RESEARCH CENTER

FIELD
Computational Sciences for Biology, Medicine and the Environment

Activity Report 2012

Section Software

Edition: 2013-04-24

ABS Project-Team

4. Software

4.1. Software

This section briefly comments on all the software distributed by ABS. On the one hand, the software released in 2012 is briefly described as the context is presented in the sections dedicated to new results. On the other hand, the software made available before 2012 is briefly specified in terms of applications targeted.

In any case, the website advertising a given software also makes related publications available.

4.1.1. addict: Stoichiometry Determination for Mass Spectrometry Data

Participants: Deepesh Agarwal, Frédéric Cazals, Noël Malod-Dognin.

Context. Our work on the stoichiometry determination (SD) problem for noisy data in structural proteomics is described in section 5.2.1 . The `addict` software suite not only implements our algorithms `DP++` and `DIOPHANTINE`, but also important algorithms to determine the so-called Frobenius number of a vector of protein masses, and also to estimate the number of solutions of a SD problem, from an unbounded knapsack problem.

Distribution. Binaries for the `addict` software suite are made available from http://team.inria.fr/abs/software/voratom/.

4.1.2. vorpatch and compatch: Modeling and Comparing Protein Binding Patches

Participants: Frédéric Cazals, Noël Malod-Dognin.

Context. Modeling protein binding patches is a central problem to foster our understanding of the stability and of the specificity of macro-molecular interactions. We developed a binding patch model which encodes morphological properties, allows an atomic-level comparison of binding patches at the geometric and topological levels, and allows estimating binding affinities—with state-of-the-art results on the protein complexes of the binding affinity benchmark. Given a protein complex, `vorpatch` compute the binding patches, while the program `compatch` allows comparing two patches.

Distribution. Binaries for `VORPATCH` and `COMPATCH` are available from http://team.inria.fr/abs/software/vorpatch-compatch.

4.1.3. voratom: Modeling Protein Assemblies with Toleranced Models

Participants: Frédéric Cazals, Tom Dreyfus.

Context. Large protein assemblies such as the Nuclear Pore Complex (NPC), chaperonin cavities, the proteasome or ATP synthases, to name a few, are key to numerous biological functions. Modeling such assemblies is especially challenging due to their plasticity (the proteins involved may change along the cell cycle), their size, and also the flexibility of the sub-units. To cope with these difficulties, a reconstruction strategy known as Reconstruction by Data Integration (RDI), aims at integrating diverse experimental data. But the uncertainties on the input data yield equally uncertain reconstructed models, calling for quantitative assessment strategies.

To leverage thee reconstruction results, we introduced TOleranced Model (TOM) framework, which inherently accommodates uncertainties on the shape and position of proteins. The corresponding software package, `VORATOM`, includes programs to (i) perform the segmentation of (probability) density maps, (ii) construct toleranced models, (iii) explore toleranced models (geometrically and topologically), (iv) compute Maximal Common Induced Sub-graphs (MCIS) and Maximal Common Edge Sub-graphs (MCES) to assess the pairwise contacts encoded in a TOM.

Distribution. Binaries for the software package `VORATOM` are made available from http://team.inria.fr/abs/software/voratom/.

4.1.4. wsheller: Selecting Water Layers in Solvated Protein Structures

Participants: Frédéric Cazals, Christine Roth.

Context. Given a snapshot of a molecular dynamics simulation, a classical problem consists of *quenching* that structure—minimizing the potential energy of the solute together with selected layers of solvent molecules. The program `wsheller` provides a solution to the water layer selection, and incorporates a topological control of the layers selected.

Distribution. Binaries for `wsheller` are available from http://team.inria.fr/abs/software/wsheller.

4.1.5. intervor: Modeling Macro-molecular Interfaces

Participant: Frédéric Cazals.

In collaboration with S. Loriot (The GEOMETRY FACTORY*)*

Context. Modeling the interfaces of macro-molecular complexes is key to improve our understanding of the stability and specificity of such interactions. We proposed a simple parameter-free model for macro-molecular interfaces, which enables a multi-scale investigation —from the atomic scale to the whole interface scale. Our interface model improves the state-of-the-art to (i) identify interface atoms, (ii) define interface patches, (iii) assess the interface curvature, (iv) investigate correlations between the interface geometry and water dynamics / conservation patterns / polarity of residues.

Distribution. The following website http://team.inria.fr/abs/software/intervor serves two purposes: on the one hand, calculations can be run from the website; on the other hand, binaries are made available. To the best of our knowledge, this software is the only publicly available one for analyzing Voronoi interfaces in macro-molecular complexes.

4.1.6. vorlume: Computing Molecular Surfaces and Volumes with Certificates

Participant: Frédéric Cazals.

In collaboration with S. Loriot (The GEOMETRY FACTORY*, France)*

Context. Molecular surfaces and volumes are paramount to molecular modeling, with applications to electrostatic and energy calculations, interface modeling, scoring and model evaluation, pocket and cavity detection, etc. However, for molecular models represented by collections of balls (Van der Waals and solvent accessible models), such calculations are challenging in particular regarding numerics. Because all available programs are overlooking numerical issues, which in particular prevents them from qualifying the accuracy of the results returned, we developed the first certified algorithm, called `vorlume`. This program is based on so-called certified predicates to guarantee the branching operations of the program, as well as interval arithmetic to return an interval certified to contain the exact value of each statistic of interest—in particular the exact surface area and the exact volume of the molecular model processed.

Distribution. Binaries for `Vorlume` is available from http://team.inria.fr/abs/software/vorlume.

4.1.7. ESBTL: theEasy Structural Biology Template Library

Participant: Frédéric Cazals.

In collaboration with S. Loriot (The GEOMETRY FACTORY*, France) and J. Bernauer (Inria AMIB, France).*

Context. The ESBTL (Easy Structural Biology Template Library) is a lightweight C++ library that allows the handling of PDB data and provides a data structure suitable for geometric constructions and analyses.

Distribution. The C++ source code is available from http://esbtl.sourceforge.net/http://esbtl.sourceforge.net/.

4.1.8. A_purva: Comparing Protein Structure by Contact Map Overlap Maximization

Participant: Noël Malod-Dognin.

In collaboration with N. Yanev (University of Sofia, and IMI at Bulgarian Academy of Sciences, Bulgaria), and R. Andonov (Inria Rennes - Bretagne Atlantique, and IRISA/University of Rennes 1, France).

Context. Structural similarity between proteins provides significant insights about their functions. Maximum Contact Map Overlap maximization (CMO) received sustained attention during the past decade and can be considered today as a credible protein structure measure. The solver `A_purva` is an exact CMO solver that is both efficient (notably faster than the previous exact algorithms), and reliable (providing accurate upper and lower bounds of the solution). These properties make it applicable for large-scale protein comparison and classification.

Distribution. The software is available from http://apurva.genouest.orghttp://apurva.genouest.org.

AMIB Project-Team

4. Software

4.1. Varna

Participants: Yann Ponty [correspondant], Alain Denise.

