core is about to be complete. It includes among others full HPC functionalities, high-order finite elements, physics coupling and topology capabilities. Our purpose will then be to use the library to implement the sophisticated cardiovascular models of the team and couple them with Verdandi (data assimilation library) to provide patient-specific simulations.

- Participants: Gautier Bureau, Federica Caforio, Dominique Chapelle, Sébastien Gilles, Sébastien Imperiale, Philippe Moireau,
- Contact: Sébastien Gilles
- URL: http://felisce.gforge.inria.fr

6.2. HeartLab

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

SCIENTIFIC DESCRIPTION

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

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: Gautier Bureau, Radomir Chabiniok, Dominique Chapelle and Philippe Moireau
- Contact: Philippe Moireau
- URL: https://raweb.inria.fr/rapportsactivite/RA2013/m3disim/uid14.html

6.3. Verdandi

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

FUNCTIONAL DESCRIPTION

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

- Participants: Gautier Bureau, Dominique Chapelle, Philippe Moireau
- Contact: Philippe Moireau
- URL: http://verdandi.gforge.inria.fr/

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

6. New Software and Platforms

6.1. TiQuant

Tissue Quantifier

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

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 recognised. 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 [72]. It is implemented in portable object-oriented ANSI C++. The GUI is based on QT and supports real-time visualisation using OpenGL. TiQuant is embedded in the tissue modelling framework CellSys and thus is tightly linked with TiSim, a versatile and efficient simulation environment for tissue models. TiQuant provides an interface to VolView and further complements its functionality by linking to the open-source libraries ITK and VTK (itk/vtk.org). The image/volume processing chains currently implemented in TiQuant for example include techniques to segment conduit and cell segmentation from 3D confocal micrographs of liver tissue based on the Adaptive Otsu Thresholding method and a number of morphological operators [75]. TiQuant is currently extended by a machine learning component.

FUNCTIONAL DESCRIPTION

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.

- Contact: Dirk Drasdo
- URL: http://www.msysbio.com

6.2. TiSim

Tissue Simulator

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

FUNCTIONAL DESCRIPTION

TiSim (Tissue Simulator) is a software for agent-based models of multicellular systems. It permits model development with centre-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. A non-interactive mode to use the software also exists, accepting a combination of XML and HDF5 (hierarchical data format v5) as input, which produces output data in VTP (VTK) and HDF5 format. SBML, SBML_ODESolver and sundials are deployed for the creation and solution of the differential equations of metabolic networks and signalling pathways presented in SBML data format. TiSim permits agent-based simulations of multicellular systems and can be directly fed by processed image data from TiQuant.

- Contact: Dirk Drasdo
- URL: (No url yet)

MONC Project-Team

6. New Software and Platforms

6.1. CADMOS

KEYWORDS: Health - Cancer - Partial differential equation - Cartesian grid

- Participants: Olivier Saut, Julien Jouganous, Annabelle Collin and Olivier Gallinato
- Partners: CNRS - INP Bordeaux - Université de Bordeaux
- Contact: Olivier Saut
- URL: https://team.inria.fr/monc/software/

6.2. Carcinom

Computer-Assisted Research about Cancer growth and INsights on Oncological Mechanisms
KEYWORDS: Cancer - Data modeling - Regression

- Participants: Vivien Pianet and Simon Evain
- Contact: Sébastien Benzekry
- URL: https://team.inria.fr/monc/software/

6.3. MetaPoumon

KEYWORDS: Health - Evolution - Cancer - Medical imaging
FUNCTIONAL DESCRIPTION

The software evaluates the aggressiveness of pulmonary metastasis or response to treatment for predictive goal. To do this, we use a mathematical model based on a set of equations to nonlinear partial differential equations. This model is calibrated to the patient data using a longitudinal sequence of CT or MRI of the patient.

