



RESEARCH CENTER

FIELD

Digital Health, Biology and Earth

Activity Report 2015

Section Software

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COMPUTATIONAL BIOLOGY

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ABS Project-Team

5. New Software and Platforms

5.1. The Structural Bioinformatics Library

5.1.1. Web site:

<http://sbl.inria.fr>

5.1.2. The SBL : Overview

The SBL is a generic C++/python library providing algorithms and applications to solve complex problems in computational structural biology (CSB).

For Biologists, the key advantages are:

- comprehensive in silico environment providing applications,
- answering complex bio-physical problems,
- 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.

5.1.3. 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 Waals 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++ concepts⁰.
- **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.

⁰The design has been guided by that used in the Computational Geometry Algorithm Library (CGAL), see <http://www.cgal.org>. In a nutshell, concepts are a type system for types, and models are specific classes following this system.

5.1.4. 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.

5.1.5. 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.

5.1.6. SBL-CORE: the SBL for Low-level Developers and Contributors

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 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.

5.1.7. 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 (e.g. molecular dynamics 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/>).

5.1.8. 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.

AMIB Project-Team

5. New Software and Platforms

5.1. VARNA

KEYWORDS: Bioinformatics - Structural Biology

FUNCTIONAL DESCRIPTION

A lightweight Java Applet dedicated to the quick drawing of an RNA secondary structure. VARNA is open-source and distributed under the terms of the GNU GPL license. Automatically scales up and down to make the most out of a limited space. Can draw multiple structures simultaneously. Accepts a wide range of documented and illustrated options, and offers editing interactions. Exports the final diagrams in various file formats (svg,eps,jpeg,png,xfig)

- Participants: Yann Ponty
- Contact: Yann Ponty
- URL: <http://varna.lri.fr/>

5.2. KGS

KEYWORDS: Bioinformatics - Structural Biology -protein kinematics -RNA kinematics

FUNCTIONAL DESCRIPTION

The Kino-Geometric Sampling (KGS) software suite uses advanced, robotics-inspired algorithms to rapidly explore the conformational landscape of folded proteins, RNA, and their complexes. Combined with powerful statistical techniques, it structurally characterizes collective motions and excited substates from sparse, spatiotemporally averaged data.

- Participants: Amélie Héliou.
- Contact: Amélie Héliou
- URL: <https://simtk.org/home/kgs/>

5.3. SV-BAY

KEYWORDS: Bioinformatics - NGS- Cancer

FUNCTIONAL DESCRIPTION

SV-BAY is a software to detect structural variants in cancer genomes. It relies on a Bayesian approach and a correction for GC-content and read mappability is provided. SV-BAY is written in Python with small insertions in C++ code.

- Participants: Daria Iakovishina and M. Régnier
- Contact: M. Régnier
- URL: <https://github.com/InstitutCurie/SV-Bay>

5.4. DeClone

KEYWORDS: Bioinformatics - Comparative Genomics - Genome rearrangements

FUNCTIONAL DESCRIPTION

DECLONE is a software to predict ancestral adjacencies from reconciled gene trees. It offers multiple indicators to assess the robustness of predictions, including individual supports, the (stochastic) generation of (co/sub)-optimal solutions, and the domain of validity of a given prediction in the parameter space.

- Participants: Y. Ponty
- Contact: Y. Ponty
- URL: <https://github.com/yannponty/DeClone>

BEAGLE Project-Team

6. New Software and Platforms

6.1. DeCo

Detection of Co-evolution

KEYWORDS: Bioinformatics - Evolution

SCIENTIFIC DESCRIPTION

The software DeCo computes adjacencies (or any type of relation, like regulation, interaction, functional relationships) between ancestral genes from gene phylogenies reconciled with a species phylogeny according to duplications and losses. It takes as input (1) a species tree (2) a set of extant genes (3) a set of extant adjacencies (relations) between extant genes and (4) gene trees which leaves are the extant genes. It outputs ancestral species, genes, and adjacencies. It also highlights the duplications involving several genes.

FUNCTIONAL DESCRIPTION

DeCo for Detection of Co-evolution, reconstructs neighborhood relationships between genes of ancient genomes, in the presence of gene duplications, transfer and losses.

- Participant: Eric Tannier
- Contact: Eric Tannier
- URL: <http://pbil.univ-lyon1.fr/software/DeCo/>

6.2. DeCoLT

Detection of Co-evolution with Lateral gene Transfer

KEYWORDS: Bioinformatics - Evolution

SCIENTIFIC DESCRIPTION

The software DeCoLT computes adjacencies (or any type of relation, like regulation, interaction, functional relationships) between ancestral genes from gene phylogenies reconciled with a species phylogeny according to duplications, losses and lateral gene transfer. It takes as input a species tree a set of extant genes a set of extant adjacencies (relations) between extant genes and reconciled gene trees which leaves are the extant genes. It outputs ancestral species, genes, and adjacencies. It also highlights the duplications or transfers involving several genes.

FUNCTIONAL DESCRIPTION

The software DeCoLT computes adjacencies (or any type of relation, like regulation, interaction, functional relationships) between ancestral genes from gene phylogenies reconciled with a species phylogeny according to duplications, losses and lateral gene transfer.

- Participant: Eric Tannier
- Contact: Eric Tannier
- URL: <http://pbil.univ-lyon1.fr/software/DeCoLT/>

6.3. 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, Priscila Do Nascimento Biller, Yoram Vadee Le Brun, David Parsons and Vincent Liard
- Partners: UCBL Lyon 1 - INSERM - Universite Paris-Descartes - Insa de Lyon
- Contact: Carole Knibbe
- URL: <http://www.aevol.fr/>

6.4. EvoEvo

In silico experimental 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/>

6.5. 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 : i) Select regions of interest in each image (detect the colony), (ii) Denoise and renormalize the images, (iii) Identify each cells in each image (segmentation), (iv) Follow cells through the whole movie (tracking) and (v) Detect divisions and construct cell lineage in the population

- Participants: Magali Vangkeosay, David Parsons and Hugues Berry
- Partner: Universite Descartes
- Contact: Hugues Berry
- URL: <http://fluobacktracker.inrialpes.fr/>

BIGS Project-Team

6. New Software and Platforms

6.1. SesIndexCreator: An R Package for Socioeconomic Indices Computation and Visualization

KEYWORDS: socioeconomic status, multidimensional index, principal component analysis, hierarchical classification, R

SCIENTIFIC DESCRIPTION

In order to study social inequalities, indices can be used to summarize the multiple dimensions of the socioeconomic status. As a part of the Equit'Area Project, a public health program focused on social and environmental health inequalities, a statistical procedure to create (neighborhood) socioeconomic indices was developed. This procedure uses successive principal components analyses to select variables and create the index. In order to simplify the application of the procedure for non-specialists, the R package SesIndexCreator was created. It allows the creation of the index with all the possible options of the procedure, the classification of the resulting index in categories using several classical methods, the visualization of the results, and the generation of automatic reports. [8]

FUNCTIONAL DESCRIPTION

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

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

6.2. Angio-Analytics

KEYWORDS: Health - Cancer - Biomedical imaging

SCIENTIFIC DESCRIPTION

Angio Analytics at l'APP under identification N° FR001.280027.000.R.P.2015.000.10000 - Software for image analysis and statistical analysis of parameters issued from these images

Angiogenesis is the phenomenon by which new blood vessels are created from preexisting ones. But this natural process is also involved, in a chaotic way, in tumor development. Many molecules have shown particular efficiency in inhibiting this phenomenon, hopefully leading to either: (i) a reorganization of the neovessels allowing a better tumor uptake of cytotoxic molecules (as chemotherapy) or (ii) a deprivation of the tumor vascular network with the view to starve it. However, characterizing the anti-angiogenic effects of a molecule remains difficult, mainly because the proposed physical modeling approaches have barely been confronted to in vivo data, which are not directly available. We have developed an original approach to characterize and analyze the anti-angiogenic responses in cancerology that allows biologists to account for spatial and dynamical dimensions of the problem. The proposed solution relies on the association of a specific biological in vivo protocol using skinfold chambers, image processing and dynamic system identification. An empirical model structure of the anti-angiogenic effect of a tested molecule is selected according to experimental data. Finally the model is identified and its parameters are used to characterize and compare responses of the tested molecule. The solution has been implemented in a software developed in The Matlab environment.

FUNCTIONAL DESCRIPTION

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

- Participant: Thierry Bastogne
- Contact: Thierry Bastogne

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

KEYWORDS: Bioinformatics - Cancer - Drug development

FUNCTIONAL DESCRIPTION

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

- Participant: Thierry Bastogne
- Contact: Thierry Bastogne

BONSAI Project-Team

6. New Software and Platforms

6.1. Iedera

Iedera : subset seed design tool

KEYWORDS: Computational biology - Sequence alignment - Spaced seeds

SCIENTIFIC DESCRIPTION

Iedera is a tool based on a weighted automata framework that enables to compute spaced seeds, associated probability distributions, scores/costs, counts, and even polynomials on a classical semi-ring framework. Seed design is computed by full enumeration or hill-climbing optimization.

FUNCTIONAL DESCRIPTION

Iedera is a tool to select and design subset seed and vectorized subset seed patterns. Spaced seeds and transition-constrained spaced seeds can be perfectly represented in the subset seed model.

- Participants: Laurent Noé, Grégory Kucherov and Mikhail Roytberg
- Partners: CNRS - Université de Nancy - Université de Lille
- Contact: Laurent Noé
- URL: <http://bioinfo.lifl.fr/yass/iedera.php>

6.2. NORINE

Nonribosomal peptides resource

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

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 Leclère, Laurent Noé, Yoann Dufresne, Juraj Michalik and Stéphane Janot
- Partners: CNRS - Université Lille 1 - Institut Charles Violette
- Contact: Maude Pupin
- URL: <http://bioinfo.lille.inria.fr/NRP>

6.3. ProCARs

PROgressive Contiguous Ancestral RegionS

KEYWORDS: Bioinformatics - Evolution - Metagenomics

SCIENTIFIC DESCRIPTION

ProCars is a program used to reconstruct ancestral gene orders as CARs (Contiguous Ancestral Regions) with a progressive homology-based method. The method runs from a phylogeny tree (without branch lengths needed) with a marked ancestor and a block file. This homology-based method is based on iteratively detecting and assembling ancestral adjacencies, while allowing some micro-rearrangements of synteny blocks at the extremities of the progressively assembled CARs. The method starts with a set of blocks as initial set of CARs, and detects iteratively the potential ancestral adjacencies between extremities of CARs, while building up the CARs progressively by adding, at each step, new non-conflicting adjacencies that induce the less homoplasmy phenomenon. The species tree is used, in some additional internal steps, to compute a score for the remaining conflicting adjacencies, and to detect other reliable adjacencies, in order to reach completely assembled ancestral genomes.

FUNCTIONAL DESCRIPTION

ProCARs is a program used to reconstruct ancestral gene orders as CARs (Contiguous Ancestral Regions) with a progressive homology-based method. The method runs from a phylogeny tree with a marked ancestor and a block file.

- Participants: Aïda Ouangraoua, Samuel Blanquart, Jean-Stéphane Varré and Amandine Perrin
- Partners: CNRS - Université de Lille
- Contact: Jean-Stéphane Varré
- URL: <http://bioinfo.lifl.fr/procars>

6.4. SortMeRNA

KEYWORDS: Bioinformatics - NGS - Genomic sequence

SCIENTIFIC DESCRIPTION

SortMeRNA is a biological sequence analysis tool for metatranscriptomic and metagenomic data filtering, mapping and OTU-picking. The main application of SortMeRNA is filtering and mapping ribosomal RNA from NGS reads.

FUNCTIONAL DESCRIPTION The core algorithm is based on approximate seeds as well as an optimized text index data structure. It allows for fast and sensitive analyses of nucleotide sequences.

SortMeRNA takes as input a file of reads (fasta or fastq format) and one or multiple rRNA database file(s), and sorts apart rRNA and rejected reads into two files specified by the user. Optionally, it can provide high quality local alignments of rRNA reads against the rRNA database. SortMeRNA works with Illumina, 454, Ion Torrent and PacBio data, and can produce SAM and BLAST-like alignments. It is implemented in C++.

- Participants: H el ene Touzet, Laurent No e and Evguenia Kopylova
- Contact: H el ene Touzet
- URL: <http://bioinfo.lille.inria.fr/RNA/sortmerna/>

6.5. 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, Mik  l Salson, Marc Duez, Ryan Herbert, Tatiana Rocher and Florian Thonier
- Partners: CNRS - Inria - Universit   de Lille
- Contact: Mathieu Giraud
- URL: <http://www.vidjil.org>

6.6. Yass

KEYWORDS: Bioinformatics - Genomic sequence - Computational biology - Sequence alignment

SCIENTIFIC DESCRIPTION

As most of the heuristic DNA local alignment softwares (BLAST, FASTA, PATTERNHUNTER, BLASTZ, LAST...) YASS uses seeds to detect potential similarity regions, and then tries to extend them to actual alignments.

This genomic search tool uses multiple transition-constrained spaced seeds (most of the design of these seeds is provided by the Iedera tool) to search for more fuzzy repeats, such as non-coding DNA/RNA.

Main features of YASS are: (i) multiple, possibly overlapping seeds and a new hit criterion to ensure a good sensitivity/selectivity trade-off (ii) transition-constrained spaced seeds to improve sensitivity (transition mutations are purine to purine [AG] or pyrimidine to pyrimidine [CT]) (iii) using different scoring schemes with bit-score and E-value evaluated according to the sequence background frequencies (iv) parameterizable output filter for low complexity repeats (v) reporting of various alignment statistical parameters (mutation bias along triplets, transition/transversion), and (vi) post-processing step to group gapped alignments.

FUNCTIONAL DESCRIPTION

YASS is a genomic similarity search tool, for nucleic (DNA/RNA) sequences in fasta or plain text format : it produces local pairwise alignments.

- Participants: Laurent No   and Gr  gory Kucherov
- Partners: CNRS - Universit   de Nancy - Universit   de Lille
- Contact: Laurent No  
- URL: <http://bioinfo.lifl.fr/yass>

6.7. miRkwood

KEYWORDS: Bioinformatics - Genomics

SCIENTIFIC DESCRIPTION

miRkwood is a bioinformatic pipeline that allows for the fast and easy identification of microRNAs in plant genomes. It is both available as a webserver and a stand-alone software. It offers an user-friendly interface to navigate in the data, as well as many export options to allow the user to conduct further analyses on a local computer.

FUNCTIONAL DESCRIPTION

The method takes as input a set of small reads, that have been previously trimmed and aligned onto the reference genome. It identifies novel microRNAs on the basis of the distributions of reads and the potential of flanking genomic sequence to fold into a stem-loop secondary structure. Then the result is refined through a variety of additional complementary features that bring new evidence to the prediction: duplex stability, thermodynamic stability, phylogenetic conservation, repeats, etc.

- Participants: H  l  ne Touzet, Mohcen Benmounah, Jean-Fr  d  ric Berthelot, Isabelle Guigon and Sylvain Legrand
- Contact: H  l  ne Touzet
- URL: <http://bioinfo.lille.inria.fr/mirkwood/>

CAPSID Project-Team

6. New Software and Platforms

6.1. Kpax

KEYWORDS: Protein Structure Alignment

SCIENTIFIC DESCRIPTION

Kpax is a program for flexibly aligning two or more protein structures and for searching databases of protein structures.

FUNCTIONAL DESCRIPTION

The Kpax program exploits the fact that each amino acid residue has a carbon atom with a highly predictable tetrahedral geometry. This allows the local environment of each residue to be transformed into a canonical orientation, thus allowing easy comparison between the canonical orientations of residues within pairs of proteins using a novel scoring function based on Gaussian overlaps. Kpax is now used by the KBDOCK web server [3] to find structural templates for docking which might be beyond the reach of sequence-based homology modeling approaches. In 2015, the Kpax program was extended to allow the flexible alignment and superposition of multiple protein structures, and a new multiple alignment quality measure has been developed. According to this quality measure, Kpax gives higher quality multiple structural alignments than all other published approaches. A journal article describing these new developments is under review.

- Contact: David Ritchie
- URL: <http://kpax.loria.fr>

6.2. KBDOCK

KEYWORDS: Protein Binding Sites

SCIENTIFIC DESCRIPTION

KBDOCK is a database of all known protein-protein interactions that have experimentally determined 3D structures. In 2015, we used the latest version of KBDOCK in several rounds of the community-wide “CAPRI” blind docking experiment [36]. A journal article has been accepted for publication in *Proteins*.