VARNA is a tool for the automated drawing, visualization and annotation of the secondary structure of RNA, designed as a companion software for web servers and databases. VARNA implements four drawing algorithms, supports input/output using the classic formats *dbn, ct, bpseq* and *RNAML* and exports the drawing, either as a bitmap (*JPEG, PNG*) or as a vector picture (*SVG, EPS* and *XFIG*). It also allows manual modification and structural annotation of the resulting drawings using either an interactive *point and click* approach, within a web server or through command-line arguments. VARNA is a free software distributed under the terms of the GPLv3.0 license and available at http://varna.lri.fr.

VARNA is currently used by RNA scientists (Cited by 92 research articles since its presentation in Fall of 2009, according to Google scholar), web servers such as the BOULDEALE (http://www.microbio.me/boulderale/), TFOLD (http://tfold.ibisc.univ-evry.fr/TFold/), CYLOFOLD (http://cylofold.abcc.ncifcrf.gov/) webservers, and by databases such as IRESITE (http://iresite.org/), SRNATARBASE (http://ccb.bmi.ac.cn/srnatarbase/)and RFAM (http://rfam.sanger.ac.uk/), the main source of sequence/structure data for RNA scientist, to display secondary structures. It is also used as an integrated component within JALVIEW, arguably one of the leading sequence alignment editor (http://www.jalview.org/), and Y. Ponty co-supervised with Jim Procter (University of Dundee, Jalview Project Leader) two internships (including a Google Summer of Code) in the summer of 2012 to further the interactions between the two software.

4.2. SPFlow

Participants: Jiuqiang Chen, Sarah Cohen-Boulakia [correspondant], Christine Froidevaux [correspondant].

SPFLOW is a scientific workflow rewriting tool. SPFlow aims at transforming complex workflow structures (non series-parallel structures) into provenance-equivalent simple workflow structures (series-parallel structures). SPFlow takes as an input a file representing one scientific workflow from Taverna and produces another file in which the structure of the original workflow is made series-parallel while ensuring that both workflows have the same provenance (more information available at [32], [39]). The tool is freely available at http://www.lri.fr/~chenj/SPFlow.

4.3. GeneValorization

Participants: Bryan Brancotte, Sarah Cohen-Boulakia [correspondant].

High-throughput technologies provide fundamental information concerning thousands of genes. Many of the current research laboratories daily use one or more of these technologies and end-up with lists of genes. Assessing the originality of the results obtained includes being aware of the number of publications available concerning individual or multiple genes and accessing information about these publications. Faced with the exponential growth of publications available and number of genes involved in a study, this task is becoming particularly difficult to achieve. We introduce GENEVALORIZATION, a web-based tool which gives a clear and handful overview of the bibliography available corresponding to the user input formed by (i) a gene list (expressed by gene names or ids from ENTREZGENE) and (ii) a context of study (expressed by keywords). From this input, GENEVALORIZATION provides a matrix containing the number of publications with co-occurrences of gene names and keywords. Graphics are automatically generated to assess the relative importance of genes within various contexts. Links to publications and other databases offering information on genes and keywords are also available. To illustrate how helpful GENEVALORIZATION is, we have considered the gene list of the OncotypeDX prognostic marker test. it is available at http://bioguide-project.net/gv.

4.4. HSIM

Participant: Patrick Amar [correspondant].

HSIM is a simulation tool for studying the dynamics of biochemical processes in a virtual bacteria. The model is given using a language based on probabilistic rewriting rules that mimics the reactions between biochemical species. HSIM is a stochastic automaton which implements an entity-centered model of objects. This kind of modelling approach is an attractive alternative to differential equations for studying the diffusion and interaction of the many different enzymes and metabolites in cells which may be present in either small or large numbers.

The new version of HSIM includes a Stochastic Simulation Algorithm *a la* Gillespie that can be used with the same model in a standalone way or in a mixed way with the entity-centered algorithm. This new version offers also the possibility to export the model in SciLab for a ODE integration. Last, HSIM can export the differential equations system, equivalent to the model, to LaTeX for pretty-printing.

This software is freely available at http://www.lri.fr/~pa/Hsim; A compiled version is available for the Windows, Linux and MacOSX operating systems.

4.5. Cartaj

Participant: Alain Denise [correspondant].

CARTAJ is a software that automatically predicts the topological family of three-way junctions in RNA molecules, from their secondary structure only. The Cartaj software http://cartaj.lri.fr that implements our method can be used online. It is also meant for being part of RNA modelling softwares and platforms. The methodology and the results of CARTAJ are presented in [14].

BAMBOO Project-Team

5. Software

5.1. AcypiCyc

Participants: Hubert Charles [EPI], Patrice Baa Puyoule [Contact, Patrice.Baa-Puyoulet@lyon.inra.fr], Stefano Colella [Contact, stefano.colella@lyon.inra.fr], Ludovic Cottret, Marie-France Sagot [EPI], Augusto Vellozo [Contact, augusto@cycadsys.org], Amélie Véron.

Database of the metabolic network of *Acyrthosiphon pisum*.
http://acypicyc.cycadsys.org/

5.2. AlViE

Participants: Pierluigi Crescenzi [Contact, pierluigi.crescenzi@unifi.it, ext. member EPI], Giorgio Gambosi, Roberto Grossi, Carlo Nocentini, Tommaso Papini, Walter Verdese.

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

5.3. Cassis

Participants: Christian Baudet [EPI, Contact, christian.baudet@univ-lyon1.fr], Christian Gautier [EPI], Claire Lemaitre [Contact, claire.lemaitre@inria.fr], Marie-France Sagot [EPI], Eric Tannier.

Algorithm for precisely detecting genomic rearrangement breakpoints.
http://pbil.univ-lyon1.fr/software/Cassis/

5.4. Cravela

Participants: Ana Teresa Freitas, Nuno Mendes [Contact, ndm@kdbio.inesc-id.pt], Marie-France Sagot [EPI, Contact, marie-france.sagot@inria.fr].

Framework for the identification and evaluation of miRNA precursors (finished), targets (in development) and regulatory modules(in development).
http://www.cravela.org/

5.5. C3P

Participants: Frédéric Boyer, Anne Morgat [EPI, ext. member], Alain Viari [EPI, Contact, alain.viari@inria.fr].

Merging two or more graphs representing biological data (e.g. pathways, ...).
http://www.inrialpes.fr/helix/people/viari/cccpart

5.6. CycADS

Participants: Hubert Charles [EPI], Patrice Baa Puyoule [Contact, Patrice.Baa-Puyoulet@lyon.inra.fr], Stefano Colella [Contact, stefano.colella@lyon.inra.fr], Ludovic Cottret, Marie-France Sagot [EPI], Augusto Vellozo [Contact, augusto@cycadsys.org].

Cyc annotation database system.

http://www.cycadsys.org/

5.7. Gobbolino

Participants: Vicente Acuña [EPI], Etienne Birmelé [EPI, délégation], Ludovic Cottret, Pierluigi Crescenzi, Fabien Jourdan, Vincent Lacroix, Alberto Marchetti-Spaccamela [EPI, ext. member], Andrea Marino, Paulo Vieira Milreu [EPI, Contact, pvmilreu@gmail.com], Marie-France Sagot [EPI], Leen Stougie [EPI, ext. member].

Algorithm to enumerate all metabolic stories in a metabolic network given a set of metabolites of interest.
Code available on request.