- Participants: Olivier Saut, Thierry Colin, Marie Martin and Julien Jouganous
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Olivier Saut
- URL: https://team.inria.fr/monc/software/

6.4. Nenuphar

KEYWORDS: Modeling - Oncologie - Cancer - Partial differential equation - Medical - Medical imaging
FUNCTIONAL DESCRIPTION

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

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

6.5. PapriK

- Contact: Cynthia Perier
- URL: https://team.inria.fr/monc/software/

6.6. SESAR

Monitor of the effect of RT on Retroperitoneal Sarcoma
KEYWORDS: Segmentation - Health - DICOM - Cancer - Medical imaging

- Partner: Institut Bergonié
- Contact: Cynthia Perier
- URL: https://team.inria.fr/monc/software/

6.7. SegmentIt

KEYWORDS: Health - Signal - Registration of 2D and 3D multimodal images - 3D - Image analysis - Image - Processing - Medical imaging
FUNCTIONAL DESCRIPTION

Image processing software for anatomical and functional data. Segmentation, registration and digital filtering. Assessement of the kidney perfusion and the kidney function (to be continued).

- Participants: Thierry Colin, Olivier Saut, Vivien Pianet, Agathe Peretti, Marie Martin, Sébastien Benzekry, Baudoin Denis De Senneville, Cynthia Perier, Benjamin Taton, Nicolas Grenier and Christian Combe
- Contact: Benjamin Taton
- URL: https://team.inria.fr/monc/software/

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

6. New Software and Platforms

6.1. DynPeak

KEYWORDS: Biology - Health - Physiology
SCIENTIFIC DESCRIPTION

DynPeak is an algorithm for pulse detection and frequency analysis in hormonal time series. A new release of the DynPeak Scilab atom toolbox has been delivered in 2016 https://atoms.scilab.org/toolboxes/Dynpeak/2.1.0

- Participants: Frédérique Clement, Serge Steer, Thierry Martinez
- Partner: INRA
- Contact: Frédérique Clement
- URL: https://team.inria.fr/mycenae/en/software/

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

5. New Software and Platforms

5.1. 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: Paul Vigneaux

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

5.3. 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 et 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: Paul Vigneaux and Ehouarn Maguet
- Partner: ENS Lyon
- Contact: Paul Vigneaux

5.4. 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: Emmanuel Grenier

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

6. New Software and Platforms

6.1. cardioXcomp

KEYWORDS: Cardiac Electrophysiology - Safety Pharmacology
FUNCTIONAL DESCRIPTION

cardioXcomp is a software dedicated to the safety pharmacology industry. It is developed in the framework of the joint laboratory (LabCom) "cardioXcomp" with the software company Notocord. Its purpose is to model the electrical potential of cardiomyocytes measured by a microelectrode array (MEA), and to model the effect of drugs on this signal. It was registered in November 2015 at the Agence pour la Protection des Programmes under the Inter Deposit Digital Number IDDNFR.001.480003.000.S.P.2015.000.31230.

- Participants: Jean-Frédéric Gerbeau, Fabien Raphel, Nejib Zemzemi
- Contact: Jean-Frédéric Gerbeau

6.2. FELiScE

Finite Elements for Life SCiences and Engineering problems
KEYWORDS: Finite element modeling - 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: Dominique Chapelle, Miguel Ángel Fernández Varela, Jean-Frédéric Gerbeau, Philippe Moireau, Marina Vidrascu, Sebastien Gilles, Benoit Fabreges, Axel Fourmont, Mikel Landajuela Larma, Damiano Lombardi, Matteo Aletti, Irene Vignon-Clementel and Faisal Amlani
- Contact: Jean-Frédéric Gerbeau
- URL: http://felisce.gforge.inria.fr

6.3. MODULEF

FUNCTIONAL DESCRIPTION

MODULEF is a legacy finite element library developed at Inria since the 1980's. Here, we limit ourselves to recent developments done within this library.

A numerical method to approximate the constitutive laws for rubber elasticity derived from polymer physics are implemented in Modulef.

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

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

6.4. SHELDDON

SHELls and structural Dynamics with DOmain decomposition in Nonlinear analysis

FUNCTIONAL DESCRIPTION

SHELDDON is a finite element library based on the Modulef package which contains shell elements, nonlinear procedures and PVM subroutines used in domain decomposition or coupling methods, in particular fluid-structure interaction.

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