FUNCTIONAL DESCRIPTION

KBDOCK combines coordinate data from the PDB with the Pfam protein domain family classification [28] in order to describe and analyze all known protein-protein interactions for which the 3D structures are available.

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

6.3. Hex

KEYWORDS: Protein Docking - 3D rendering - 3D interaction

SCIENTIFIC DESCRIPTION

Hex is an interactive protein docking and molecular superposition program. The underlying approach uses our polar Fourier correlation technique to accelerate the search for close-fitting orientations of the two protein molecules.

FUNCTIONAL DESCRIPTION

Hex understands protein and DNA structures in PDB format, and it can also read small-molecule SDF files. Hex will run on most Windows, Linux and Mac OS X computers. The recent versions 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. In 2015, the Hex code base was re-organised to separate the GUI and computational components into separate libraries. The computational library is now used in our Sam and Kpax software.

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

6.4. Sam

KEYWORDS: Protein Symmetry Assembly - Protein Docking

SCIENTIFIC DESCRIPTION

Sam is a program for building models of protein complexes having arbitrary point group symmetry. The Sam program was developed in the frame of the ANR “PEPSI” project with The Nano-D team at Inria Grenoble – Rhône Alpes. A journal article describing Sam has been accepted for publication in the Journal of Applied Crystallography [16].

FUNCTIONAL DESCRIPTION

The underlying approach makes use of multiple one-dimensional polar Fourier correlations (implemented in the Hex code-base) to search rapidly a symmetry-constrained rigid body protein docking search space. The approach may be used to build symmetrical multi-component protein complexes having a given cyclic (C_n), dihedral (D_n), tetrahedral (T), octahedral (O) or icosahedral (I) point group symmetry.

- Contact: David Ritchie
- URL: <http://sam.loria.fr>

6.5. EC-DomainMiner

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. MD-Kmean

KEYWORDS: Molecular Dynamics Analysis

SCIENTIFIC DESCRIPTION

MD-Kmean is a fast program for the analysis of large numbers of Molecular Dynamics frames. The accurate comparison of different protein structures plays important roles in structural biology, structure prediction and functional annotation. The root-mean-square-deviation (RMSD) after optimal superposition is the predominant measure of similarity due to the ease and speed of computation. MD-Kmean was designed to perform both the RMSD and the clustering step necessary to compare large numbers of protein 3D structures stored in large datasets and was applied to a set of 2 microsecond MD simulations producing 2 million frames to be compared and clustered.

FUNCTIONAL DESCRIPTION

We have implemented a very fast version of RMSD for graphics processing units (GPUs) using a quaternion method for calculating the optimal superposition and RMSD that is designed for parallel applications. This acceleration in speed allows RMSD calculations to be used efficiently in computationally intensive applications such as the clustering of large number of molecular dynamics frames. MD-Kmean is 50 times faster on a Nvidia GPU, on average, than the original single-threaded CPU implementation on an Intel quad-core processor.

- Contact: Bernard Maigret

6.7. Protein-Marshmallow

KEYWORDS: Coarse-Grained Representation

SCIENTIFIC DESCRIPTION

A Protein-protein interaction may be considered in terms of physical interaction between two deformable objects. The description at the atomic level of such complex objects is beginning to be feasible by MD simulations, but this requires the use of petaflop machines which are out of reach of most laboratories.

FUNCTIONAL DESCRIPTION

The Protein-Marshmallow program represents the surface of a protein as “coarse grained” 3D triangle mesh. In this mesh, each triangle is colored according to some biological property. In this way, a large complex object may be represented by a much smaller number of samples in a 3D mesh. The Marshmallow program describes deformations of such meshes under the influence of an external force field to simulate the strains that one object may undergo over time due to the interaction with another one.

- Contact: Bernard Maigret

6.8. Platforms

6.8.1. *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: Bioinformatics - Linked data - Networks - Semantic Web - Omics

FUNCTIONAL DESCRIPTION

This tool was designed in 2015 in the framework of the MIRNadapt project. Biological studies and bioinformatical analysis produce numerous heterogeneous data, calling for their integration. AskOmics is an integration and interrogation software relying on an RDF model and the SPARQL query language. Its purpose is to obtain quick answers to biological questions demanding currently hours of manual search in several spreadsheet results files. New study perspectives will arise from these answers and from this integration work. Using AskOmics, we integrated an omic dataset borrowed from the MiRNAdapt ANR project that aims to describe the networks of the genes involved in aphids adaptation to seasons. AskOmics allows biologists to integrate and interrogate themselves their data without needing any knowledge about RDF and SPARQL. The query process consists in linking sets of biological entities as nodes in a graphical interface, optionally specifying biological attributes for these nodes. The graph is then converted into a SPARQL query to provide the user an answer to his biological questions. The answers are the elements of the sets that match the query constraints.

- Participants: Charles Bettembourg, Anthony Bretaudeau, Olivier Dameron, Aurélie Evrard, Yvanne Chaussin, Anne Siegel, Fabrice Legeai
- Partners: INRA IGEPP
- Contact: Fabrice Legeai
- URL: http://bipaa.genouest.org/askomics_aphid/

6.2. VIRALpro

FUNCTIONAL DESCRIPTION

VIRALpro is a predictor capable of identifying capsid and tail protein sequences using support vector machines (SVM) with an estimated accuracy between 90% and 97%. Predictions are based on the protein amino acid composition, on the protein predicted secondary structure, as predicted by SSpro, and on a boosted linear combination of HMM e-values obtained from 3,380 HMMs built from multiple sequence alignments of specific fragments - called contact fragments - of both capsid and tail sequences. This tool was designed in the context of a 2015 Explorer Program visit at University of California, Irvine

- Participants: Clovis Galiez, François Coste
- Partner: Pierre Baldi, University of California, Irvine
- Contact: Clovis Galiez

6.3. Shogen

KEYWORDS: Systems Biology - Bioinformatics - Genomics

FUNCTIONAL DESCRIPTION

This ASP-based software aims at identifying every segments of consecutive genes in a bacterial genome with a maximum number of genes that participates in a given metabolic pathway. Through this selection, the shogen tool deciphers putative sets of genes that (1) take an active part in metabolic pathways while being closely connected via metabolic networks and (2) are consecutive on each of the genomes involved. In practice, our approach connects genomic and metabolic knowledge by considering the genome organization and the biochemical reactions catalyzed by enzymes encoded by its genes. The underline parsimonious principle assumes that genes must be jointly regulated to activate a metabolic reaction cascade, and should be close enough in the genome organization. In 2015, the tool was simplified to handle standardized data formats, enabling its application to the modelling of a bacterial community [17]

- Participants: Philippe Bordron, Damien Eveillard, Alejandro Maass and Anne Siegel
- Partners: LINA - University of Chile
- Contact: Anne Siegel
- URL: <http://aspforbiology.genouest.org/wiki.php/Software%20&%20Biological%20applications>

6.4. Caspo

Cell ASP Optimizer

FUNCTIONAL DESCRIPTION

Cell ASP Optimizer (caspo) is a pipeline for 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. Caspo-learn performs an automated inference of logical networks from experimental data. It identifies admissible large-scale families of logic models without any a priori bias, thus saving a lot of efforts. Next, once a family a logical networks has been identified, caspo-design can suggest or design new experiments in order to reduce the uncertainty associated to this family. Finally, caspo-control computes 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. In 2015, the tool was extended to compute experimental design proposition [23], and to handle time-series datasets [31].

- Participants: Santiago Videla, Carito Guziolowski, Sven Thiele, Thomas Cokelaer, Torsten Schaub, Anne Siegel, Loic Paulevé and Max Ostrowski
- Partners: Ecole Centrale de Nantes - University of Potsdam - EMBL - LRI - Laboratoire de Recherche en Informatique
- Contact: Anne Siegel
- URL: <http://bioasp.github.io/caspo/>

6.5. Platforms and toolboxes

Among others, a goal of the team is to facilitate interplays between tools for biological data analysis and integration. Our tools are based on formal systems. They 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 available both as stand-alone software and through portals such as Mobylye or Galaxy interfaces. Tools are developed in collaboration with the GenOuest resource and data center hosted in the IRISA laboratory, including their computer facilities [\[more info\]](#).

We present here three toolboxes which each contains complementary tools with respect to their targeted sub-domain of bioinformatics.

6.5.1. Integrative Biology: (constraint-based) toolbox for network filtering

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.

MeMap and MeMerge. We develop a workflow for the **Automatic Reconstruction of Metabolic networks** (AuReMe). In this workflow, we use heterogeneous sources of data with identifiers from different namespaces. MeMap (**M**etabolic network **M**apping) consists in mapping identifiers from different namespaces to a unified namespace. Then, MeMerge (**M**etabolic network **M**erge) merges two metabolic networks previously mapped on the same namespace. [web server].

meneco [*input*: draft metabolic network & metabolic profiles. *output*: metabolic network]. It is a qualitative approach to elaborate the biosynthetic capacities of metabolic networks and solve incompleteness of large-scale metabolic networks. Since November 2015, a new version of Meneco has been available with Python 3, and a new functionality of topological producibility checking has been set up. [82] [60] [python package][web server].

shogen [*input*: genome & metabolic network. *output* : functional regulatory modules]. This software is able to identify genome portions which contain a large density of genes coding for enzymes that regulate successive reactions of metabolic pathways. See section 6.3 for details. [55][python package].

lombarde [*input*: genome, modules & several gene-expression datasets. *output*: oriented regulation network]. This tool is useful to enhance key causalities within a regulatory transcriptional network when it is challenged by several environmental perturbations. In 2015, the tool was simplified to handle standardized data formats. [41] [web server].

ingranalysis [*input*: signed regulation network & one gene-expression dataset. *output*: network repair gene-expression prediction] This tool is an extension to the bioquali tool. 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. The tool has evolved to the *iggy* tool recently [5] [21] [Python package][web server].

6.5.2. Dynamics and invariant-based prediction

We develop tools predicting some characteristics of a biological system behavior from incomplete sets of parameters or observations.

cadbiom. Based on Guarded transition semantic, this software provides a formal framework to help the modeling of biological systems such as cell signaling network. It allows investigating synchronization events in biological networks. [software][web server].

caspo: Cell ASP Optimizer This soft provides an easy to use software for learning Boolean logic models describing the immediate-early response of protein signaling networks. See Sec. 6.4 for details. The tool is included in the cellNopt package⁰. [python package][web server].

nutritionAnalyzer. This tool is dedicated to the computation of allocation for an extremal flux distribution. It allows quantifying the precursor composition of each system output (AIO) and to discuss the biological relevance of a set of flux in a given metabolic network by computing the extremal values of AIO coefficients. This approach enables to discriminate diets without making any assumption on the internal behaviour of the system [40][webservice][software and doc].

POGG. The POGG software allows scoring the importance and sensibility of regulatory interactions with a biological system with respect to the observation of a time-series quantitative phenotype. This is done by solving nonlinear problems to infer and explore the family of weighted Markov chains having a relevant asymptotic behavior at the population scale. Its possible application fields are systems biology, sensitive interactions, maximal entropy models, natural language processing. It results from our collaboration with the LINA-Nantes [2][matlab package].

6.5.3. Sequence annotation

We develop tools for discovery and search of complex signatures within biological sequences.

⁰<http://www.cellnopt.org/>

Logol Logol is a swiss-army-knife for pattern matching on DNA/RNA/Protein sequences, using a high-level grammar to permit a large expressivity [48]. In 2015, the efficiency of the tool was improved by slight evolutions of the underlying grammar. Possible fields of application are the detection of mutated binding sites or stem-loop identification (e.g. in CRISPR⁰ [10]) [software].

Protomata learner Protomata software suite provides a grammatical inference framework for learning the specific signature of a functional protein family from unaligned sequences by partial and local multiple alignment and automata modeling. In 2015, motivated by the characterization of viral protein sequences during the internship of Maud Jusot [38], we have begun a refactoring of the parsing part of Protomata and we implemented a new mode returning the sum of the scores over all paths (Forward score), besides the classical score on best path (Viterbi score), to improve parsing's sensitivity on divergent but conserved families of sequences. [web server].

6.5.4. Integration of toolboxes and platforms in webservice

Most of our software were designed as "bricks" that can be combined through workflow application such as Mobylye. It worths considering them into larger dedicated environments to benefit from the expertise of other research groups.

Platform for data storage, expertise sharing and application inventory In collaboration with the GenOuest ressource center, the BII platform (Bio Investigation Index) is a good way to enhance knowledge and expertise sharing, improve the visibility on the team's work in progress and record the History of the team's discoveries and main results. It enables experiment reproducibility, reporting on experiment process details, storing all scripts and softwares (in the corresponding versions) and linking all input files, results and not reproducible intermediate data. [web access].

Web servers In collaboration with the GenOuest ressource center, most our tools are made available through several web portals.

- The **mobylye@GenOuest portal** is the generic web server of our ressource center. It hosts the ingranalysis, meneco, caspo, lombarde and shogun tools [website].
- The **Mobylye@Biotempo server** is a mobylye portal for system biology with formal approaches. It hosts the memap, memerge, meneco, ingranalysis, cadbiom and pogg tools [website].
- The **GenOuest galaxy portal** now provides access to most tools for integrative biology and sequence annotation (access on demand).

Dr Motif This resource aims at the integration of different software commonly used in pattern discovery and matching. This resource also integrates Dyliss pattern search and discovery software.

ASP4biology and BioASP It is a meta-package to create a powerful environment of biological data integration and analysis in system biology, based on knowledge representation and combinatorial optimization technologies (ASP). It provides a collection of python applications which encapsulates ASP tools and several encodings making them easy to use by non-expert users out-of-the-box. [Python package][website].

ASP encodings repository This suite comprises projects related to applications of Answer Set Programming using Potassco systems (the Potsdam Answer Set Solving Collection, bundles tools for Answer Set Programming developed at the University of Potsdam). These are usually a set of encodings possibly including auxiliary software and scripts [repository].

⁰<http://crispi.genouest.org/>

ERABLE Project-Team

5. New Software and Platforms

5.1. AcypiCyc

FUNCTIONAL DESCRIPTION

Database of the metabolic network of *Acyrtosiphon 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. AIViE

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 Verdesi
- 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 DESCRIPTIONCIDANE 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 Sinimeri
- Contact: Christian Baudet (not Inria), Marie-France Sagot and Blerina Sinimeri
- URL: <http://coala.gforge.inria.fr/>

5.6. CophyTrees

FUNCTIONAL DESCRIPTION

COPHYTREES is a visualisator for host-parasite and gene-specie trees evolution..

- Participants: Laurent Bulteau
- Contact: Laurent Bulteau (not Inria), Blerina Sinimeri (for Inria)
- 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 Deniérou, 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
- 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, Pierluigi Crescenzi, Marie-France Sagot, Blerina Sinimeri,
- Contact: Christian Baudet (not Inria), Beatrice Donati (not Inria), and Marie-France Sagot
- 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
- 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: <https://github.com/AlgoLab/HapCol>

5.13. KisSNP & DiscoSNP

FUNCTIONAL DESCRIPTION

Algorithm for identifying SNPs without a reference genome by comparing raw reads. KISNP has now given birth to DISCOSNP in a work involving V. Lacroix from ERABLE and the GenScale Inria Team at Rennes.

- Participants: Vincent Lacroix, Pierre Peterlongo
- Contact: Pierre Peterlongo (EPI GenScale)

5.14. KisSplice & KisSplice2igv7

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. KISSPLICE2IGV is a pipeline that combines the outputs of KISSPLICE to a reference transcriptome (obtained with a full-length transcriptome assembler or a reference database). It provides a visualisation of the events found by KISSPLICE in a longer context using a genome browser (IGV).

- 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://kisssplice.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: 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, H el ene 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-Lafferri re, 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 Scaffold) 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. PhEVER

FUNCTIONAL DESCRIPTION

Database of homologous gene families built from the complete genomes of all available viruses, prokaryotes and eukaryotes and aimed at the detection of virus/virus and virus/host lateral gene transfers.

- Participants: Christian Gautier, Vincent Lotteau, Leonor Palmeira, Simon Penel, Chantal Rabourdin-Combe
- Contact: Christian Gautier, Leonor Palmeira (not EPI)
- URL: <http://pbil.univ-lyon1.fr/databases/phever>

5.25. PepLine

FUNCTIONAL DESCRIPTION

Pipeline for the high-throughput analysis of proteomic data.