5.8. kisSNP

Participants: Vincent Lacroix [EPI], Pierre Peterlongo [Contact, pierre.peterlongo@inria.fr], Nadia Pisanti, Marie-France Sagot [EPI], Nicolas Schnel.

Algorithm for identifying SNPs without a reference genome by comparing raw reads.
http://alcovna.genouest.org/kissnp/

5.9. kisSplice

Participants: Rayan Chikhi, Janice Kielbassa [EPI], Vincent Lacroix [Contact, EPI], Pierre Peterlongo [Contact, pierre.peterlongo@inria.fr], Gustavo Sacomoto [EPI], Marie-France Sagot [EPI], Raluca Uricaru.

Algorithm for de-novo calling alternative splicing events from RNA-seq data.
http://alcovna.genouest.org/kissplice/

5.10. LASAGNE

Participants: Pierluigi Crescenzi [Contact, pierluigi.crescenzi@unifi.it, ext. member EPI], Roberto Grossi, Michel Habib, Claudio Imbrenda, Leonardo Lanzi, Andrea Marino.

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.
http://amici.dsi.unifi.it/lasagne/

5.11. MetExplore

Participants: Michael Barrett, Hubert Charles [EPI], Ludovic Cottret [Contact, Ludovic.Cottret@toulouse.inra.fr], Fabien Jourdan, Marie-France Sagot [EPI], Florence Vinson, David Wildridge.

Web server to link metabolomic experiments and genome-scale metabolic networks.
http://metexplore.toulouse.inra.fr/metexplore/

5.12. Migal

Participants: Julien Allali [Contact, julien.allali@labri.fr], Marie-France Sagot [EPI, Contact, marie-france.sagot@inria.fr].

RNA, tree comparison
Algorithm for comparing RNA structures.
http://www-igm.univ-mlv.fr/~allali/logiciels/index.en.php

5.13. MotusWEB

Participants: Ludovic Cottret, Fabien Jourdan, Vincent Lacroix [EPI, Contact, vincent.lacroix@univ-lyon1.fr], Odile Rogier, Marie-France Sagot [EPI].

Algorithm for searching and inferring coloured motifs in metabolic networks (web-based version - offers different functionalities from the downloadable version).
http://pbil.univ-lyon1.fr/software/motus_web/

5.14. Motus

Participants: Ludovic Cottret, Fabien Jourdan, Vincent Lacroix [EPI, Contact, vincent.lacroix@univ-lyon1.fr], Odile Rogier, Marie-France Sagot [EPI].

Algorithm for searching and inferring coloured motifs in undirected graphs (downloable version - offers different functionalities from the web-based version).
http://pbil.univ-lyon1.fr/software/motus/

5.15. PhEVER

Participants: Christian Gautier [EPI], Vincent Lotteau, Leonor Palmeira [Contact, mlpalmeira@ulg.ac.be], Chantal Rabourdin-Combe, Simon Penel.

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.
http://pbil.univ-lyon1.fr/databases/phever/

5.16. PepLine

Participants: Jérôme Garin, Alain Viari [EPI, Contact, alain.viari@inria.fr].

Pipeline for the high-throughput analysis of proteomic data.
http://www.grenoble.prabi.fr/protehome/software/pepline

5.17. Pitufo and family

Participants: Vicente Acuña [EPI], Ludovic Cottret [Contact, Ludovic.Cottret@toulouse.inra.fr], Alberto Marchetti-Spaccamela [EPI, ext. member], Paulo Vieira Milreu [EPI, Contact, pvmilreu@gmail.com], Marie-France Sagot [EPI], Leen Stougie [EPI, ext. member], Fabio Viduani-Martinez.

Algorithms to enumerate all minimal sets of precursors of target compounds in a metabolic network.
http://sites.google.com/site/pitufosoftware/

5.18. PSbR

Participants: Yoan Diekmann, Marie-France Sagot [EPI, Contact, marie-france.sagot@inria.fr], Eric Tannier.

Algorithm for testing the evolution and conservation of common clusters of genes.
http://pbil.univ-lyon1.fr/members/sagot/htdocs/team/software/PSbR/

5.19. Repseek

Participants: Guillaume Achaz [Contact, achaz@abi.snv.jussieu.fr], Eric Coissac, Alain Viari [EPI].

Finding approximate repeats in large DNA sequences.
http://wwwabi.snv.jussieu.fr/public/RepSeek/

5.20. Smile

Participants: Laurent Marsan, Marie-France Sagot [EPI, Contact, marie-france.sagot@inria.fr].

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

5.21. Tuiuiu

Participants: Alair Pereira do Lago, Pierre Peterlongo [Contact, pierre.peterlongo@inria.fr], Nadia Pisanti, Gustavo Sacomoto [EPI], Marie-France Sagot [EPI].

Multiple repeat search filter with edit distance.
http://mobyle.genouest.org/cgi-bin/Mobyle/portal.py?form=tuiuiu

5.22. UniPathway

Participants: Eric Coissac, Anne Morgat [EPI, Contact, anne.morgat@inria.fr], Alain Viari [EPI].

Database of manually curated pathways developed with the Swiss-Prot group.
http://www.unipathway.org

BEAGLE Team

5. Software

5.1. aevol (artificial evolution)

Participants: Guillaume Beslon, Stephan Fischer, Carole Knibbe, David P Parsons, Bérénice Batut.

- Contact: Carole Knibbe (carole.knibbe@inria.fr).
- Aevol is a simulation software dedicated to the study of genome evolution. It allows to carry out *in silico* experimental evolution. Populations of digital organisms reproduce and mutate randomly, with both small mutations and large chromosomic rearrangements, in a steady or varying environment. A curve-fitting task is used to determine the fitness of the organisms and thus their rate of reproduction. The number of genes, their order, their sequences, their intergenic distances are all free to evolve.
- URL: http://www.aevol.fr

5.2. FluoBacTracker

Participants: Hugues Berry, David P Parsons, Magali Vangkeosay.

- contact: Hugues Berry (hugues.berry@inria.fr)
- FluoBacTracker is a software for automated quantification of bacterial cells in microscopy movies, developed in collaboration with INSERM U1001 and Paris 5 MAP (Applied Mathematics) Labs. The development (started october 2012) is supported by is a 2-year grant (ADT) funded by Inria's Technological Development Department (Sept 2012- July 2014, project name: "MultiPop"). We hope this software will be useful to all the experimental biology labs that tries to derive single-cell data from bacteria growth microscopy movies. Codeveloppers include Magali Vangkeosay (Beagle), David P Parsons (SED, Inria Grenoble) and Xiaohu Song (INSERM U1001).

5.3. Ancestral Genome Reconstructions

Participant: Eric Tannier.

- Contact: Eric Tannier (eric.tannier@inria.fr).
- We participated in the development of a series of softwares for genome organization analysis:
  - ANGES, for ANcestral GEnomeS maps, is a toolkit for ordering ancestral genomic markers in chromosomes. An application note has been published in *Bioinformatics* in 2012 to advertise its first release. It is hosted at SFU in Vancouver, URL: http://paleogenomics.irmacs.sfu.ca/ANGES/, under a GNU license, 2012.
  - DeCo, for Detection of Co-evolution, reconstructs neighborhood relationships between genes of ancient genomes, in the presence of gene duplications and losses. It is hosted at the PRABI, the bioinformatics platform in Lyon, URL: http://pbil.univ-lyon1.fr/software/DeCo/, under a Cecill license, 2012.
  - DCJ2HP provides bayesian samples of rearrangements scenarios between 2 genomes. It is hosted at the Renyi Institute in Budapest, URL http://www.renyi.hu/~miklosi/DCJ2HP/

BONSAI Project-Team

5. Software

5.1. YASS – Local homology search

Actively maintained.
Software self-assessment following the mechanisms provided by Inria Evaluation Committee for software evaluation: **A-4**, **SO-3**, **SM-2**, **EM-3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://bioinfo.lifl.fr/yass/

Licence: GPL

YASS is a software devoted to the classical problem of genomic pairwise alignment, and use most of our knowledge to design and implement efficient seeding techniques these last years. It is frequently used, it always receives more than 300 web queries per month (excluding local queries), and is also frequently downloaded and cited.

5.2. Carnac – RNA structure prediction

Actively maintained.
Software self-assessment: **A-4**, **SO-3**, **SM-2**, **EM-3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://bioinfo.lifl.fr/carnac/

Licence: Cecill

The CARNAC program is for RNA structure prediction by comprative analysis. The web interface also offers 2D visualisation tools and alignment functionalities with Gardenia. It has proven to be very fast and very specific compared to its competitors [19].

5.3. TFM-Explorer – Identification and analysis of transcription factor binding sites

Actively maintained.
Software self-assessment: **A-4**, **SO-3**, **SM-2**, **EM-3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://bioinfo.lifl.fr/TFM/

Licence: GPL

The TFM suite is a set of tools for analysis of transcription factor binding sites modeled by Position Weight Matrices. In this suite, the TFM-EXPLORER tool is designed to analyze regulatory regions of eukaryotic genomes using comparative genomics and local over-representation.

5.4. Regliss – RNA locally optimal structures

Actively maintained.
Software self-assessment: **A-2**, **SO-4**, **SM-2**, **EM-2**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://bioinfo.lifl.fr/RNA/regliss/

REGLISS is a tool that studies the energy landscape of a given RNA sequence by generating all locally optimal structures, that are maximal thermodynamically stable structures.

5.5. RNAspace – A platform for noncoding RNA annotation

Actively developped.

Software self-assessment: **A-5**, **SO-3**, **SM-3-up4**, **EM-2-up3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://www.rnaspace.org/

Licence: GPL

RNAspace is a national collaborative initiative conducted with Genopole Midi-Pyrénées and originally supported by IBISA [1]. The goal is to develop an open source platform for structural and functional noncoding RNA annotation in genomes (see Section 6.2): http://www.rnaspace.org. The project will be pursued within France Génomique (see Section 7.2.1).

5.6. CGseq – A toolbox for comparative analysis

Actively maintained.
Software self-assessment: **A-4**, **SO-3**, **SM-2**, **EM-3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://bioinfo.lifl.fr/CGseq/

Licence: GPL

CG-seq is a toolbox for identifying functional regions in a genomic sequence by comparative analysis using multispecies comparison.

5.7. SortMeRNA – Metatranscriptome classification

Actively developed.
Software self-assessment: **A-4**, **SO-3**, **SM-2**, **EM-3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site: http://bioinfo.lifl.fr/RNA/sortmerna

Licence: GPL

SortMeRNA is a software designed to rapidly filter ribosomal RNA fragments from metatransriptomic data produced by next-generation sequencers. It is capable of handling large RNA databases and sorting out all fragments matching to the database with high accuracy and specificity.

5.8. Biomanycores.org – A community for bioinformatics on manycore processors

Actively developped.
Software self-assessment: **A-3**, **SO-2**, **SM-3**, **EM-3down2**, **SDL-4up5**, OC-4 (DA-4, CD-4, MS-4, TPM-4)

Software web site : http://biomanycores.org/

Manycore architectures are an emerging field of research full of promises for parallel bioinformatics. However the usage of GPUs is not so widespread in the end-user bioinformatics community. The goal of the `biomanycores.org` project is to gather open-source CUDA and OpenCL parallel codes and to provide easy installation, benchmarking, and interoperability. The last point includes interfaces to popular frameworks such as Biopython, BioPerl and BioJava.

The development of Biomanycores was supported by a national ADT [2] between BONSAI, SYMBIOSE (CRI Rennes) and DOLPHIN (CRI Lille), from October 2010 to October 2012. This ADT led to the hiring of J.-F. Berthelot (IJD) who completely redesigned the existing code and added more applications. Biomanycores has now a comprehensive developer and user documentation, large test suites and continuous integration. In June 2012, the project has been presented during a workshop dedicated to manycore programming (see Section 8.1).

[1] IBISA is a French consortium for evaluating and funding national technological platforms in life sciences.
[2] ADT (Action for Technological Development) is an Inria internal call

5.9. Norine – A resource for nonribosomal peptides

Actively maintained.
Software self-assessment: **A-5**, **SO-3**, **SM-3-up4**, **EM-2-up3**, **SDL-4**, DA-4, CD-4, MS-4, TPM-4

Software web site : http://bioinfo.lifl.fr/norine/ Norine is a public computational resource that contains a database of NRPs with a web interface and dedicated tools, such as a 2D graph viewer and editor for peptides or comparison of NRPs. Norine was created and is maintained by members of BONSAI team, in tight collaboration with members of the ProBioGEM lab, a microbial laboratory of Lille1 University. Since its creation in 2006, Norine has gained an international recognition as the unique database dedicated to non-ribosomal peptides because of its high quality and manually curated annotations, and has been selected by wwPDB as a reference database. It is queried from all around the world by biologists or biochemists. It receives more than 3000 queries per month. Norine main users come for 13% from the United States of America, for 12% from the United Kingdom, for 5% from China or for 4% from Germany where renowned biology laboratories work on nonribosomal peptides (NRPs) or on their synthetases.

5.10. GkArrays – Indexing high throughput sequencer reads

Actively maintained.
Software self-assessment: **A-3**, **SO-3**, **SM-3**, **EM-2**, **SDL-4**, DA-4, CD-4, MS-4, TPM-3

Software web site : http://crac.gforge.inria.fr/gkarrays/

Objective : Gk-Arrays is a C++ library specifically dedicated to indexing reads produced by high-throughput sequencers. This index allows to answer queries centred on reads. It also takes benefits from the input specificity to lower space consumption.

This library is the result of a collaboration with N. Philippe and T. Commes (IGH laboratory, Montpellier), M. Léonard and T. Lecroq (LITIS laboratory, Rouen) and É. Rivals (LIRMM laboratory, Montpellier).

DYLISS Team

5. Software

5.1. Data integration: actors involved in the response of a living system

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.

- **Mobyle@GenOuest network portal** We are developing a web service [2] to use several tools to confront knowledge and data towards the correction of large-scale networks, based either on decision diagrams or on answer set programming. BioQuali [3][4] allows one to confront model and data, localize errors and, when model and data are consistent, to predict the variation of non observed nodes [6]. BioASP [5] was developed in Potsdam and allows one to perform prediction even if model and observations are contradictory, by considering all possible repairs of data and models and computing the common predictions of all repaired models [5]. The portal also include tools for the completion of metabolic networks [32].
- **Combined set of key actors in reaction-based networks: Cadbiom**[6]. This tool is based on state-chart like graphical language. It allows investigating synchronization events in biological networks. It is applied to cancer signaling networks [10].