- Participant: Jérôme Garin, Alain Viari
- Contact: Alain Viari

5.26. Pitufu 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. Smile

FUNCTIONAL DESCRIPTION

Motif inference algorithm taking as input a set of biological sequences.

- Participants: Laurent Marsan, Marie-France Sagot
- Contact: Marie-France Sagot
- URL: Not available

5.30. UniPathway

FUNCTIONAL DESCRIPTION

Database of manually curated pathways developed with the Swiss-Prot group.

- Participants: Eric Coissac, Anne Morgat, Alain Viari
- Contact: Anne Morgat
- URL: <http://www.unipathway.org/>

5.31. WhatsHap and pWH

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. PWH 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 Schön-huth, Leen Stougie, Leo van Iersel
- Contact: Alexander Schönhuth(not Inria), Gunnar Klau, Nadia Pisanti
- URL: <https://bitbucket.org/whatschap/whatschap>

GENSCALE Project-Team

6. New Software and Platforms

6.1. HTS data processing

6.1.1. GATB: Genome Assembly & Analysis Tool Box

The GATB software toolbox 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 processors (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 library is written in C++.

Contact: Dominique Lavenier

URL: <https://gatb.inria.fr/>

6.1.2. LEON: Genomic Data Compression

Leon is a lossless compression software that achieves compression of DNA sequences of high throughput sequencing data, without the need of a reference genome. Techniques are derived from assembly principles that better exploit NGS data redundancy. A reference is built de novo from the set of reads as a probabilistic de-Bruijn graph stored in a Bloom filter. Each read is encoded as a path in this graph, storing only an anchoring kmer and a list of bifurcations indicating which path to follow in the graph. This new method will allow to have compressed read files containing its underlying de-Bruijn Graph, thus directly re-usable by many tools relying on this structure. Leon achieved the encoding of a *C. elegans* reads set with 0.7 bits per base, outperforming state of the art reference-free methods.

Contact: Claire Lemaitre

URL: <https://gatb.inria.fr/software/leon/>

6.1.3. BLOOCOO: Genomic Data Correction

Bloocoo is a k-mer spectrum-based read error corrector, designed to correct large datasets with a very low memory footprint. It uses the disk streaming k-mer counting algorithm included in the GATB library, and inserts solid k-mers in a bloom-filter. The correction procedure is similar to the Musket multistage approach. Bloocoo yields similar results while requiring far less memory: as an example, it can correct whole human genome re-sequencing reads at 70 x coverage with less than 4GB of memory.

Contact: Claire Lemaitre

URL: <https://gatb.inria.fr/bloocoo-read-corrector/>

6.1.4. DiscoSnp++: DISCOVering Single Nucleotide Polymorphism

DiscoSnp++ is designed for discovering Single Nucleotide Polymorphism (SNP) and insertions/deletions (indels) from raw set(s) of reads obtained with Next Generation Sequencers (NGS). The number of input read sets is not constrained, it can be one, two, or more. No other data as reference genome or annotations are needed. The software is composed of three modules: (1) kissnp2, that detects SNPs and indels from read sets; (2) kissreads2, that enhances the kissnp2 results by providing for each variant a read coverage mean and a (phred) quality; (3) VCF_creator, that provides a file in the Variant Calling Format (VCF). A VCF file using or not a reference genome is also created.

Contact: Pierre Peterlongo

URL: <http://colibread.inria.fr/software/discosnp/>

6.1.5. *MindTheGap: Detection of insertion*

MindTheGap is a software that performs detection and assembly of DNA insertion variants in NGS read datasets with respect to a reference genome. It takes as input a set of reads and a reference genome. It outputs two sets of FASTA sequences: one is the set of breakpoints of detected insertion sites, the other is the set of assembled insertions for each breakpoint. For each breakpoint, MindTheGap either returns a single insertion sequence (when there is no assembly ambiguity), or a set of candidate insertion sequences (due to ambiguities) or nothing at all (when the insertion is too complex to be assembled). 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.

Contact: Claire Lemaitre

URL: <http://mindthegap.genouest.org/>

6.1.6. *TakeABreak: Detection of inversion breakpoints*

TakeABreak is a tool that can detect inversion breakpoints directly from raw NGS reads, without the need of any reference genome and without de novo assembling the genomes. Its implementation is based on the Genome Assembly Tool Box (GATB) library, and has a very limited memory impact allowing its usage on common desktop computers and acceptable runtime (Illumina reads simulated at 80x coverage from human chromosome 22 can be treated in less than two hours, with less than 1GB of memory).

Contact: Claire Lemaitre

URL: <http://colibread.inria.fr/software/takeabreak/>

6.2. Sequence comparison

6.2.1. *PLAST: Parallel Local Alignment Search Tool*

PLAST is a fast, accurate and NGS scalable bank-to-bank sequence similarity search tool providing significant accelerations of seeds-based heuristic comparison methods, such as the Blast suite. PLAST is fully designed to compare query and subject comprised of large sets of DNA, RNA and protein sequences. It is significantly faster than BLAST, while providing comparable sensitivity. PLAST contains a fully integrated data-filtering engine capable of selecting relevant hits with user-defined criteria (E-Value, identity, coverage, alignment length, etc.).

Contact: Dominique Lavenier

URL: <https://plast.inria.fr>

6.2.2. *SIMKA: Comparison of metagenomic datasets*

Simka rapidly compares a large number of metagenomics datasets using efficient kmer-based method. Datasets may contains hundreds of millions of NGS sequences. Kmers of each datasets are rapidly counted and identified to estimate the pairwise similarities between datasets. The output of Simka can be used for clustering purpose or for checking correlation between metadata.

Contact: Gaëtan Benoit

URL: <https://gatb.inria.fr/software/simka/>

6.2.3. *BGREAT: read mapper on de-Bruijn graph*

BGREAT maps reads on a de-Bruijn Graph, usually used for genome assembly. Mapping reads on graphs offers the possibility to conserve all the pieces of information lost during the assembly process and to avoid multi-mapping problems due to genomic repeats. BGREAT rewrites a read sequence as a succession of unitigs sequences. It can map millions of reads per CPU hour on a de-Bruijn graph built from a large set of human genomic reads.

Contact: Antoine Limasset

URL: <http://github.com/Malfoy/BGREAT/>

IBIS Project-Team

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 the implementation of methods 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 8.7.1. In comparison with the previously distributed versions, GNA 8.7.1 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 Joseph Fourier, Université Pierre Mendès-France
- 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, Michel Page, Delphine Ropers, Valentin Zulkower
- Partners: Université Joseph Fourier, Université Pierre Mendès-France
- Contact: Hidde de Jong
- URL: <https://github.com/ibis-inria/welfare>

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, Michel Page, Delphine Ropers, Valentin Zulkower
- Partners: Université Joseph Fourier, Université Pierre Mendès-France
- Contact: Hidde de Jong
- URL: <http://ibis.inrialpes.fr/article1080.html>

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 Joseph Fourier, Université Pierre Mendès-France
- 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, making simulations, performing static analyses, specifying behaviors in temporal logic.

- Participants: François Fages, François-Marie Floch, Thierry Martinez, Sylvain Soliman
- Contact: François Fages
- URL: <http://lifeware.inria.fr/biocham/>

6.2. BIOCHAM-WEB

KEYWORDS: Systems Biology - Bioinformatics

FUNCTIONAL DESCRIPTION

BIOCHAM-web is a web service which makes it possible to try BIOCHAM on line without any installation, through a spreadsheet.

- Participants: François Fages, François-Marie Floch and Thierry Martinez
- Contact: François Fages
- URL: <http://lifeware.inria.fr/biocham/online/>

6.3. CellStar

KEYWORDS: Systems Biology - Bioinformatics

FUNCTIONAL DESCRIPTION

In close collaboration with Kirill Batmanov, Cédric Lhoussaine and Cristian Versari from the LIFL (CNRS/Lille Univ) and with Pascal Hersen (MSC lab; CNRS/Paris 7), 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 methods. 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
- Contact: Grégory Batt
- URL: <http://yeast-image-toolkit.biosim.eu/pmwiki.php>

6.4. ClpZinc

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 is 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, Philippe Morignot and Sylvain Soliman
- Contact: Thierry Martinez
- URL: <http://lifeware.inria.fr/~tmartine/clp2zinc/>

MORPHEME Project-Team

5. New Software and Platforms

5.1. BioLib

KEYWORD: Biomedical imaging

FUNCTIONAL DESCRIPTION

Library of image analysis for biology: object detection, tracking. This year some new developments for embedding attractive interactions in the Multiple Births and Cut algorithm have been included.

- Participants: Sylvain Prigent, Xavier Descombes, Grégoire Malandain, Étienne Delclaux, Emmanuel Soubies and Sen Wang.
- Contact: Xavier Descombes

5.2. PIB

Biological imaging platform

FUNCTIONAL DESCRIPTION

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

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

5.3. Stracking

KEYWORDS: Bioinformatics - Biology - Biomedical imaging

SCIENTIFIC DESCRIPTION

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

FUNCTIONAL DESCRIPTION

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

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

PLEIADE Team

5. New Software and Platforms

5.1. Magus

KEYWORDS: Bioinformatics - Genomic sequence - Knowledge database

SCIENTIFIC DESCRIPTION

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

FUNCTIONAL DESCRIPTION

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

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

5.2. 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 a zoomable representation of a model submitted by the user in SBML format. The most general view represents the compartments of the model, the next view shows the visualization of generalized versions of reactions and metabolites in each compartment, and the most detailed view visualizes the initial model with the generalization-based layout (where similar metabolites and reactions are placed next to each other). The 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/>

5.3. 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/>

5.4. 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/>

5.5. Platforms

5.5.1. 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.

5.5.2. 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.

SERPICO Project-Team

6. New Software and Platforms

6.1. 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://mobylye-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:** [26]

6.2. 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://mobylye-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::ATLAS>
- **Language:** C/C++
- **Reference:** [12]

6.3. 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 shapes-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://mobylye-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/>)

6.4. 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://mobylye-serpico.rennes.inria.fr/cgi-bin/portal.py#forms::Motion2D>
- **Languages:** C/C++ and JAVA (plug-in IMAGEJ: <http://rsbweb.nih.gov/ij/>)

6.5. 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) [4]. 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://mobylye-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 Scientific, Photometrics, Nikon Europe BV (2016).
- **Reference:** [4]

6.6. 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++

6.7. 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.

- **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://equip.es.igdr.univ-rennes1.fr/en/tips/Software/TubuleJ/>
- **Language:** JAVA (plug-in IMAGEJ: <http://rsbweb.nih.gov/ij/>)

6.8. 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/>)

6.9. Platforms

6.9.1. MobyLe@Serpico platform and software distribution

MobyLe@SERPICO (guest)
set email | sign-in | activate | sign-out
refresh workspace

SERPICO team (INRIA Rennes - Bretagne Atlantique) is partner of France-BioImaging

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Welcome to MobyLe, a portal for bioinformatics analyses

Space time RePresentation, Imaging
and cellular dynamics of molecular
Complexes

Programs available

- o **Backwarping:** Warp sequence with parametric motion model
- o **CRFMovingSpotDetection:** Detecting moving spots/vesicles using Conditional Random Fields
- o **HotSpotDetection:** Robust detection of fluorescence accumulation over time in video-microscopy
- o **Hullkground:** Separation of moving and non moving part in a sequence
- o **KLTracker:** Track vesicle and POI in image sequences
- o **Motion2D:** Estimate 2D parametric motion model
- o **MS-Detect:** Detecting moving objects in image sequences by background subtraction
- o **ND-SAFIR:** Denoise N-Dimensional images
- o **Optical-flow:** Compute Optical Flow between 2 images
- o **OpticalFlowStack:** Compute Optical Flow between each pair of images in a TIFF stack

Credits
MobyLe is a platform developed jointly by the Institut Pasteur Biology IT Center and the Ressource Parisienne en Bioinformatique Structurale. More information about this project can be found here.

SERPICO FRANCE-BIOIMAGING Inria

Figure 2. MobyLe@SERPICO web portal.

The objective is to disseminate the distribution of SERPICO image processing software for biologist users: *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 developed using the MobyLe framework (Institut Pasteur, see <http://mobyLe.pasteur.fr/>). The main role of this web portal (see Fig. 2) is to demonstrate the performance of the programs developed by the team: C-CRAFT[26], ATLAS[12], HOTSPOTDETECTION[57], HULLKGROUND[43], KLTRACKER[55], MOTION2D[54], MS-DETECT[45], ND-SAFIR[4], OPTICALFLOW and FLUX ESTIMATION [26]. The web interface makes our image processing methods available for biologist users at MobyLe@SERPICO (<http://mobyLe-serpico.rennes.inria.fr/cgi-bin/portal.py#welcome>) without any installation or configuration on their own. The size of submitted images is limited to 200 MegaBytes per user and all the results are kept 15 days. The web portal and calculations run on a server with 2 CPU x 8 cores, 64 GigaBytes of RAM (500 MegaBytes for each user / Data is saved for 3 months).

IMAGEJ 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 [4], HULLKGROUND [43], MOTION2D [54], HOTSPOTDETECTION [57], STLAS [12]. The C-CRAFT algorithm [26] has been developed for the image processing ICY platform (<http://icy.bioimageanalysis.org/>).

Institut Curie CID iManage database: The microscopy facility of Institut Curie has co-developped 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.

6.9.2. 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).

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, Guillaume Baty, Julien Coste, 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 studies plant morphogenesis at the scale of 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 enables the visualization, 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, Gregoire Malandain, Christophe Pradal, Christophe Godin.
- Contact: Christophe Godin
- URL: <https://gforge.inria.fr/projects/oalab>

5.3. TissueMeca

KEYWORDS: Bioinformatics - Biology - Mechanics - Morphogenesis

FUNCTIONAL DESCRIPTION

A mechanical model of growing tissue has been implemented using the open source software SOFA and OpenAlea. Using OpenAlea, a generic tissue representation can be defined with attributes giving structural, geometrical and physical parameters of the simulation. Then, based on SOFA and its modular approach, it is possible to combine different element types (triangle and edge elements), forces (elastic forces and turgor) and positional constraints within the same model to find the static elastic equilibrium, given a current configuration. The use of an implicit integration scheme makes it possible to achieve close-to interactive simulation of growth. The module implements also growth equations for the different cell walls after each elastic equilibrium step. Algorithms to simulate division and refinement of each element of the modelled tissue are also available.

- Participants: Frédéric Boudon, Olivier Ali, Jean-Philippe Bernard, Benjamin Gilles, Christophe Godin.
- Contact: Frédéric Boudon
- <https://gforge.inria.fr/projects/tissuemeca/>

5.4. PlantScan3D

KEYWORDS: Bioinformatics - Biology - Laser scanners - 3D Reconstruction

FUNCTIONAL DESCRIPTION

This software aims at semi-automatically reconstructing the 3D structures of plants from laser scans. For this, it encapsulates automatic reconstruction method developed by the Virtual Plants team (Preuksakarn et al., 2010) or by the literature (Vernoust and Lazarus, 2000). Once reconstructed the structure can be graphically edited by adding, deleting, repositioning or reorganizing segments in the structure. The original pointset can be processed with contraction operators to shift the points toward the center of the shape. Some post processing procedures are available to retrieve automatically botanical features such as divergence angle sequences.

- Participants: Frédéric Boudon, Chakkrit Preuksakarn, Christophe Godin
- Contact: Frédéric Boudon
- URL: <http://plantscan3d.gforge.inria.fr/>

5.5. 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 knowledge on the studied system, allows to constrain the segmentation and to track cells throughout time simultaneously. Moreover, the propagation allows to bound the potential mistakes of segmentation (e.g. a cells cannot disappear) which enables powerfull post-correction based on the study of the resulting tracking.

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

5.6. Alep

KEYWORDS: Foliar Fungus, Pathogen, FSPM, Epidemics, Infectious Cycle, Modelling framework

LONG: Architecture & Leaf Pathogens

FUNCTIONAL DESCRIPTION

Alep is a FSPM library implemented in Python that adapts the concepts and tools of OpenAlea to pathosystem modelling. The key components of Alep are two abstract classes that represent Dispersal Units and Lesions of foliar fungi in a generic form. The equations in these classes are specified to model a given species of fungus. Alep also contains several generic functions to manipulate these objects and define their contract: functions of dispersal by rain and by wind, functions managing the growth and competition of several lesions on the same leaf. A particular pathosystem is modeled by assembling a coherent set of components via a plugin system. This strategy allows the composition of existing algorithms as well as the extension or the inclusion of new algorithms. Their assembly and scheduling of execution uses scientific workflows defined in OpenAlea. This way, models can run at different time and spatial scales.

- Participants: Guillaume Garin, Christophe Pradal, Christian Fournier, Vianey Houles, Corinne Robert, Bruno Andrieu
- Contact: Christophe Pradal
- URL: <https://gforge.inria.fr/projects/openaleapkg>

5.7. AutoWIG

KEYWORDS: Syntactic Analysis

FUNCTIONAL DESCRIPTION

The goal of AutoWIG (Automatic Wrapper and Interface Generator) is to provide an automatic approach for the process of Python interfacing of C++ libraries. This Python library relies on two main principles: i) automatic C++ code parsing using LLVM/clang, and ii) Python wrapper generation with C++ code introspection.

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

5.8. Phenomenal

KEYWORDS: Image Analysis

FUNCTIONAL DESCRIPTION

Phenomenal is a Python library that provides a set of algorithms to process images produce by Image-based phenotyping platforms. The library contains algorithms for i) plant image segmentation, ii) 3D reconstruction of plant organs and plant canopies, iii) calculation of intercepted light and radiation use efficiency. All these algorithms are integrated in the OpenAlea platform.

- Participants: Simon Artzet, Jérôme Chopard, Michael Mielewczik, Nicolas Brichet, Christian Fournier, Christophe Pradal
- Contact: Christophe Pradal
- URL: <https://gforge.inria.fr/projects/phenomenal/>

5.9. Platforms

5.9.1. 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.).

5.9.2. 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. 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>

6.2. Deformetrica

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

SCIENTIFIC DESCRIPTION

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

Deformetrica comes with two applications:

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

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

FUNCTIONAL DESCRIPTION

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

Deformetrica comes with two applications:

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

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

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

6.3. 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
- URL: <http://www.brainvisa.info>

6.4. 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 abnormalities and with different acquisition characteristics.

- Participants: Marie Chupin, Ludovic Fillon and Thomas Samaille
- Contact: Marie Chupin
- URL: <http://www.brainvisa.info/>

6.5. 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
- URL: <http://www.fil.ion.ucl.ac.uk/spm/>

ASCLEPIOS Project-Team

5. New Software and Platforms

5.1. MedInria

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

FUNCTIONAL DESCRIPTION:

MedInria is a medical imaging software platform developed by the Asclepios research project in collaboration with the Athena, Parietal and Visages Inria research projects. It aims at providing clinicians with state of the art algorithms dedicated to medical image processing and visualization. Efforts have been made to simplify the user interface, while keeping high-level algorithms.

The core of medInria is Open Source with a BSD license; additional plug-ins can have any license.

The latest release of medInria, 2.2.3, was made in September 2015.

- Participants: Théodore Papadopoulo, Olivier Commowick, René-Paul Debroize, Florian Vichot, Loïc Cadour, Michael Buckingham, Maxime Sermesant and Hakim Fadil
- Partners: HARVARD Medical School - IHU - LIRYC - IHU - Strasbourg - NIH
- Contact: Olivier Commowick
- URL: <http://med.inria.fr>

5.2. MUSIC

KEYWORDS: Health - Cardiac - Computer-Assisted Surgery - Cardiac Electrophysiology - Medical Imaging

FUNCTIONAL DESCRIPTION:

MUSIC (Multi-modality Platform for Specific Imaging in Cardiology) is 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.

For more information, see the [web page](#) or [this video](#) on the MUSIC software application.

- Participants: Loïc Cadour, Maxime Sermesant, Hakim Fadil, Florent Collot and Mathilde Merle (Software Engineer at IHU LIRYC)
- Contact: Maxime Sermesant
- URL: <https://team.inria.fr/asclepios/software/music/>

5.3. SOFA

KEYWORDS: Simulation of the Human Body - Physical Simulation - Health - Biomechanics - GPU - Computer-Assisted Surgery

FUNCTIONAL DESCRIPTION:

SOFA (Simulation Open Framework Architecture) 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 it can also be used as a 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 a 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 is developed mainly by the Inria team projects Shacra, Evasion and Asclepios and it is available under the LGPL licence.

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

5.4. VP2HF

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

FUNCTIONAL DESCRIPTION:

The proprietary 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 and KCL, and specific tools provided by Philips (algorithms of segmentation, scar segmentation, etc.). 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 Loic Cadour
- Contact: Maxime Sermesant
- URL: <http://www.vp2hf.eu>

5.5. 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/lclogdemons/>

ATHENA Project-Team

5. New Software and Platforms

5.1. 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 transferred to the company Olea Medical where it is currently under test and validation, thanks to the contributions of Aurobrata Ghosh.

- Participants: Demian Wassermann, Théodore Papadopoulo and Rachid Deriche
- Contact: Demian Wassermann
- URL: <https://gforge.inria.fr/projects/athenadmri2013>

5.2. 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/>

5.3. The White Matter Query Language

KEYWORDS: Health - Neuroimaging - Medical imaging

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.

- Participant: Demian Wassermann
- Contact: Demian Wassermann
- URL: <http://tract-querier.readthedocs.org/en/latest/>

5.4. 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, René-Paul Debroize, Guillaume Pasquier, Laurence Catanese, Alexandre Abadie, Benoît Bleuzé, Clément 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, Nicolas Schnitzler and Hakim Fadil
- Partners: HARVARD Medical School - IHU - LIRYC - IHU - Strasbourg - NIH
- Contact: Olivier Commowick
- URL: <http://med.inria.fr>

5.5. 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.

- Participants: Dieter Devlaminck, Loïc Mahé, Maureen Clerc, Théodore Papadopoulo, Emmanuel Maby and Jérémie Mattout
- Partner: INSERM
- Contact: Maureen Clerc

5.6. 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 electroencephalography (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>

5.7. 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.

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

5.8. 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 Legény, Jussi Tapio Lindgren, Alison Cellard, Loïc Mahé, Guillaume Serriere and Marsel Mano
- Partners: INSERM - CEA-List - GIPSA-Lab
- Contact: Anatole Lécuyer
- URL: <http://openvibe.inria.fr>

DEMAR Project-Team

4. New Software and Platforms

4.1. Synergy Neurostimulation Software

Participants: Arthur Hiairassary, David Andreu, David Guiraud.

We have developed a specific software environment called Synergy Neurostimulation Software (fig.1), allowing to remotely manage a stimulation architecture based on one controller piloting a set of distributed stimulation units, connected by means of a dedicated network. The controller embeds the set of FES functions according to which it controls stimulation units, in real-time.

This FES distributed architecture is based on our last version of stimulation units that embed stimulation sequencing and a more efficient modulation mechanism.

Synergy Neurostimulation Software has been registered at the french Agence de Protection des Programmes (APP).

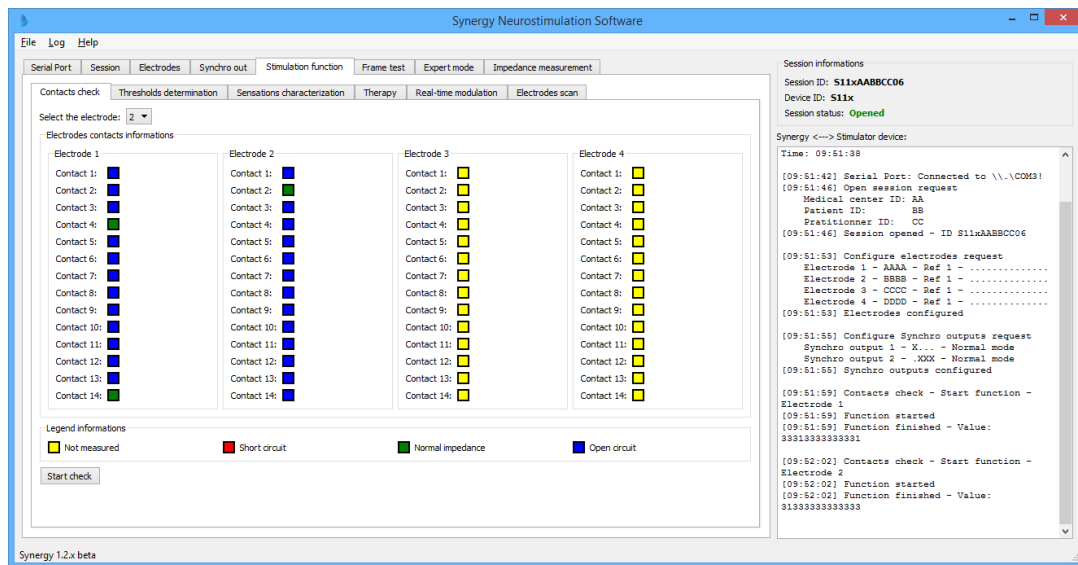


Figure 1. Synergy Neuromodulation Software

4.2. HILECOP

High Level hardware Component Programming

FUNCTIONAL DESCRIPTION

Our SENIS (Stimulation Electrique Neurale dIStribuee) based FES architecture relies on distributed stimulation units (DSU) which are interconnected by means of a 2-wire based network. A DSU is a complex digital system since it embeds among others a dedicated processor (micro-machine with a specific reduced instruction set), a monitoring module and a 3-layer protocol stack. To face the complexity of the units digital part and to ease its prototyping on programmable digital devices (e.g. FPGA), we developed an approach for high level hardware component programming (HILECOP). To support the modularity and the reusability of sub-parts of complex hardware systems, the HILECOP methodology is based on components. An HILECOP component has: a Petri Net (PN) based behavior (fig.2), 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 of 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 aggregation 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).

- Participants: Baptiste Colombani, David Andreu, Thierry Gil, Robin Passama
- Contact: David Andreu

4.3. MOS2SENS

Model Optimization and Simulation To Selective Electrical Neural Stimulation

KEYWORDS: Neurosciences - Health - Physiology

FUNCTIONAL DESCRIPTION

This model can predict nerve fiber activation through multipolar electrode stimulation. Furthermore the models provide an optimal current configuration to activate accurately the targeted muscle or organ (indeed a targeted group of fiber).

The new software MOS2SENS is an adjustment support tool for neuroprosthetics devices. It models and optimizes the current injected by multipolar CUFF electrodes inside the nerve in order to activate selective fiber targets in terms of spatial criterion.

- Participants: Melissa Dali, Olivier Rossel and David Guiraud
- Contact: David Guiraud

4.4. PALGate

KEYWORDS: Health - Home care - Handicap

- Contact: David Daney

4.5. PersoBalance

PersoBalance: A Personalized Balance Assessment in Home Rehabilitation

KEYWORDS: Health - Home care - Handicap

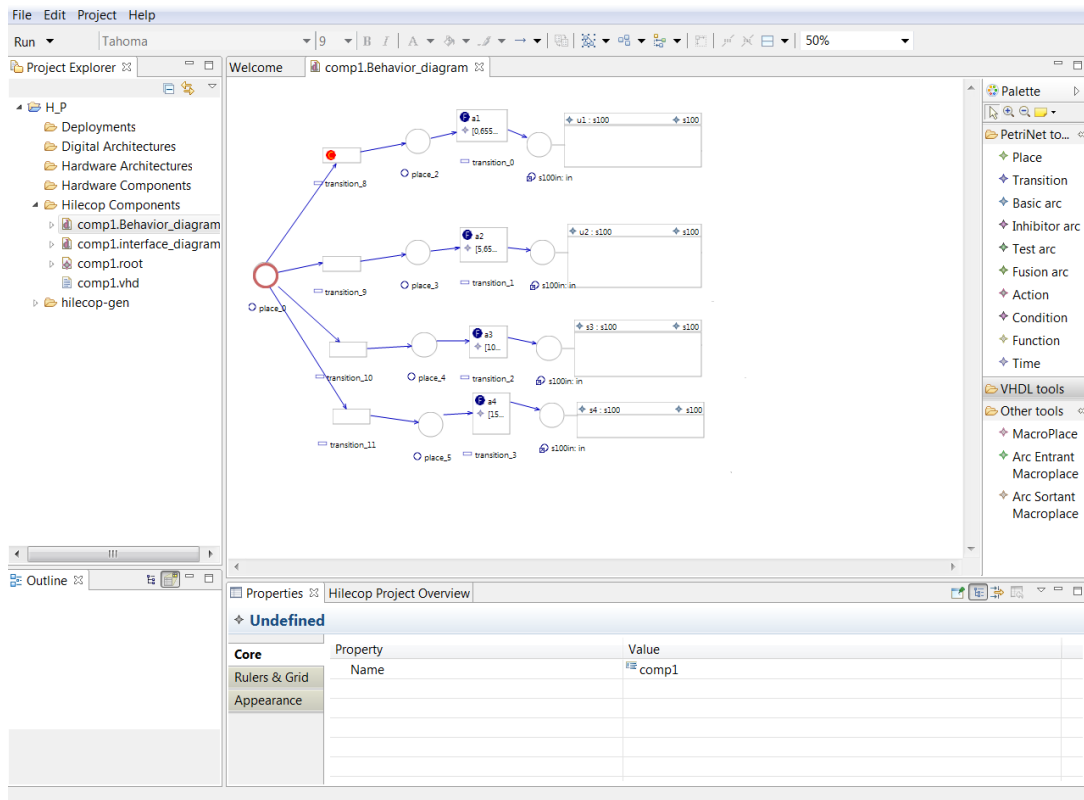


Figure 2. HILECOP screenshot

4.5.1. PersoBalance: A Personalized Balance Assessment in Home Rehabilitation

Participants: Mitsuhiro Hayashibe, Alejandro Gonzalez [Euromov], Philippe Fraisse.

The objective of this software is to realize a personalized evaluation of the postural balance to be used in home-based rehabilitation, by using portable sensors such as Kinect and wii board. After the one time of identification, the system provide us the personalized estimation of the center of mass (CoM) for the whole body only with Kinect information, through Statically Equivalent Serial Chain method.

The first function is the adaptive identification interface for the CoM parameters based on Kalman filter which allows a subject to provide different postures interactively with minimized time length. The second function is the balance measure visualization (stable or instable) based on the identified model for each subject considering subject-specific body differences on the segment mass distribution.

Recently, this software was demonstrated at the event of Rencontre Inria-Industrie 13/10/2015 at Bordeaux. <https://www.inria.fr/centre/bordeaux/innovation/rii-sante/demonstrations2> It is also filed at Software Catalogue of Inria. <https://www.inria.fr/centre/bordeaux/innovation/rii-sante/catalogue-logiciels>

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

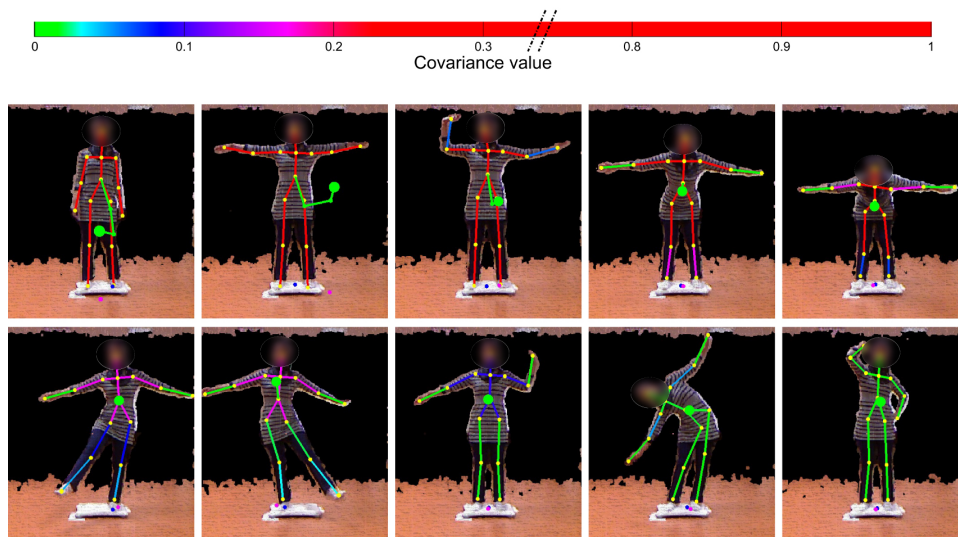


Figure 3. PersoBalance: A Personalized Balance Assessment in Home Rehabilitation: This scene shows the process how the CoM is being identified through different postures information with portable sensors.

4.6. SENISManager

Stimulation Electrique Neurale dIStribuee
FUNCTIONAL DESCRIPTION

SENISManager is a specific software environment allowing to remotely manage and control a network of DSUs, i.e. the distributed FES architecture. SENISManager performs self-detection of the architecture being deployed. This environment allows the manipulation of micro-programs from their edition to their remote control. It also allows the programming of control sequences executed by an external controller in charge of automatically piloting a stimulator.