5.2. Dynamics: actor/parameter combination controlling the response of a system

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

- **caspo: Cell ASP Optimizer**. We have implemented a Python package which combines BioASP [7] and CellNOpt[8] to provide an easy to use software for learning Boolean logic models using ASP [19]. The software is available for download[9] and also as a web service through the Mobyle framework.
- **Event network and quantitative time-series data: POGG**[10]. POGG is a tool developed in collaboration with the LINA lab (Nantes) that uses mean dynamics to score the respective relevance of regulatory pathways in a higher-scale phenotype. It was applied to the quantitative prediction of protein quantities under exponential growth [2]. It predicts the main features of a Markov chain model derived from a reaction-based model when confronted to a single time-series quantitative observation.

[2] http://mobyle.genouest.org/cgi-bin/Mobyle/portal.py
[3] http://www.irisa.fr/symbiose/bioquali/
[4] http://www.irisa.fr/symbiose/projects/bioqualiCytoscapePlugin/
[5] http://www.cs.uni-potsdam.de/bioasp/
[6] http://cadbiom.genouest.org/
[7] http://www.cellnopt.org/
[8]

;sthiele/bioasp/http://www.cs.uni-potsdam.de/ ~sthiele/bioasp/
[9] http://pypi.python.org/pypi/caspo
[10] http://pogg.genouest.org/wiki.php/Home

5.3. Sequence annotation

We develop tools for discovery and search of complex pattern signatures within biological sequences, with a focus on protein sequences. An integrated environment, Dr Motif [11] is available on the GenOuest Platform that gathers state-of-the-art tools for pattern discovery and pattern matching including our own developments.

- **Complex pattern discovery: Protomata learner**[12] is a grammatical inference framework suitable for the inference of accurate protein signatures [3], [4]. It was completely redesigned in 2010-2011 thanks to a specific Inria action (ADT support). It is currently applied to the recognition of olfactory receptor genes.
- **Complex pattern matching: Logol [13].** We have completely redesigned Stan (suffix-tree analyser), a former tool to search for nucleotidic and peptidic patterns within whole chromosomes [7]. The result is Logol, a software suite accepting a syntax based on String Variable Grammars, which allows the description of realistic complex patterns including ambiguities, insertions/ deletions, gaps, repeats and palindromes. It has been presented for the first time in [21]. Logol has been applied to the detection of -1 frameshifts, a structure including pseudo knots, on a reference benchmark (Recode2).

[11] http://www.drmotifs.org/
[12] http://protomata-learner.genouest.org/
[13] **http://webapps.genouest.org/LogolDesigner/**

GENSCALE Team

5. Software

5.1. Next Generation Sequencing

Participants: Alexan Andrieux, Rayan Chikhi, Dominique Lavenier, Claire Lemaitre, Nicolas Maillet, Pierre Peterlongo, Raluca Uricaru.

- **Genome assembly** [contact: P. Peterlongo]
  - **Minia : ultra low memory assembly** Minia is a short-read assembler based on a de Bruijn graph, capable of assembling a human genome on a desktop computer in a day. The output of Minia is a set of contigs. Minia produces results of similar contiguity and accuracy to other de Bruijn assemblers (e.g. Velvet). http://minia.genouest.org/
  - **Mapsembler: targeted assembly software.** Mapsembler is a targeted assembly software. From sets of NGS raw reads and a set of input sequences (starters), it determines if each starter could be constructed from the reads. Then for each "read-coherent" starter, Mapsembler outputs its sequence neighborhood as a linear sequence or as a graph, depending on the user choice. http://alcovna.genouest.org/mapsembler/
- **Variant detection** [contact: C. Lemaitre]
  - **kisSnp and kisSplice : variant identification without the use of a reference genome**. kisSnp is a tool to find single nucleotide polymorphisms (SNP) by comparing two sets of raw NGS reads. http://alcovna.genouest.org/kissnp/ KisSplice finds alternative splicings but also short insertions, deletions and duplications, SNPs and sequencing errors in one or two RNA-seq sets, without assembly nor mapping on a reference genome. http://alcovna.genouest.org/kissplice/
  - **Kissreads: quantification of variants** Kissreads considers sets of NGS raw reads and a set of input sequences (starters). Mapping reads to each starter, it provides quantitative (coverage depth) and qualitative (mapped read quality) information about each starter.
- **Read mapping** [contact: D. Lavenier]
  - **GASSST: short reads mapper** The GASSST software (Global Alignment Short Sequence Search Tool) is a general purpose mapper. GASSST finds global alignments of short DNA sequences against large DNA banks. One main characteristic of GASSST is its ability to perform fast gapped alignments and to process long reads compared to other current similar tools. http://www.irisa.fr/symbiose/projects/gassst/

5.2. High throughput sequence analysis

Participants: Rayan Chikhi, Erwan Drezen, Dominique Lavenier, Claire Lemaitre, Nicolas Maillet, Pierre Peterlongo.

- **PLAST : efficient bank-to-bank alignments** PLAST (Parallel Local Alignment Search Tool) is a parallel alignment search tool for comparing large protein banks. PLAST runs 3 to 5 times faster than the NCBI-BLAST software. An improved version is commercialized by the Korilog Company, including the DNA bank-to-bank option. [contact: D. Lavenier] http://www.irisa.fr/symbiose/projects/plast/
- **Compareads : efficient comparison of large metagenomics NGS datasets** This software extracts similar DNA sequences (reads) between two metagenomic datasets. It requires a small and fixed amount of memory and can thus be used on huge datasets. [contact: P. Peterlongo] http://alcovna.genouest.org/compareads/

5.3. 3D Protein structures

Participants: Rumen Andonov, Guillaume Chapuis, Mathilde Le Boudic-Jamin, Antonio Mucherino.

- **CSA and DALIX** CSA (Comparative Structural Alignment) is a webserver for computing and comparing protein structure alignments. CSA is able to compute score-optimal alignments with respect to various inter-residue distance-based scoring schemes. [contact: R. Andonov] http://csa.project.cwi.nl/
- **A_purva** A_purva is a Contact Map Overlap maximization (CMO) solver. Given two protein structures represented by two contact maps, A_purva computes the amino-acid alignment which maximize the number of common contacts. [contact: R. Andonov] http://mobyle.genouest.org/cgi-bin/Mobyle/portal.py?forms::A_Purva
- **MD-Jeep** MD-jeep is a software tool for solving distance geometry problems. It is able to solve a subclass of instances of the problem for which a discrete reformulation can be supplied. We refer to this subclass of instances as the Discretizable Molecular Distance Geometry Problem (DMDGP). We employ a Branch & Prune (BP) algorithm for the solution of DMDGPs. [contact: A. Mucherino] http://www.antoniomucherino.it/en/mdjeep.php

5.4. HPC and Parallelism

Participants: Guillaume Chapuis, Dominique Lavenier, François Moreews.