- Participants: David Andreu and Robin Passama
- Contact: David Andreu

4.7. sensbiotk

KEYWORDS: Motion analysis - Sensors

SCIENTIFIC DESCRIPTION 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.

FUNCTIONAL DESCRIPTION

sensbiotk toolbox for Python. for the calibration, acquisition, analysis and visualization of motion capture using IMU

- Participants: Christine Azevedo Coste, Roger Pissard-Gibollet and Benoît Sijobert
- Contact: Roger Pissard Gibollet
- URL: <http://sensbio.github.io/sensbiotk/>

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. DROP

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

FUNCTIONAL DESCRIPTION

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

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

6.4. FastPD

KEYWORD: Medical imaging

FUNCTIONAL DESCRIPTION

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

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

6.5. GraPeS

Grammar Parser for Shapes

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

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

6.6. HOAP-SVM

High-Order Average Precision SVM

SCIENTIFIC DESCRIPTION

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

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

FUNCTIONAL DESCRIPTION

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

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

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

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

6.7. LBSD

Learning-Based Symmetry Detection

FUNCTIONAL DESCRIPTION

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

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

6.8. 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/>

6.9. 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: Nikolaos Paragyios
- Contact: Nikolaos Paragyios
- URL: <http://www.mrf-registration.net/>

MIMESIS Team

5. New Software and Platforms

5.1. The SOFA Framework

5.1.1. Description

SOFA⁰ is an open-source software framework targeted at real-time multi-physics simulation, with an emphasis on medical simulation. The idea of SOFA was initiated by members of the MIMESIS team, strongly supported by Inria and still actively developed within the MIMESIS team. Based on C++, the SOFA engine provides many algorithms, physiological models and anatomical data, made available within a plugin architecture. With its high level of modularity, SOFA appears to be an efficient tools to benchmark and develop new medical technologies using existing algorithms.



Figure 7. Logo of the SOFA framework

The SOFA framework relies on a multi-model representation which allows for having several representations (e.g. mechanical, thermal and visual) of the same object. Those different representations are connected together through a mechanism called mapping. With these features, it is also possible to have models of very different natures interacting with each other, for instance rigid bodies, deformable objects, and fluids. CPU and GPU implementations can be transparently combined to exploit the computational power of modern hardware architectures.

SOFA is at the heart of a number of research projects, including cardiac electro-physiology modeling, interventional radiology planning and guidance, planning for cryosurgery and deep brain stimulation, robotics, percutaneous procedures, laparoscopic surgery, non-rigid registration, etc. As a proof of its success, SOFA has been downloaded nearly 150,000 times, and is used today by many research groups around the world, as well as a number of companies. The mailing list used to exchange with the community includes several hundreds of researchers, from about 50 different institutions. SOFA is currently used by several industrial partners (Siemens Corporate Research, Epona Medical, Moog, SenseGraphics, etc.) and also provides the key technology on which our newly created start-up (InSimo) is relying. We strongly believe that today SOFA has become a reference for academic research, and is increasingly gaining recognition for product prototyping and development. The best illustration of this worldwide positioning is the role of SOFA in the challenge set by the HelpMeSee foundation to win the contract for the development of a very ambitious and high-risk project on cataract surgery simulation.

⁰More information about SOFA at <http://www.sofa-framework.org>

5.1.2. The SOFA Consortium

SOFA started ten years ago as an Inria collaborative research project. Now, SOFA includes many different functionalities, several companies rely on the framework as a physics engine and a large community rose over the years. To better meet the expectations of the community, Inria and the SOFA architects decided to create the SOFA Consortium in which the MIMESIS is strongly involved. The official kick-off of the Consortium took place in Strasbourg on the 25. November 2015.



Figure 8. The SOFA Consortium was created around the SOFA platform in 2015: here are some fields of application of SOFA

The **objectives of the SOFA Consortium** can be defined as:

- Represent the identity of SOFA,
- Structure and develop the community,
- Coordinate the development of SOFA to make it always more efficient and stable.

The Consortium has to represent the identity of SOFA. As a consequence, the first mission of the Consortium is to promote SOFA in conferences, forums or any other event. The Consortium must present SOFA to researchers and industrials and inform about all activities around the simulation platform and the available applications. By advertising all this work, the Consortium will bring more visibility to the entire SOFA community, encourage partnership and stimulate technology transfer.

Second, the Consortium now becomes a privileged contact point for any question or request. Members, users, beginners or any interested partner can contact us. We will find the answer to their needs and thus increase the interactions outside and within the community.

Third, the Consortium is in charge of coordinating the developments made in SOFA. Through regular meetings, and bi-annual technical committee, the Consortium makes sure the development follows the road map. Moreover, the Consortium sticks to the vision of SOFA as an open-source software, that has to become more and more stable and easy to use.

Finally, a free support is provided by the Consortium on the public version of SOFA, with the help of the entire SOFA community.

MNEMOSYNE Project-Team

6. New Software and Platforms

6.1. Positioning

Our previous works in the domain of well-defined distributed asynchronous adaptive computations [62], [59], [64] have already made us define a library (DANA [58]), 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 sub-neural or neural models [48], 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. Virtual Enaction

KEYWORDS: Neurosciences - Simulation - Health
FUNCTIONAL DESCRIPTION

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

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

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

NEUROMATHCOMP Project-Team

5. New Software and Platforms

5.1. ENAS

Event Neural Assembly Simulation

KEYWORDS: Neurosciences - Health - Physiology

FUNCTIONAL DESCRIPTION Enas is a software for the analysis of spike trains either coming from neural simulators or from biological experiments. Spike trains statistical analysis is based on the estimation of a Gibbs distribution with a spatio-temporal potential optimally characterizing the statistics of empirical spike trains by minimisation of the Kullback-Leibler divergence between the empirical measure and the Gibbs measure. From this, classical statistical indicators such as firing rate, correlations, higher order moments statistical entropy, effective connectivity graph, confidence plots and so on are obtained. Also, the form of the Gibbs potential provides essential informations on the underlying neural network and its structure. This method does not only allows us to estimate the spikes statistics but also to compare different models, thus answering such questions about the neural code as, e.g., are correlations (or time synchrony or a given set of spike patterns, etc.) significant with respect to rate coding? The software includes classical Maximum Entropy Models such as Ising model, but also more general forms of potentials with spatio-temporal interactions. It also has a functionality attempting to guess the shape of the potential from data and a procedure fitting an Integrate and Fire Neural Network reproducing the empirical rasters statistics. Finally, it allows to generate artificial rasters having a given distribution (e.g. corresponding to biological spike trains).

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

5.2. Virtual Retina

KEYWORDS: Neurosciences - Simulation - Biology

FUNCTIONAL DESCRIPTION Virtual Retina [14] 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 [79], [82], [83], [56]. It has recently been shown to predict spikes in a mouse retina more accurately than linear-nonlinear (LN) models [93]. 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 retinal ganglion cells (RGCs). All parameters for the different stages of the model are customizable so that the visual field can be paved with different RGC types.

- Participants: Bruno Cessac, Maria-Jose Escobar, Pierre Kornprobst, Adrien Wohrer and Thierry Viéville
- Contact: Pierre Kornprobst
- URL: <http://www-sop.inria.fr/neuromathcomp/public/software/virtualretina/>

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 can be visualized in a 2D and 3D-plot evolving in time. It is written in Python, open-source and involves heavily the simulation package BRIAN⁰.

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

6.2. NeuralFieldSimulator

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.

- Participants: Axel Hutt and Eric Nichols
- Partner: Kevin Green, University of Ontario, Canada
- Contact: Axel Hutt
- URL: <https://gforge.inria.fr/projects/nfsimulator/>

6.3. 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.

⁰<http://briansimulator.org/>

This year, Neurosys was in charge of the linux release. the main development efforts concern machine learning: Multi-layer perceptrons have been added as classification methods and evaluation plugins allow to get standalone visualization for Kappa coefficient, Receiving Operative Curve (ROC) curve and general statistics.

- 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 Serrière, Marsel Mano, Maureen Clerc Gallagher, Théodore Papadopoulo, Laurent Bougrain, Jérémy Frey and Nathanaël Foy
- Partners: INSERM - CEA-List - GIPSA-Lab
- Contact: Anatole Lécuyer
- URL: <http://openvibe.inria.fr>

6.4. BRIAN Contributions

KEYWORDS: Spiking neurons models - Neurosciences - BRIAN

FUNCTIONAL DESCRIPTION

6.4.1. Spiking Neuron Templates

BRIAN-compatible libraries has been developed by the team for various ionic currents to be assembled together to create template neurons. The purpose of these is to speed up simulation set-up time 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 (leak, sodium and potassium)
- Hodgkin-Huxley pyramidal neuron with calcium-activated non-specific (CAN) receptors (leak, sodium, potassium, m-current, calcium, CAN)
- Hodgkin-Huxley fast-spiking inhibitory hippocampal (leak, sodium, potassium, m-current)

Implemented ionic current libraries include:

- Traub and Miles Hodgkin-Huxley (I_{Leak} , I_K , I_{Na}) implementation;
- M-Current (I_M) implementation;
- Calcium current (I_L) implementation;
- Calcium pump mechanisms ($\frac{dCa}{dt}$) implementation;
- Calcium-activated non-selective current (I_{CAN}) implementation;
- Wang and Buszáki inhibitory Hodgkin-Huxley (I_{Leak} , I_K , I_{Na}) implementation;

The current library is easily extensible by third-party users due to its hierarchical design. The template neurons and their currents are defined as YAML⁰ files, which are conveniently parsed by a Python library which acts as an interface to the BRIAN simulator API's.

6.4.2. BRIAN Simulation Parameters

A python library which acts as a wrapper for BRIAN simulations, allowing the user to define simulation parameters in external YAML files, which are then parsed and forwarded to the BRIAN simulator. In addition, simulation parameters can be overridden via the command-line when invoking the python script containing the simulation.

- Participants: Francesco Giovannini
- Contact: Francesco Giovannini
- URL: <http://www.briansimulator.org>

⁰<http://www.yaml.org/>

PARIETAL Project-Team

6. New Software and Platforms

6.1. Scikit-learn

KEYWORDS: Classification - Learning - Clustering - Regression - 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 and Fabian Pedregosa Izquierdo
- Partners: CEA - Logilab - Nuxeo - Saint Gobain - Tinyclues - Telecom Paris
- Contact: Olivier Grisel
- URL: <http://scikit-learn.org>

6.2. Nilearn

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.
- Contact: Bertrand Thirion
- URL: <http://nilearn.github.io>

6.3. Mayavi

FUNCTIONAL DESCRIPTION

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

- Contact: Gaël Varoquaux
- URL: <http://mayavi.sourceforge.net/>

6.4. 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, Aina Frau Pascual and Lotfi Chaari
- Partners: CEA - NeuroSpin
- Contact: Florence Forbes
- URL: <http://pyhrf.org>

POPIX Team

6. New Software and Platforms

6.1. Clinical Trial Simulator

KEYWORDS: Statistics - Bioinformatics - Drug development

FUNCTIONAL DESCRIPTION

A clinical trial simulator (CTS) enables effective implementation of the learn-and-confirm paradigm in drug development. Through simulations the anticipated success rate of a future trial can be estimated. For various reasons industry has not embraced currently available software for trial simulation. A new tool is essential for Model Based Drug Development (MBDD).

POPIX is developing the mlxR R package for the model based simulation of clinical trials.

- Participants: Marc Lavielle
- URL: <http://simulx.webpopix.org>

6.2. Monolix

KEYWORDS: Statistics - Bioinformatics - Health - Drug development

FUNCTIONAL DESCRIPTION

MONOLIX is an easy, fast and powerful tool for parameter estimation in nonlinear mixed-effect models, model diagnosis and assessment, and advanced graphical representation. It is a platform of reference for model-based drug development. Pharmacometricians and biostatisticians can rely on MONOLIX for population analysis and to model PK/PD and other complex biochemical and physiological processes.

MONOLIX was developed by Inria until June 2011. The start-up Lixoft now develops and supports MONOLIX. POPIX collaborates closely with Lixoft to convert research results into new user features available in MONOLIX.

A first extension of MONOLIX for partial differential equations (PDEs) based models was developed by POPIX in 2015.

- Participants: Marc Lavielle, Raphael Kuate

6.3. MLXtran

KEYWORDS: Statistics - Bioinformatics - Health - Drug development

FUNCTIONAL DESCRIPTION

Monolix is associated with MLXtran, a powerful and immediately readable declarative language for describing complex pharmacometric and statistical models. MLXtran can be used and interfaced with various environments, e.g., R, Matlab, etc.

POPIX collaborates closely with Lixoft on the definition of the specifications and the syntax of MLXtran. Implementation is then ensured by Lixoft.

- Participants: Marc Lavielle

SISTM Project-Team

6. New Software and Platforms

6.1. New Software

6.1.1. *sgPLS*

Sparse Group Partial Least Square

KEYWORD: Bioinformatics

FUNCTIONAL DESCRIPTION

The Sparse Group Partial Least Square package (sgPLS) provides sparse, group, and sparse group versions of partial least square regression models.

- Contact: Benoît Liquet
- URL: <https://cran.r-project.org/web/packages/sgPLS/index.html>

6.2. Upgraded Software

6.2.1. *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. 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>

6.2.2. *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: <http://cran.r-project.org/web/packages/VSURF/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: Laurence Catanese, Olivier Commowick, René-Paul Debroize, Florent Leray, Renaud Hédouin and Guillaume Pasquier
- Contact: Olivier Commowick
- URL: <https://github.com/Inria-Visages/Anima-Public/wiki>
- APP number: IDDN.FR.001.460020.000.S.P.2015.000.31230

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.

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

- Participants: Olivier Commowick, René-Paul Debroize, Guillaume Pasquier, Laurence Catanese
- 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. autoMRI

KEYWORDS: Magnetic Resonance Imaging (MRI) - functional MRI (fMRI) - Arterial Spin Labeling (ASL) - functional ASL (fASL) - Statistical Parametric Mapping (SPM) - Automation

SCIENTIFIC DESCRIPTION This software is highly configurable in order to fit to a wide range of needs. Pre-processing includes segmentation of anatomical data, as well as co-registration, spatial normalization and atlas building of all data types. The analysis pipelines perform either within-group analysis or between-group or one subject-versus-group comparison and produce statistical maps of regions with significant differences. These pipelines can be applied to structural data to exhibit patterns of atrophy or lesions, to ASL (both pulsed or pseudo-continuous sequences) or PET data to detect perfusion or metabolic abnormalities (see figure 3 , left), to relaxometry data to detect deviations from a template (see figure 3 , right), 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.

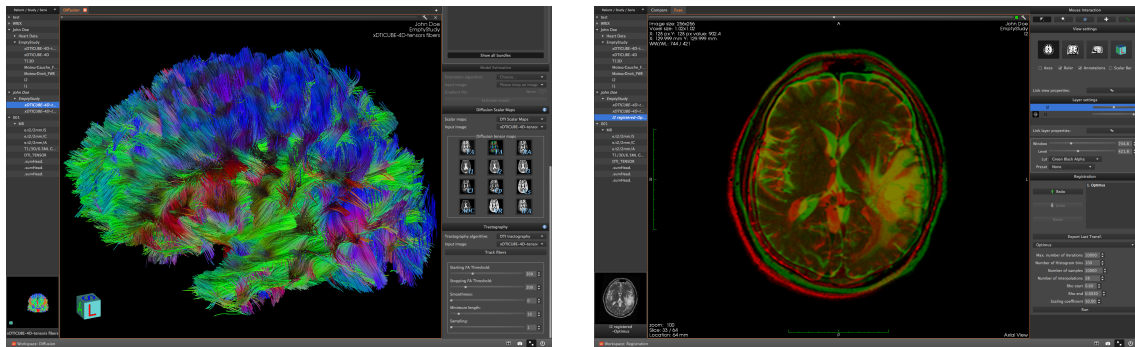


Figure 2. The medInria software platform: Tractography overlapped with 3D image (left), and Fused view of registered images (right)

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). A new version of the ASL post-processing part was developed in Python and Nipype, therefore not requiring the disponibility of Matlab licences.

- Participants: Isabelle Corouge, Cédric Meurée, Pierre Maurel and Elise Banner
- Contact: Isabelle Corouge
- URL: <http://www.irisa.fr/visages/>

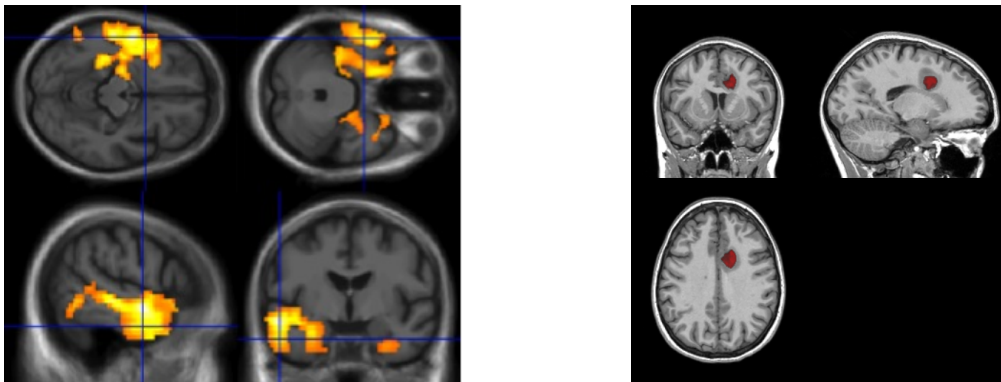


Figure 3. Illustrations of results obtained with autoMRI: Conjunction map showing areas of hypoperfusion and hypometabolism in semantic dementia (left) and detection of relaxometry defect in an MS patient (right).

6.4. Shanoir

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

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 figure 4).

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 holding meta-data. The data model, based on OntoNeurolog, an ontology devoted to the neuroimaging field, is structured around the concept of "research study". A research study includes patients who themselves have examinations that 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 file imports are possible from various sources (DICOM CDs, PACs, image files in NIfTI / Analyze format) using either online wizards, with completions of related meta-data, or commande line tools. Once de-identified during the import phase, DICOM header's customizable feature. Shanoir can also record any executed processing allowing to retrieve workflows applied to a particular dataset along with the intermediate data.

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

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

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

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

- Participants: Michael Kain, Justine Guillaumont, Christian Barillot, Anthony Baire and Yao Yao
- Partners: Université de Rennes 1 - CNRS - INSERM
- Contact: Christian Barillot
- URL: <http://shanoir.gforge.inria.fr>
- APP number: IDDN.FR.001.520021.003.S.A.2008.000.31230 (2014/08/20)

6.5. 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.

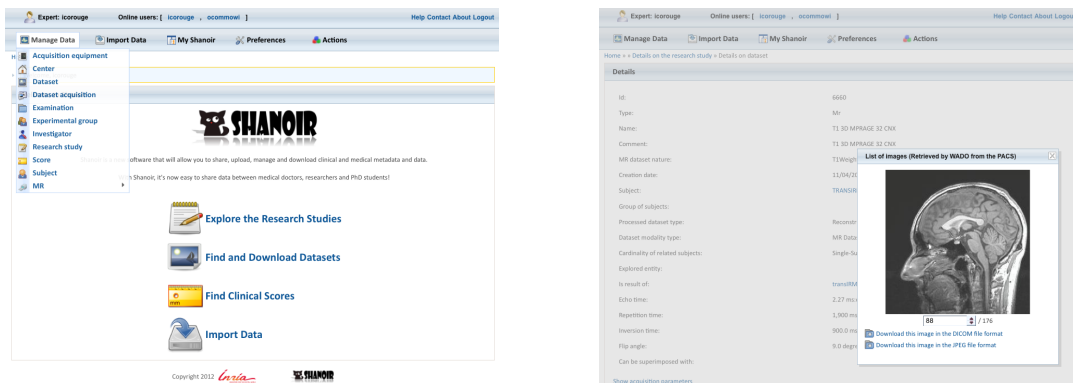


Figure 4. The SHANOIR software is a web application to share, archive, search and visualize neuroimaging data.

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-platform for medical image processing and visualization.

- Participants: Olivier Commowick, Justine Guillaumont, Florent Leray, and Wefa Hakem
- Contact: Olivier Commowick
- URL: <http://qtshanoir.gforge.inria.fr>
- APP number: IDDN.FR.001.130017.000.S.A.2012.000.31230 (2012/02/08)

6.6. 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 figure 5 . After this ShanoirUploader sends the data to a Shanoir server instance in order to import these data. This application bypasses the situation, that in most of the clinical network infrastructures a server to server connection is complicated to set up between the PACS and a Shanoir server instance.

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

- Participants: Justine Guillaumont, Michael Kain, Christian Barillot, Yao Yao, Inès Fakhfakh
- Contact: Christian Barillot
- URL: <http://shanoir.gforge.inria.fr>
- APP number: IDDN.FR.001.380026.000.S.P.2015.000.31230 (2015/09/11)

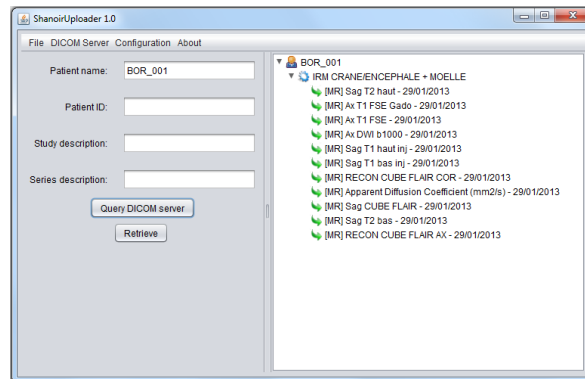


Figure 5. The ShanoirUploader software is a desktop application designed to interact with a PACS to query and retrieve the data stored on any PACS.

6.7. 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. For this the Shanoir SOAP web-services are called. As shown in figure 6 , 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 viewer that the user has already installed on his device.

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

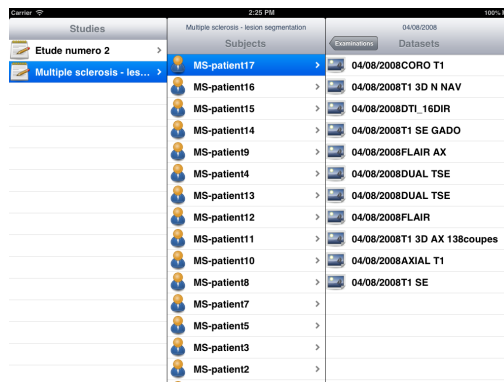


Figure 6. The iShanoir software is a desktop application designed to...

6.8. Integration of EEG and fMRI

Participants: Marsel Mano, Lorraine Perronnet.

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)

- Keywords: medical imaging, EEG, fMRI
- Software benefit: integration of EEG and fMRI processing
- Type of human computer interaction: C++ API, shell scripts
- OS/Middleware: Windows, Mac and Linux.
- Required library or software : SPM, pnet.
- Programming language: C++, shell scripts

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 (<http://www.neurinfo.org>). This platform has been supported under the “Contrat de Projets Etat-Région” (C. 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 4010 k€ (600 k€ for the infrastructures, 2850 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 U 650 - 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.

AIRSEA Team

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
- Contact: Laurent Debreu
- URL: <http://www-ljk.imag.fr/MOISE/AGRIF>

6.2. BALAISE

Bibliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement
KEYWORDS: Multi-scale analysis - Data assimilation - Optimal control
FUNCTIONAL DESCRIPTION

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

- Contact: Arthur Vidard

6.3. NEMOVAR

Variational data assimilation for NEMO
KEYWORDS: Oceanography - Data assimilation - Adjoint method - Optimal control
FUNCTIONAL DESCRIPTION

NEMOVAR is a state-of-the-art multi-incremental variational data assimilation system with both 3D and 4D 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

6.4. Sensitivity

FUNCTIONAL DESCRIPTION

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

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

ANGE Project-Team

6. New Software and Platforms

6.1. Freshkiss3D (FREe Surface Hydrodynamics using KInetic SchemeS)

FUNCTIONAL DESCRIPTION

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

- Participants: Jacques Sainte-Marie, Emmanuel Audusse, Marie-Odile Bristeau, Raouf Hamouda, David Froger and Anne-Céline Boulanger
- Partners: UPMC - CEREMA
- Contact: Jacques Sainte-Marie

For a list of recent developments, refer to §7.5.1 .

6.2. TSUNAMATHS

FUNCTIONAL DESCRIPTION

Tsunamaths is an educational platform aiming at simulating historical tsunamis. Real data and mathematical explanations are provided to enable people to better understand the overall process of tsunamis.

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

CASTOR Project-Team

4. New Software and Platforms

4.1. CEDRES++

FUNCTIONAL DESCRIPTION

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

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

- Participants: Cédric Boulbe, Jacques Blum, Blaise Faugeras and Holger Heumann
- Partners: CNRS - CEA - Université de Nice Sophia Antipolis (UNS)
- Contact: Cédric Boulbe
- Reference: [16]

4.2. 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.

- Participants: Jacques Blum, Cédric Boulbe and Blaise Faugeras
- Contact: Blaise Faugeras
- Reference: [1]

4.3. FBGKI (Full Braginskii)

FUNCTIONAL DESCRIPTION The Full Braginskii solver considers the equations proposed by Braginskii (1965), in order to describe the plasma turbulent transport in the edge part of tokamaks. These equations rely on a two fluid (ion - electron) description of the plasma and on the electroneutrality and electrostatic assumptions. One has then a set of 10 coupled non-linear and strongly anisotropic PDEs. FBGKI makes use in space of high order methods: Fourier in the toroidal periodic direction and spectral elements in the poloidal plane. The 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 FBGKI presents two layers of parallelization: The first one corresponds to the

poloidal plane and the second one to the toroidal direction. In the poloidal plane, the domain decomposition is achieved using the software METIS. For the parallel linear algebra, one uses the software PETSC (Portable Extensible Toolkit for Scientific Computation). The time discretization makes use of a Strang splitting, that decouples the explicit treatment of the advection and Braginskii terms, from the implicit treatment of the Lorentz forces and the computation of the electric potential. Whereas the explicit part is easily parallelized, the implicit one requires solving a strongly anisotropic elliptic problem for the potential. In the parallel version of FBGKI the system matrix is assembled in sparse manner, in order to allow using the multigrid HYPRE preconditionner implemented in PETSC. Till now results have only been obtained for computations done on a few tens of processors. Both the weak and strong scalings look satisfactory. Numerical experiments are still required to go up to hundreds or thousands of processors.

- Participants: Sébastien Minjeaud and Richard Pasquetti
- Contact: Sebastian Minjeaud
- Reference: [25]

4.4. FEEQS.M

FUNCTIONAL DESCRIPTION

FEEQS.M (Finite Element Equilibrium Solver in Matlab) is a MATLAB implementation of the numerical methods in [16] to solve equilibrium problems for toroidal plasmas. Direct and inverse problems for both the static and transient formulations of plasma equilibrium can be solved. FEEQS.M exploits MATLAB's evolved sparse matrix methods and uses heavily the vectorization programming paradigm, which results in running times comparable to C/C++ implementations. FEEQS.M complements the production code CEDRES++ in being considered as fast prototyping test bed for computational methods for equilibrium problems. This includes aspects of numerics such as improved robustness of the Newton iterations or optimization algorithms for inverse problems. The latest developments aim at incorporating the resistive diffusion equation.

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

4.6. Jorek-Django

FUNCTIONAL DESCRIPTION

Jorek-Django is a non-production version of the JOREK software, for MHD modeling of plasma dynamic in tokamak 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 (EPI Tonus), Ayoub Iaagoubi and Ahmed Ratnani (IPP, Garching)
- Contact: Hervé Guillard
- URL: <https://gforge.inria.fr/projects/jorek/>

4.7. 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 Estivals
- Contact: Hervé Guillard

4.8. 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. The proposed method and algorithm are detailed in [4] and results from numerous numerical experiments are presented. The method is foreseen to be used in the real-time plasma control loop on the WEST tokamak.

- Contact: Blaise Faugeras

CLIME Project-Team

5. New Software and Platforms

5.1. Data assimilation library: Verdandi

Participants: Nicolas Claude, Vivien Mallet, Gautier Bureau [M3DISIM], Dominique Chapelle [M3DISIM], Sébastien Gilles [M3DISIM], Philippe Moireau [M3DISIM].

The leading idea is to develop a data assimilation library (see the web site <http://verdandi.sourceforge.net/>) intended to be generic, at least for high-dimensional systems. Data assimilation methods, developed and used by several teams at Inria, are generic enough to be coded independently of the system to which they are applied. Therefore these methods can be put together in a library aiming at:

- making easier the application of methods to a great number of problems,
- making the developments perennial and sharing them,
- improving the broadcast of data assimilation works.

An object-oriented language (C++) has been chosen for the core of the library. A high-level interface to Python is automatically built. The design study raised many questions, related to high dimensional scientific computing, the limits of the object contents and their interfaces. The chosen object-oriented design is mainly based on three class hierarchies: the methods, the observation managers and the models. Several base facilities have also been included, for message exchanges between the objects, output saves, logging capabilities, computing with sparse matrices.

In 2015, version 1.7 was released. We introduced an implementation of nudging. A level-set observation manager was added. Further tests were included. We added the option to build Verdandi as a library.

5.2. Image processing library: Heimdali

Participants: Isabelle Herlin, Dominique Béréziat [UPMC], David Froger [SED].

The initial aim of the image processing library Heimdali was to develop 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 image assimilation based on ITK (Insight Segmentation and Registration Toolkit <http://www.itk.org>).
- in reverse, providing tools to ITK and contribute to the ITK community.

The main components of Heimdali concern:

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

In 2015, additional functions were introduced in the library in order to allow more pre/post processing tools.

5.3. Polyphemus

Participants: Vivien Mallet, Sylvain Doré [CEREA], Karine Sartelet [CEREA], Yelva Roustan [CEREA].

Polyphemus (see the web site <http://cerea.enpc.fr/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 forecasts 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.

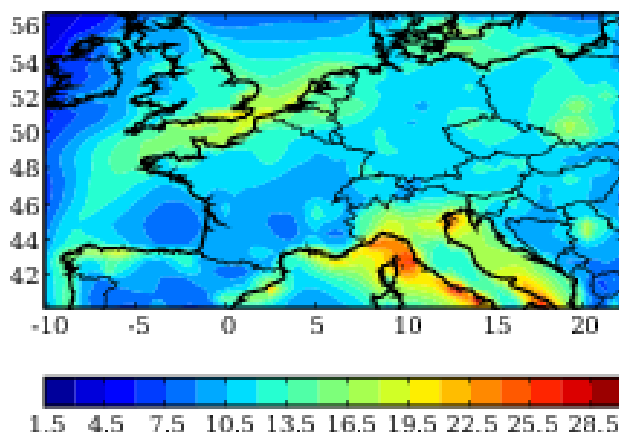


Figure 1. Map of the relative standard deviation (or spread, %) of an ensemble built with Polyphemus (ozone simulations, $\mu\text{g m}^{-3}$). The standard deviations are averaged over the summer of 2001. They provide an estimation of the simulation uncertainties.

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).

In 2015, version 1.9 was released, with all previous developments on the interface between Verdandi and Polyphemus. The other improvements were developed by CEREAs on aerosol modeling.

COFFEE Project-Team

5. New Software and Platforms

5.1. NS2DDV

The code NS2DDV is developed jointly with the team SIMPAF, of the Inria Research Centre Lille Nord Europe. 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. Further details can be found in the research papers J. Comput. Phys., 227, 4671–4696, 2008 and J. Comput. Phys., 229 (17), 6027–6046, 2010. The code exists in two versions: a Matlab public version, a C++ prototype version allowing more ambitious simulations. Both versions are still subject to developments. The current versions is restricted to incompressible flows but ongoing progress are concerned with the simulation of avalanches. The source code of the public version is downloadable and several benchmarks tests can be reproduced directly.

- Contact: Emmanuel Creusé
- URL: math.univ-lille1.fr/~simpaf/SITE-NS2DDV/home.html
- The code has been subject to an APP deposit many years ago, but we never received any registration number.

5.2. Compass

for Computing Parallel Architecture to Speed up Simulation 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. A first step in the code development has been made during the 2012 edition of CEMRACS and then pursued by C. Guichard, R. Masson and R. Eymard in 2013. A first version of the code has been deposited at the Agency for the Protection of Programs (APP). This current version of ComPASS has been tested on a gas storage two phase flow benchmark with GDFSuez using the Vertex Approximate Gradient spatial discretization. The results have shown a very good parallel scalability on the CICADA Cluster at UNS with a few millions of cells and up to 1024 cores. The objective is to develop a generic simulator for multiphase Darcy flows. This simulator will implement advanced finite volume methods on general 3D meshes and on heterogeneous anisotropic media, taking into account discrete fracture networks represented as interfaces of codimension one and coupled with the surrounding matrix. It will be able to treat a large range of multiphase Darcy flow models accounting for thermodynamical equilibrium and the coupling with an energy conservation equation. The simulator will run on massively parallel architectures with a few thousands of cores. It will be applied to several type of industrial applications starting with the simulation of high energy geothermal systems as a carbon-free source of power production.