- **QTLmap** QTLMap is a tool dedicated to the detection of Quantitative Trait Loci (QTL) from experimental designs in outbred population. QTLMap was recently ported to GPU and offers reduced run times. [contact: D. Lavenier] http://www.inra.fr/qtlmap/
- **SLICEE** (Service Layer for Intensive Computation Execution Environment) is part of the BioWIC project. This software proposes (1) to abstract the calls to the cluster scheduler by handling command submission; (2) to take care of exploiting the data parallelism with data specific methods; (3) to manage data using a cache references mecanism and route data between tasks. [contact: F. Moreews] http://vapor.gforge.inria.fr/

IBIS Project-Team

4. Software

4.1. Genetic Network Analyzer (GNA)

Participants: Hidde de Jong [Correspondent], Michel Page, François Rechenmann, Delphine Ropers.

Gene regulatory networks, qualitative simulation, model checking

GENETIC NETWORK ANALYZER (GNA) is the implementation of a method 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, 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 8.3. In comparison with the previously distributed versions, GNA 8.3 has the following additional functionalities. First, it supports the editing and visualization of regulatory networks, in an SBGN-compatible format, and second it semi-automatically generates a prototype model from the network structure, thus accelerating the modeling process. For more information, see http://www-helix.inrialpes.fr/gna.

4.2. WellReader

Participants: Guillaume Baptist, Johannes Geiselmann, Jérôme Izard, Hidde de Jong [Correspondent], Delphine Ropers.

Gene expression, reporter gene data

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). For more information, see: http://ibis.inrialpes.fr/article957.html.

MAGNOME Project-Team

5. Software

5.1. Inria Bioscience Resources

Participants: Olivier Collin [correspondant], Frédéric Cazals, Mireille Régnier, Marie-France Sagot, Hélène Touzet, Hidde de Jong, David James Sherman, Marie-Dominique Devignes, Dominique Lavenier.

Inria Bioscience Resources is a portal designed to improve the visibility of bioinformatics tools and resources developed by Inria teams. This portal will help the community of biologists and bioinformatians understand the variety of bioinformatics projects in Inria, test the different applications, and contact project-teams. Eight project-teams participate in the development of this portal. Inria Bioscience Resources is developed in an Inria Technology Development Action (ADT).

5.2. Magus: Collaborative Genome Annotation

Participants: David James Sherman [correspondant], Pascal Durrens, Natalia Golenetskaya, Florian Lajus, Tiphaine Martin.

As part of our contribution the Génolevures Consortium, we have developed over the past few years an efficient set of tools for web-based collaborative annotation of eukaryote genomes. 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 the 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 Génolevures standards of high-quality manual annotation while efficiently using the time of our volunteer curators.

MAGUS is built on: a standard sequence feature database, the Stein lab generic genome browser [61], various biomedical ontologies (http://obo.sf.net), and a web interface implementing a representational state transfer (REST) architecture [39].

For more information see magus.gforge.inria.fr, the MAGUS Gforge web site. MAGUS is developed in an Inria Technology Development Action (ADT).

5.3. YAGA: Yeast Genome Annotation

Participants: Tiphaine Martin, Pascal Durrens [correspondant], Elisabeth Bon, Aurélie Goulielmakis.

With the arrival of new generations of sequencers, laboratories, at a lower cost, can be sequenced groups of genomes. You can no longer manually annotate these genomes. The YAGA (Yeast Automatic Genome Annotation) software's objective is to annotate a raw sequence syntactically and functionally as well as generate EMBL files for publication. The annotation takes into account data from comparative genomics, such as protein family profiles.

After determining the constraints of the annotation, the YAGA software can automatically annotate *de novo* all genomes from their raw sequences.The predictors used by the YAGA software can also take into account the data RNAseq to reinforce the prediction of genes.The current settings of the software are intended for annotation of the genomes of yeast, but the software is adaptable for all types of species, and has been trained and used for the annotation of bacterial genomes.

5.4. BioRica: Multi-scale Stochastic Modeling

Participants: David James Sherman [correspondant], Rodrigo Assar Cuevas.

BioRica is a high-level modeling framework integrating discrete and continuous multi-scale dynamics within the same semantics field. A model in BioRica node is hierarchically composed of nodes, which may be existing models. Individual nodes can be of two types:

- Discrete nodes are composed of states, and transitions described by constrained events, which can be non deterministic. This captures a range of existing discrete formalisms (Petri nets, finite automata, etc.). Stochastic behavior can be added by associating the likelihood that an event fires when activated. Markov chains or Markov decision processes can be concisely described. Timed behavior is added by defining the delay between an event's activation and the moment that its transition occurs.
- Continuous nodes are described by ODE systems, potentially a hybrid system whose internal state flows continuously while having discrete jumps.

The system has been implemented as a distributable software package

The BioRica compiler reads a specification for hierarchical model and compiles it into an executable simulator. The modeling language is a stochastic extension to the AltaRica Dataflow language, inspired by work of Antoine Rauzy. Input parsers for SBML 2 version 4 are curently being validated. The compiled code uses the Python runtime environment and can be run stand-alone on most systems [40].

For more information see biorica.gforge.inria.fr, the BioRica Gforge web site. BioRica was developed as an Inria Technology Development Action (ADT).

5.5. Pathtastic: Inference of whole-genome metabolic models

Participants: David James Sherman [correspondant], Pascal Durrens, Nicolás Loira, Tiphaine Martin, Anna Zhukova.

Pathtastic is a software tool for inferring whole-genome metabolic models for eukaryote cell factories. It is based on *metabolic scaffolds*, abstract descriptions of reactions and pathways on which inferred reactions are hung are are eventually connected by an interative mapping and specialization process. Scaffold fragments can be repeatedly used to build specialized subnetworks of the complete model.

Pathtastic uses a consensus procedure to infer reactions from complementary genome comparisons, and an algebra for assisted manual editing of pathways.

For more information see pathtastic.gforge.inria.fr, the Pathtastic Gforge web site.

5.6. Génolevures On Line: Comparative Genomics of Yeasts

Participants: Pascal Durrens [correspondant], Natalia Golenetskaya, Tiphaine Martin, David James Sherman.

The Génolevures online database provides tools and data for exploring the annotated genome sequences of more than 20 genomes, determined and manually annotated by the Génolevures Consortium to facilitate comparative genomic studies of hemiascomycetous yeasts. Data are presented with a focus on relations between genes and genomes: conservation of genes and gene families, speciation, chromosomal reorganization and synteny. The Génolevures site includes an area for specific studies by members of its international community.

Génolevures online uses the MAGUS system for genome navigation, with project-specific extensions developed by David Sherman, Pascal Durrens, and Tiphaine Martin. An advanced query system for data mining in Génolevures is being developed by Natalia Golenetskaya. The contents of the knowledge base are expanded and maintained by the CNRS through GDR 2354 Génolevures. Technical support for Génolevures On Line is provided the CNRS through UMR 5800 LaBRI.

For more information see genolevures.org, the Génolevures web site.

MORPHEME Team

4. Software

4.1. Software

4.1.1. Deposits

The software MAD V2.0 was deposited with the APP in November 2012. It deals with the melasma severity scoring from multi-spectral imaging.