- Participants: Roland Masson, Cindy Guichard, Feng Xing and Robert Eymard, Thierry Goudon,
- Contact: Roland Masson
- URL: math.unice.fr/~massonr/
- The code has been subject to an APP deposit a few years ago, but we never received any registration number.

5.3. SimBiof

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: Magali Ribot

5.4. AP_PartFlow

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

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 Mémin
- Contact: Etienne Mémin
- URL: <http://fluid.irisa.fr/index.html>

5.2. 3DLayeredMotion

Estimation of 3D interconnected layered atmospheric motion fields

FUNCTIONAL DESCRIPTION

This software extends the previous 2D version. It allows 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 Mémin
- URL: <http://fluid.irisa.fr>

5.3. DenseMotion

Estimation of 2D dense motion fields

FUNCTIONAL DESCRIPTION

This code allows the computation from two consecutive images of a dense motion field. The estimator is expressed as a global energy function minimization. The code enables the choice of different data models and different regularization functionals depending on the targeted application. Generic motion estimators for video sequences or fluid flows dedicated estimators can be set up. This software allows in addition the users to specify additional correlation based matching measurements. It enables also the inclusion of a temporal smoothing prior relying on a velocity vorticity formulation of the Navier-Stoke equation for Fluid motion analysis applications. The different variants of this code correspond to research studies that have been published in IEEE transaction on Pattern Analysis and machine Intelligence, Experiments in Fluids, IEEE transaction on Image Processing, IEEE transaction on Geo-Science and Remote Sensing. The binary of this code can be freely downloaded on the FLUID web site <http://fluid.irisa.fr>.

- Participants: Étienne Mémin and Thomas Corpetti
- Contact: Étienne Mémin
- URL: <http://fluid.irisa.fr>

5.4. Low-Order-Motion - Estimation of low order representation of fluid motion

Low order description and estimation of 2D dense motion fields

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: Étienne Mémin and Anne Cuzol
- Contact: Étienne Mémin
- 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 Dérian, Christopher Mauzey and Étienne Mémin
- Contact: Étienne Mémin

LEMON Team

6. New Software and Platforms

6.1. 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. It uses fully unstructured meshes with arbitrary numbers of edges. The key features of the models and numerical techniques embedded in SW2D are

- specific momentum/energy dissipation models that are active only under transient conditions. Such models, that are not present in classical shallow water models, stem from the upscaling of the shallow water equations and prove essential in modeling the features of fast urban flow transients accurately
- modified HLLC solvers for an improved discretization of the momentum source terms stemming from porosity gradients
- higher-order reconstruction techniques that allow for faster and more stable calculations in the presence of wetting/drying fronts.

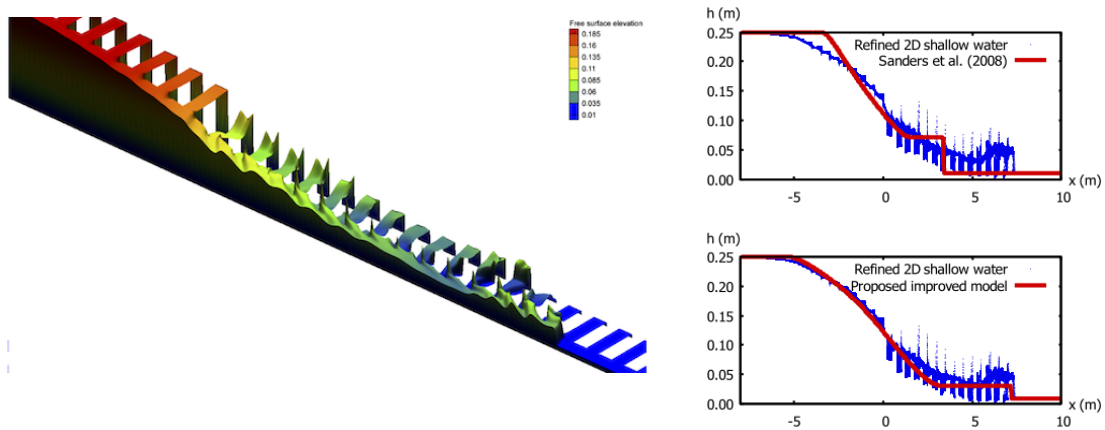


Figure 2. Propagation of a flood wave into a channel with lateral storage. Refined 2D simulation using the SW2D computational code

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

6.2. 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).

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.

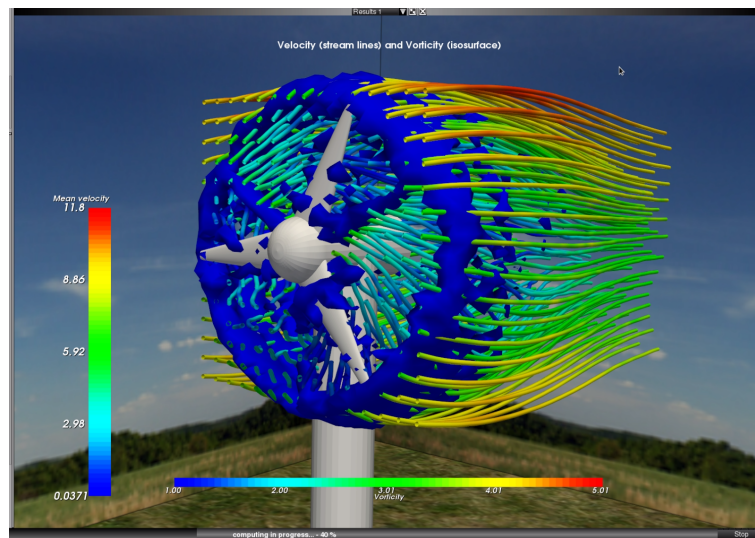


Figure 3. Velocity streamlines and vorticity around a wind mill (artistic view). WINDPOS Project.

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

- Contact: Antoine ROUSSEAU
- URL: <http://windpos.inria.fr>

MAGIQUE-3D Project-Team

5. New Software and Platforms

5.1. Elasticus

SCIENTIFIC DESCRIPTION

Elasticus simulates acoustic and elastic wave propagation in 2D and in 3D, formulated as a first order system, 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 over optimization of its performances. Developed 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.

IMPROVEMENT

The various kinds of fluxes and the RK4 time schemes were implemented by Simon Ettouati. The elasto-acoustic coupling was implemented by Elvira Shishenina in the framework of her Master internship, in collaboration with Simon Ettouati and Lionel Boillot. The TTI elastic kernel as well as the Absorbing Boundary Conditions were developed by Lionel Boillot.

- Participants: Simon Ettouati, Julien Diaz, Lionel Boillot and Elvira Shishenina.
- 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, formulated as a second order system. 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 (IPDG) 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).

IMPROVEMENT

The main improvements are related to the frequency domain part. The Hybridizable Discontinuous Galerkin was implemented in 2D and in 3D elastodynamics by Marie Bonnasse Gahot in the framework of her PhD thesis. The IPDG Method was implemented in 3D acoustics and for the 3D elasto-acoustic coupling by Conrad Hillairet in the framework of his Master thesis. The Perfectly Matched Layers were optimized (the length of the layers and the amplitude of the absorption parameters are now automatically computed) by Andrew Wang in the framework of his two months internship.

- Participants: Julien Diaz, Marie Bonnasse Gahot, Conrad Hillairet 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, elastodynamic problems.

FUNCTIONAL DESCRIPTION

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

IMPROVEMENT

This year, new high-order schemes (internship of Guillaume Marty and thesis of Mamadou N'diaye) have been implemented. The code has been strongly modified in order to obtain a fast compilation. The software has been used by Chloe team (through the internship of Laurene Hume) and compared to COMSOL providing a similar efficiency.

- Participants: Marc Duruflé, Juliette Chabassier, Mamadou N'diaye, Guillaume Marty
- Contact: Marc Duruflé
- URL: <http://montjoie.gforge.inria.fr/>

5.4. TMBM-DG

SCIENTIFIC DESCRIPTION

TMBM-DG simulates acoustic and elastic wave propagation in 2D and in 3D, formulated as a first order system, using Discontinuous Galerkin Methods. The space discretization is based on two kinds of basis functions, using Lagrange or Jacobi polynomials 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.

IMPROVEMENT

The first version of the code was recently developed jointly with our industrial partner Total. The main developer in MAGIQUE-3Dis Lionel Boillot.

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

SAGE Project-Team

6. New Software and Platforms

6.1. GENFIELD

FUNCTIONAL DESCRIPTION

GENFIELD allows the generation of log-normal correlated fields. It is based on a spectral method and uses the FFTW library. Parallelism is implemented using MPI communications. GENFIELD is used in hydrogeology to model natural fields, like hydraulic conductivity or porosity fields.

- Authors: Grégoire Lecourt, Jocelyne Erhel, Jean-Raynald De Dreuzy and Géraldine Pichot
- Contact: Jocelyne Erhel

6.2. GLiMuH

Grains with Liquid Meniscus under Heating

FUNCTIONAL DESCRIPTION

The GLiMuH code is devoted to the understanding of how heat diffuses in an assembly of solid grains separated by air and water. In the pendular regime, the quantity of water is very small, leading to liquid bridges between the grains. In the current approximation, the grains are spherical in shape, and the numerical simulation is done in a 3D axisymmetric coordinate system. The shape of the liquid/gas interface is computed by integrating a differential algebraic system of equations, with a given quantity of water per unit volume of the porous medium, and under the constraint of a given contact angle between the liquid/gas interface and the solid boundaries. The numerical results allow us to estimate the effective thermal conductivity of a real wet granular medium, which is required to establish more realistic models for the HeMaTiS code.

- Authors: Édouard Canot, Salwa Mansour and Renaud Delannay
- Contact: Édouard Canot

6.3. GRT3D

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

APP: version 2.0, April 2014, registered

Programming language: C

Current work: refactoring

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.

- Authors: Yvan Crenner, Caroline De Dieuleveult, Jocelyne Erhel, Souhila Sabit, Nadir Soualem
- Partner: ANDRA
- Contact: Jocelyne Erhel

6.4. HeMaTiS

Heat and Mass Transfer in Soils

FUNCTIONAL DESCRIPTION

HeMaTiS is a set of Finite Volume programs (variants concern different geometrical configurations: 1D, 1D-radial, 2D, 3D-axisymmetric) for computing the transient heat diffusion in soils when there is a phase change of water. Currently, the soil is modelled by a heterogeneous porous medium having constant thermo-physical properties, and the porous medium is saturated with water. The phase change is treated by means of the Apparent Heat Capacity method. In the near future, we plan to use an unsaturated model (but limited to small water content), and an effective thermal conductivity which depends on the local humidity (this latter law may reveal hysteresis behaviour). The software is written in Fortran 95 and is based on the Muesli library. A Computer Algebra System (Maple or Maxima) is used to compute the Jacobian matrix.

- Authors: Édouard Canot, Mohamad Muhieddine, Salwa Mansour and Renaud Delannay
- Contact: Édouard Canot

6.5. PALMTREE

FUNCTIONAL DESCRIPTION PALMTREE is an easy-to-use library for the parallelization of Lagrangian methods for partial differential equations and general Monte Carlo methods. The code aims at satisfying three properties:

1. Reduction of computation time by using parallel architecture,
2. Simplicity as the user just has to add the algorithm governing the behaviour of the particles,
3. Portability since one has the possibility to use the package with any compiler and OS,
4. Action-Replay which provides the ability of the package to replay a selected batch of particles.

The software also now possesses a beta version which allows to run in parallel hybrid solvers, that is solvers which use both deterministic methods (FEM, FDM, etc...) and probabilistic methods. Moreover, the engineering being this software was published in MCQMC 2014 [32].

- Authors: Lionel Lenôtre, Géraldine Pichot.
- Contact: Lionel Lenôtre.
- URL: <http://people.irisa.fr/Lionel.Lenotre/software.html>

6.6. SBM

Skew Brownian Motion

FUNCTIONAL DESCRIPTION

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

- Authors: Antoine Lejay and Géraldine Pichot
- Contact: Géraldine Pichot

6.7. TPIP

Thermal Properties by Inverse Problem

FUNCTIONAL DESCRIPTION

TPIP is a program which aims at estimating the thermo-physical of a saturated porous medium after a strong heating which leads to the phase change of the water contained in the pores, knowing the experimental heating curves history at few selected points. The least-square criterion is used, in which sensitivity coefficients are the solution of a huge, complex PDE system in order to take into account the phase change of water. These equations for the sensitivity coefficients are therefore obtained via a Computer Algebra System (Maple or Maxima). In many aspects, the forward problem is similar to the HeMaTiS code, and like it, is based on Muesli. Two different minimization algorithms may be used, Damped Gauss-Newton or Levenberg-Marquardt. A special procedure has been applied in order to obtain a robust convergence, by changing some parameters of the forward problem during the iterations.

- Authors: Édouard Canot, Mohamad Muhieddine, Salwa Mansour and Renaud Delannay
- Contact: Édouard Canot

6.8. Zohour

FUNCTIONAL DESCRIPTION

Zohour is a node-based adaptive 2D mesh algorithm, written in Fortran 2003. A basic rectangular, regular set of nodes is recursively refined. Then the cells come from the Voronoi tessellation. While the domain is currently limited to a rectangular shape, its strength is three-fold: first, computing the flux via a Finite Element or Finite Volume method is both simple and accurate because each cell-side of cells is the bisection of two nodes,

second, the transition between zones of different levels of refinement is more progressive than other methods, leading to a smaller number of nodes for the whole mesh,

third, during successive refinements when dealing with a transient problem, interpolation is needed only by the new nodes, limiting the numerical errors.

- Author: Édouard Canot
- Contact: Édouard Canot
- URL: <http://people.irisa.fr/Edouard.Canot/zohour/>

SERENA Team

6. New Software and Platforms

6.1. New Software

6.1.1. *FreeFem++ a posteriori package*

Participants: Martin Vohralík, Zuqi Tang.

The scientific calculation code FreeFem++ is an example of a complex software numerical simulation tool relying on traditional matching triangular meshes. It encompasses all specification of the problem, the choice and implementation of the numerical method, the choice and implementation of the linearization method (nonlinear solver), and the choice and implementation of the method of solution of the associated linear systems (linear solver). In the post-doc stay of Z. Tang, we have integrated here some recent advances of the theory of a posteriori error estimation and of adaptive algorithms. In particular, (local) adaptive stopping criteria for the linear and nonlinear solvers have been implemented.

Version 3.42

Programming language: C++

<http://www.freefem.org/ff++/>

<https://who.rocq.inria.fr/Zuqi.Tang/freefem++.html>

STEPP Project-Team

5. New Software and Platforms

5.1. QGISTranusReports

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 â 2D or 3D â 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.

- Contact: Peter Sturm

5.2. 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: Patrick Criqui, Constantin Ilasca, Olivier Boucher and H el ene Benveniste
- Partners: EDDEN - IPSL
- Contact: Emmanuel Prados
- URL: <http://redem.gforge.inria.fr/>

5.3. 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 is to automatize most of the work of standard input-output analysis and to visualize the results in a user-friendly way in order to efficiently address related environmental questions.

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

5.4. Contribution to the R package “sensitivity”

FUNCTIONAL DESCRIPTION

The contribution to the R package “sensitivity” includes the development of the function “sobolroahs” performing global sensitivity analysis of a numerical model. This function implements the estimation of the Sobol’ sensitivity indices introduced by [19] using two Orthogonal Array-based Latin Hypercubes. This function allows the estimation of all first-order indices or all closed second-order indices (containing the sum of the second-order effect between two inputs and the individual effects of each input) at a total cost of $2 \times N$. For closed second-order indices, $N = q^2$ where $q \geq d - 1$ is a prime number denoting the number of levels of the orthogonal array, and where d is the number of factors of the model.