4.1.2. Transfers

The software MAD V2.0 was transferred to Galderma R&D.

SERPICO Team

5. Software

5.1. Software for live cell imaging

Participants: Charles Kervrann, Patrick Bouthemy, Tristan Lecorgne.

Motion2d: parametric motion model estimation

The MOTION2D software written in C++ (APP deposit number: FR.001.520021.001.S.A.1998.000.21000 / release 1.3.11, January 2005) and JAVA (plug-in IMAGEJ (http://rsbweb.nih.gov/ij/) 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. 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.

Free academic software distribution: Motion2D Free Edition is the version of Motion2D available for development of Free and Open Source software only. More information on Motion2D can be found at http://www.irisa.fr/vista/Motion2D and the software can be downloaded at the same Web address.
On-line demo: Mobyle@GenOuest Bioinformatics http://mobyle.genouest.org/cgi-bin/Mobyle/portal.py#forms:Motion2D (see Fig. 5).

Partner: Fabien Spindler (Inria Lagadic team).

ND-Safir and Fast2D-SAFIR: Image denoising software

The ND-SAFIR software (APP deposit number: IDDN.FR.001.190033.002.S.A.2007.000.21000 / new release 3.0 in 2013) written in C++, JAVA and MATLAB, removes additive Gaussian and non-Gaussian noise in still 2D or 3D images or in 2D or 3D image sequences (with no motion computation) (see Figure 2) [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, ...).

The FAST-2D-SAFIR software (APP deposit number: IDDN.FR.001.190033.001.S.A.2007.000.21000) written in C++ 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 SAFIR-nD 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, ...).

On-line demo: Mobyle@GenOuest Bioinformatics
http://mobyle.genouest.org/cgi-bin/Mobyle/portal.py#forms::NDSafir

Free download binaries: Binaries of the software ND-SAFIR are freely and electronically distributed. Developed in standard C/C++ under Linux using the CImg library, it has been tested over several platforms such as Linux/Unix, Windows XP and Mac OS.

Academic licence agreements: Institut Curie, CNRS, ENS Ulm, Oxford university, Weizmann Institute, UCSF San-Francisco, Harvard university, Berkeley university, Stanford university, Princeton university, Georgia-Tech, Kyoto university, IMCB Singapore ...

Partners: J. Boulanger, J. Salamero (UMR 144 CNRS Institut Curie), P. Elbau (RICAM Linz, Austria), J.B. Sibarita (UMR 5091 University of Bordeaux 2).

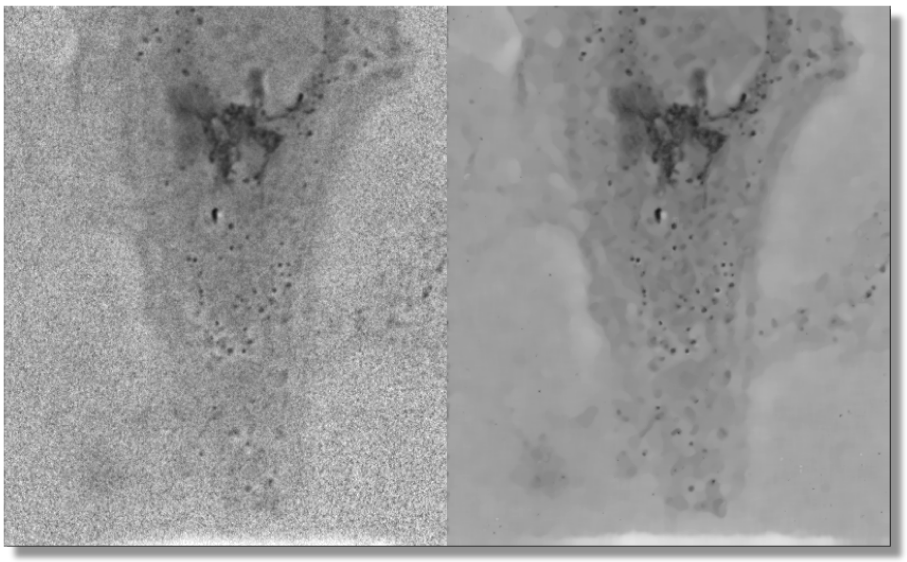


Figure 2. ND-SAFIR *software: denoising of a 3D image sequence in wide-field (WF) microscopy (GFP-Rab6A (Hela cell), UMR 144 CNRS Institut Curie).*

HullkGround: Background subtraction by convex hull estimation

The HULLKGROUND software (APP deposit number: IDDN.FR.001.400005.000.S.P.2009.000.21000) written in JAVA (plug-in IMAGEJ, see Fig. 3) 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 α shapes-based scale-space method [25].

On-line demo: Mobyle@GenOuest Bioinformatics http://mobyle.genouest.org/cgi-bin/Mobyle/portal.py#forms::Hullkground
Partners: A. Chessel and J. Salamero (UMR 144 CNRS Institut Curie)

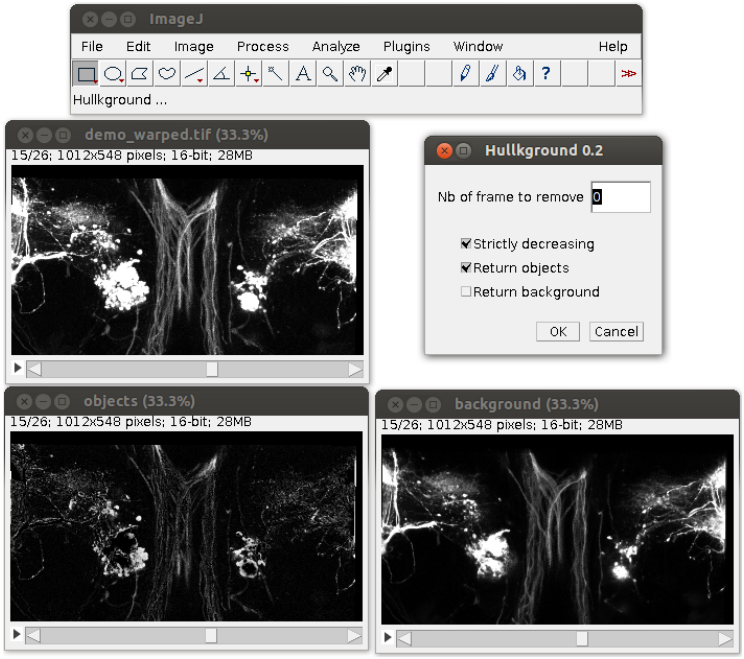


Figure 3. HULLKGROUND *software: plug-in* IMAGEJ.

5.2. Software for Cyo-electron tomography

Participant: Charles Kervrann.

TubuleJ: Straightening of microtubule cryo-EM projection views

The TUBULEJ software (APP deposit number: IDDN.FR.001.240023.000.S.P.2011.000.21000) 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 points 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. These projection views are then back projected, by using the IMOD plug-in (http://rsbweb.nih.gov/ij/), to reconstruct 3D microtubules.