- Participants: Laurent Gilquin, Elise Arnaud, Clémentine Prieur
- Partners: AIRSEA (Inria / UJF)
- Contact: Laurent Gilquin
- URL: <https://cran.r-project.org/web/packages/sensitivity/index.html>

TONUS Team

6. New Software and Platforms

6.1. SCHNAPS

Participants: Emmanuel Franck, Pierre Gerhard, Philippe Helluy [correspondent], Michel Massaro, Malcolm Roberts, Bruno Weber.

Solveur pour les lois de Conservation Hyperboliques Non-linéaires Appliqué aux PlasmaS

SCIENTIFIC DESCRIPTION

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

We have invested for several years until now into scientific computing on GPUs, using the open standard OpenCL (Open Computing Language). We were recently awarded a prize in the international AMD OpenCL innovation challenge thanks to an OpenCL two-dimensional Vlasov-Maxwell solver that fully runs on a GPU. OpenCL is a very interesting tool because it is an open standard now available on almost all brands of multicore processors and GPUs. The same parallel program can run on a GPU or a multicore processor without modification. 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 heart of the library is made of generic parallel algorithms for solving conservation laws. The parallelism can be both fine-grained (oriented towards GPUs and multicore processors) and coarse-grained (oriented towards GPU clusters). The separate modules allow managing the meshes and some specific applications. With our partner AxesSim, we also develop a C++ specific version of SCHNAPS for electromagnetic applications.

FUNCTIONAL DESCRIPTION

SCHNAPS is a generic Discontinuous Galerkin solver, written in C, based on the OpenCL, MPI and StarPU frameworks.

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

6.2. Selalib

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

SEmi-LAgrangian LIBrary

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/>

6.3. 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 physicist has obtained some important results. However to run larger and more complex test cases it is necessary to evolve the numerical methods used.
In 2014, the DJANGO code has been created, the aim of this code is double: 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 2003 with a Basic MPI framework. The code is coupled with the PETSC library for the linear solvers and the code CAID (A. Ratnani) for the mesh.
- 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:
Laura Mendoza, Mustafa Gaja (PhD), Jalal Lakhilili, Celine Caldini-Queiros, Matthias, Hoelzl, Eric Sonnendrücker (Max Planck Institut of Plasma Physic, Garching, Germany), Ayoub Iaagoubi (ADT), Hervé Guillard (University of Nice and Inria Sophia-Antipolis, France), Virginie Grandgirard, Guillaume Latu (CEA Cadarache, France)
- Year 2015:
The year 2015 is an important year for the JOREK code. Indeed, after the year 2014 where the IsoParametric (Bezier curves) finite element approach in 2D have been implemented for basic elliptic equations, in 2015 we have extended the code for more complex problems. Now the code can treat some hyperbolic, parabolic and elliptic models with different approaches (IsoParametric/IsoGeometric approach, Splines for triangle) in 2D and 3D by tensor product. The compilation of the code is more stable and some regression test cases have been added. To finish, two realistic MHD models (which come from to the JOREK code) have been implemented and must be validated. The Year 2016 will be the year of the first physical and realistic results.

BIOCORE Project-Team

6. New Software and Platforms

6.1. In@lgae

KEYWORDS: Simulation - Microalgae system - Productivity

SCIENTIFIC DESCRIPTION The in@lgae simulation platform is dedicated to the simulation of microalgae growth at different locations and for different periods of the year. The platform runs different submodels to account for the actual climate and compute biomass productivity together with the consumption of water, nitrogen, phosphorus, ... The platform runs models which describe mechanisms from fast time scale (dynamics of photosystems) down to slow time scales (growth photoacclimation). The models also include a description of the temperature evolution in the culturing systems. The simulation can also be coupled with a model of hydrodynamics as represented by the Freshkiss software developed by the Ange EPI.

FUNCTIONAL DESCRIPTION

In@lgae simulates the productivity of a microalgae production system, taking into account both the process type and its location and time of the year. The process is mainly defined by its thermal dynamics and by its associated hydrodynamics. For a given microalgal strain, a set of biological parameters describe the response to nitrogen limitation, temperature and light. As a result, the biomass production, CO₂ and nitrogen fluxes, lipid and sugar accumulation are predicted.

- Participants: Étienne Delclaux, Francis Mairet, Quentin Béchet and Olivier Bernard
- Contact: Olivier Bernard
- URL: <https://gforge.inria.fr/projects/inalgae>

6.2. Odin

KEYWORDS: Bioinformatics - Biotechnology

SCIENTIFIC DESCRIPTION

This C++ application is dedicated to deploy advanced control algorithms on real bioprocesses through the use of a Scilab interpreter. In Biocore we develop advanced algorithms for supervision and control, and ODIN is the media to apply them. 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 also contains a Scilab-based process simulator which can be harnessed for experimentation and training purposes. It is very modular in order to adapt to any plant and to run most of the algorithms.

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, Olivier Bernard and Francesco Novellis
- Contact: Olivier Bernard
- URL: <https://team.inria.fr/biocore/software/odin/>

CARMEN Team

6. New Software and Platforms

6.1. CEPS: a Cardiac ElectroPhysiology Simulator

The Carmen team develops a software code 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 easily allow the development of new numerical methods and new physical models.

As compared to other existing softwares, CEPS aims at providing a more general framework of integration for new methods or models and a better efficiency in parallel. CEPS is designed to run on massively parallel architectures, and to make use of state-of-the-art and well known computing libraries to achieve realistic and complex heart simulations. CEPS also includes software engineering and validation tools. We use the platform GForge ([ceps](#)) based on Git. This allows to keep a history of developments for developers and users. Some of our collaborators actively participate to the testing and discussion for the development of CEPS, namely:

- C. Pierre, LMA University of Pau et des Pays de l'Adour;
- R. Turpault, IMB University of Bordeaux;

Several people work and make an useful code for researchers and users.

- Development of an external procedure to compile dependencies for CEPS. This allows a very simple way to install CEPS for partners or students.
- Improve continuous integration test cases in order to have a best coverage of the code as possible.
- Overwrite C++ class for ionic models and adding new models in collaboration with A. Gérard.
- Integration of the partitionneur PTScotch in order to realise a partitioning on the nodes.
- Tutorials for beginners on the code (linear algebra, installation, compilation...).
- New implementation of the bilayer model developed by L. Simon during his PhD thesis. The most important part will be provided by M. Fuentes works. Difficulties are currently the specification of two layers in CEPS and how to connect them.
- The strategy remains at this time is to have two meshes in entry (on global mesh for the auricles and another *under-mesh* corresponding to the two layers domain). This means, that we have to create a connectivity table between the global mesh and the *under-mesh*.
- Development of an interface for users in order to specify data in a text file for the code such as physical values for ionic models or numerical values for numerical methods (especially in time) used.

6.2. IDAM

The goal of the IDAM project is to define a conceptual module in MUSIC in order to create realistic meshes for the CEPS code. Information comes from IRM done by doctors. Furthermore, objectives are the continuation of used methods in the team and the visualisation of numerical results obtained by CEPS (<https://bil.inria.fr/software/view/2630/tab>).

This project started on 1st December 2015 for two years. M. Juhor is in charge of this project in collaboration with the MedInria team and the IHU LIRYC.

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

M3DISIM Team

6. New Software and Platforms

6.1. FELiScE

Finite Elements for Life SCIences and Engineering problems

KEYWORDS: Health - Cardiac - Finite elements - Cardiac Electrophysiology

FUNCTIONAL 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.

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: Dominique Chapelle, Miguel Angel Fernandez Varela, Jean-Frédéric Gerbeau, Philippe Moireau, Marina Vidrascu, Sébastien Gilles, Sebastien Impériale and Gautier Bureau
- 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 written in (64-bit compatible) Matlab and C (mex functions), designed to perform both simulation and estimation (based on various types of measurements, e.g. images) of the heart mechanical behavior. Started in 2006, it is already quite large (about 60,000 lines), and is used within various collaborations.

FUNCTIONAL DESCRIPTION

The code relies on OpenFEM – to which the team has previously contributed, see <http://www.openfem.net> – for the finite element computations, and the implementation was performed with a particular concern for modularity, since modeling and estimation use the same finite element operators. This modularity also allows to couple the code with other FEM solvers, such as LifeV and Mistral developed in the Reo team-project. In particular, we are now able to include perfusion and electrical coupling with LifeV using PVM, and fluid-structure interaction using Mistral.

We also included 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.

We incorporated numerous non-linear data assimilation observation operators based on medical imaging post-processing to be able to now perform estimation with a large variety of medical imaging modalities. And recently we have worked on generalized micro-macro cardiac law using stochastic formulations.

- Participants: 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 an 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. Moreover, a Matlab module called VerdandinMatlab is developed in the team for pedagogical and test purposes.

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

MAMBA Project-Team

6. New Software and Platforms

6.1. TiQuant

Tissue Quantifier

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

FUNCTIONAL DESCRIPTION

Systems biology and medicine on histological scales require the 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 has been little recognised thus far. 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, allowing 3D reconstructions of liver lobules down to a resolution of less than a micrometer. The software has been made available to the public by publication in ref. [14], together with a new surface reconstruction algorithm based on the morphological Watershed algorithm. We validated that this algorithm allows reconstruction of cell shapes from nucleus and blood microvessel information, and demonstrated that it allows a reliable estimate of liver lobules, the smallest repetitive functional and micro-anatomical liver units, that besides in pig are not anatomically separated.

A separate 2D version of it (TI-Quant-BF-2D) has been used to analyse the invasion pattern of non-small cell lung cancer (NSCLC) cells *in vitro* [24] (see below).

- Contact: Dirk Drasdo
- URL: <http://www.msystbio.com>

6.2. TiSim

Tissue Simulator

KEYWORDS: Systems Biology - Bioinformatics - Biology - Physiology

FUNCTIONAL DESCRIPTION

We advanced the complementary software TiSim (Tissue Simulator) that will soon be provided. TiSim allows agent-based simulations of multicellular systems and can be directly used by processed image data provided by TiQuant.

The software has been tested over the whole year including almost all group members to prepare it for submission and will present a number of application example to introduce a potential user into the software. These will be monolayer and multicellular spheroid growth, a multiscale modeling example and liver regeneration.

- Contact: Dirk Drasdo

MODEMIC Project-Team

6. New Software and Platforms

6.1. Landfill Recirculation Management Simulator

FUNCTIONAL DESCRIPTION

Following the first works on modeling and control of landfills performed in the framework of the associated team DYMECOS with Chile, that have proposed an optimal feedback strategy for the leachate recirculation under the assumption of a perfectly mixed medium [40], a first mock-up software has been conceived in view of studying the effects of inhomogeneity along with identification procedures of spatial network structures on data (interconnection of bioreactors as in VITELBIO project). The development of the software is in progress.

- Participants: Andres Donoso-Bravo (PUCV, Chile), J.R. de Dreuzy (GéoSciences Rennes), Alain Rapaport, Hector Ramirez, Alejandro Rojas Palma
- Contact: Alain Rapaport
- URL: <https://sites.google.com/site/eadymecos/resultats>

6.2. Action Dépollution

FUNCTIONAL DESCRIPTION

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

- Participants: Alain Rapaport, Antoine Rousseau (EPI LEMON)
- Contact: Antoine Rousseau
- URL: <https://depollution.inria.fr/>

6.3. VITELBIO (VIRtual TELLuric BIOreactors)

FUNCTIONAL DESCRIPTION

Vitelbio is a simulator of the microbial activity in soils, for which the spatialization is represented as a network of interconnected reservoirs. The software allows to draw an interconnections graph, that respects the constraint of the maximum flow, and to choose the biological characteristics of various bacterial species in competition for a single nutrient. The simulator computes the time evaluations of the different populations in each compartment, and compares the overall yielding of the ecosystem in terms of bio-conversion of the substrate. This software has been developed in the framework of the INRA/Inria project VITELBIO (VIRtual TELLuric BIOreactors), with the help of the company ITK. It is today mainly used for educational purposes (in MSC and PhD lectures).

- Participants: Jérôme Harmand, Alain Rapaport
- Contact: Alain Rapaport
- URL: <http://vitelbio.itkweb.fr/vitelbio/>

Monc Team

6. New Software and Platforms

6.1. CADMOS

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

- Participants: Olivier Saut and Julien Jouganous
- Partners: Université de Bordeaux - CNRS - INP Bordeaux
- Contact: Olivier Saut

6.2. Carcinom (Computer-Assisted Research about Cancer growth and INsights on Oncological Mechanisms)

KEYWORDS: Cancer - Data modeling - Regression

- Participants: Sébastien Benzekry
- Contact: Sébastien Benzekry
- FUNCTIONAL DESCRIPTION A software for nonlinear regression of tumor growth and therapy models and statistical inference. This software is primarily designed to perform a modeling analysis of tumor growth kinetics. Given a data set of longitudinal measurements of tumor size in a population, it fits several models of tumor growth, computes several goodness-of-fit statistical metrics, identifies the parameters of the models and estimates the uncertainty associated to their determination. It provides several graphical and numerical outputs (in the form of LaTeX tables).

6.3. ELMO (Numerical Simulation of cell electroporation)

KEYWORDS: Bioinformatics - Biology - Numerical electroporation - Finite difference method in 2D-3D

- Participants: Clair Poignard and Michael Leguebe
- Partners: Université de Bordeaux - CNRS - INP Bordeaux
- Contact: Michael Leguebe
- URL: http://www.math.u-bordeaux1.fr/~mleguebe/phd_fr.html
- SCIENTIFIC DESCRIPTION 2D-3D code of finite difference method in C++ to compute the electroquasistatic field in a biological cell, with non-linear model of membrane conductance and lateral diffusion of lipids.
- FUNCTIONAL DESCRIPTION Compute the electroquasistatic field and the porated region of the cell membrane. The aim is to provide a user-friendly code for applied mathematicians and biophysicists.

6.4. Meta-poumon

KEYWORDS: Health - Evolution - Cancer - Medical imaging

- Participants: Olivier Saut, Thierry Colin, Marie Martin and Julien Jouganous
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: Olivier Saut
- 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.

6.5. Nenuphar

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

- Partners: CNRS - INP Bordeaux - Université Bordeaux 1
- Contact: Marie Martin
- 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.

6.6. SESAR (Monitor of the effect of RT on Retroperitoneal Sarcoma)

KEYWORDS: Segmentation - Health - DICOM - Cancer - Medical imaging

- Partner: Institut Bergonié
- Contact: Olivier Saut

6.7. SegmentIt

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

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

MYCENAE Project-Team (section vide)

NUMED Project-Team

4. New Software and Platforms

4.1. Bingham flows

FUNCTIONAL DESCRIPTION

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

- Contact: Paul Vigneaux

4.2. OptimChemo

FUNCTIONAL DESCRIPTION

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

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

4.3. SETIS

KEYWORDS: Health - DICOM - Medical imaging - Drug development

FUNCTIONAL DESCRIPTION

SETIS software is a GUI allowing to treat DICOM medical images to extract pathological data. These data can then be exported and used in a SAEM software (including Monolix (Inria and 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). SETIS is filed under APP number IDN.FR.001.150013.000.S.A.2014.000.21000.

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

4.4. SIMPHYT

KEYWORDS: Bioinformatics - Cancer - Drug development

FUNCTIONAL DESCRIPTION

SimPHYt is an implementation in Python of the low grad glioma model. The aim is to predict the evolution of the glioma size of patients.

- Participant: Benjamin Ribba
- Contact: Benjamin Ribba

4.5. VAXSIMSTAB

KEYWORDS: Bioinformatics - Health - Drug development

FUNCTIONAL DESCRIPTION

VAXSIMSTAB is a modeler stability prediction of vaccine software, property of Sanofi Pasteur.

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

REO Project-Team

6. New Software and Platforms

6.1. FELiScE

Finite Elements for Life SCIences and Engineering problems

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

FUNCTIONAL DESCRIPTION

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

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

6.2. LIFE-V

KEYWORD: Finite element modelling

FUNCTIONAL DESCRIPTION

LIFE-V is a finite element library providing implementations of state of the art mathematical and numerical methods. It serves both as a research and production library. LIFE-V is the joint collaboration between three institutions: Ecole Polytechnique Fédérale de Lausanne (CMCS) in Switzerland, Politecnico di Milano (MOX) in Italy and Inria (REO) in France. It is a free software under LGPL license.

- Participants: Jean-Frédéric Gerbeau and Miguel Angel Fernandez Varela
- Partners: EPFL - Ecole Polytechnique Fédérale de Lausanne - MOX Politecnico di Milano
- Contact: Miguel Angel Fernández Varela
- URL: <http://www.lifev.org/>

6.3. SHELDDON

SHELLs and structural Dynamics with DOrain 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/shelldon/>