On-line demo: see http://equipes.igdr.univ-rennes1.fr/en/tips/Software/TubuleJ/

Partners: S. Blestel and D. Chrétien (UMR 6290 CNRS University of Rennes 1)

Cryo-Seg: Segmentation of tomograms in cryo-electron microscopy

The CRYO-SEG software written in C++ and JAVA (plug-in MAGEJ) has been developed to detect microtubule structures and helical structures in 2D cryo-electron microscope images (see Figure 4). 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.

Partners: S. Blestel and D. Chrétien (UMR 6290 CNRS University of Rennes 1)

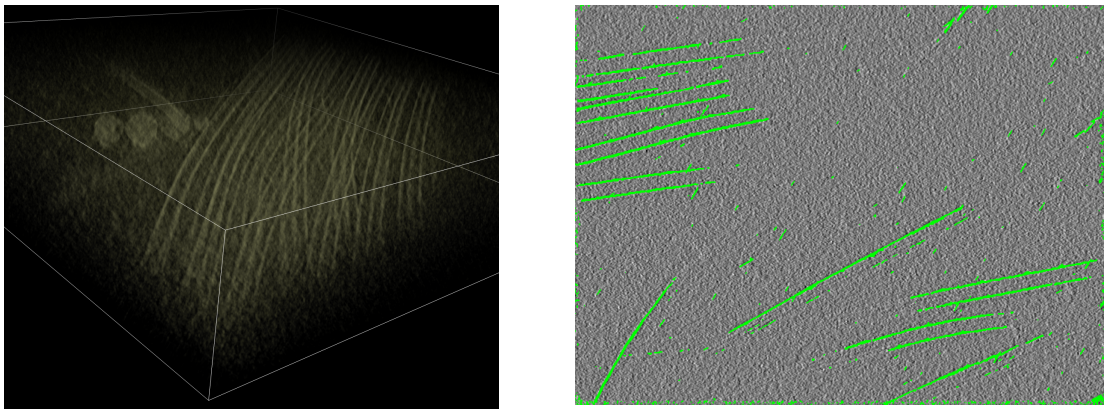


Figure 4. CRYO-SEG *software: Segmentation of 3D microtubles in a cryo-EM tomogram (left) and 2D view (right) (UMR 6290 CNRS University of Rennes 1).*

5.3. Image Processing software distribution

Participants: Tristan Lecorgne, Charles Kervrann.

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 web portal*: An online version of the software has been released using the Mobyle framework (see http://mobyle.pasteur.fr/) developed at Institut Pasteur. The main role of this web portal is to demonstrate the performance of the programs developed by the team. The web interface makes our image processing methods available for biologist users without any installation or configuration (see ND-SAFIR, HULLKGROUND, MOTION2D (see Fig. 5) at http://mobyle.genouest.org/). The size of submitted images is limited by network bandwidth. We use the computing facility of the GenOuest platform to run calculations.

- 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, HULLKGROUND (see Fig. 3), MOTION2D, HOTSPOTDETECTION and OPTICALFLOW.
- *Institut Curie database*: Institut Curie is currently acquiring a new database system to store mass of data. The database can be searched via meta-data and includes menu selections that enable to run remote processing. We have integrated ND-SAFIR in the interface environment to allow the database users to denoise images easily.

Partners: C. Deltel (Inria Rennes SED) and Perrine Paul-Gilloteux (UMR 144 PICT IBiSA CNRS Institut Curie)

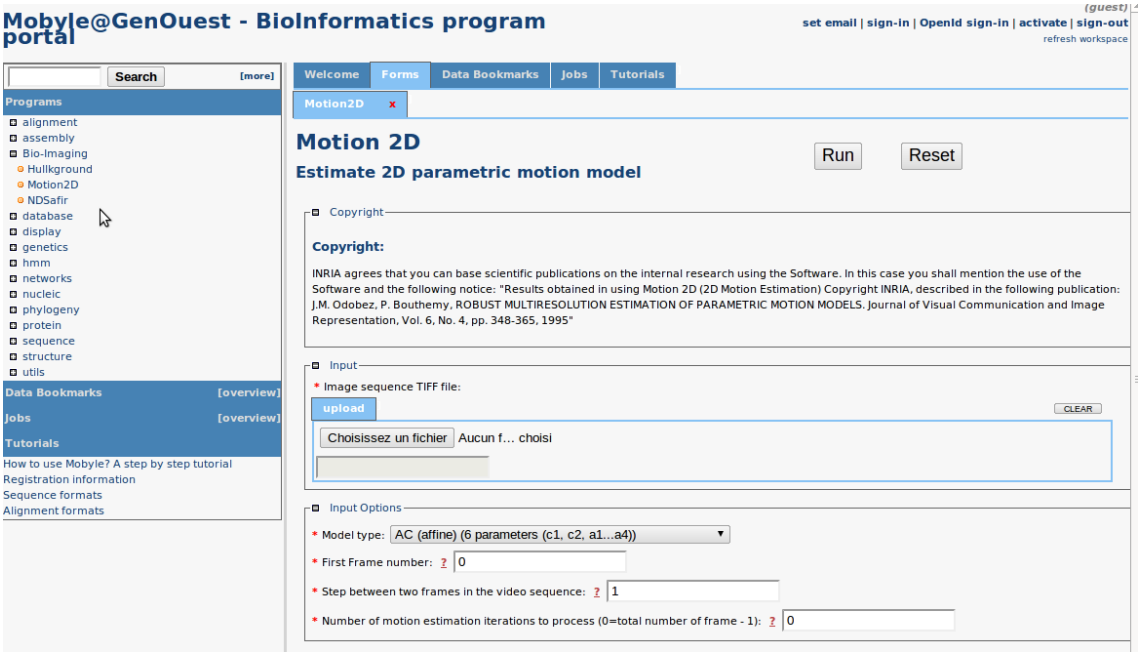


Figure 5. Motion2D on Mobyle@GenOuest Bioinformatics.

ASCLEPIOS Project-Team

4. Software

4.1. SOFA

Participants: Hervé Delingette [correspondant], Brina Goyette, Federico Spadoni, Stéphanie Marchesseau, Hugo Talbot.

SOFA is an Open Source framework primarily targeted at real-time simulation, with an emphasis on medical simulation. It is mostly intended for the research community to help develop newer algorithms, but can also be used as an efficient prototyping tool. based on an advanced software architecture, it allows to:- create complex and evolving simulations by combining new algorithms with algorithms already included in SOFA- modify most parameters of the simulation (deformable behavior, surface representation, solver, constraints, collision algorithm, etc.) by simply editing an XML file- build complex models from simpler ones using a scene-graph description- efficiently simulate the dynamics of interacting objects using abstract equation solvers- reuse and easily compare a variety of available methods. It is mainly developed by the Inria team projects Shaman, Evasion and Asclepios.
See also the web page http://www.sofa-framework.org/.

- ACM: J.2 Physics, J.3 LIFE AND MEDICAL SCIENCES
- Software benefit:- Simulation of the human body
- License: GPL
- License: LGPL
- Type of human computer interaction: console, opengl, qt
- OS/Middelware: linux, windows, mac
- Required library or software: Qt - GPL - GLEW - BSD/MIT - Tinyxml - zlib
- Programming language: C/C++
- Documentation: - each function of the core API and each class in the SOFA modules - doxygen
- ACM: J.3
- Programming language: C/C++

4.2. MedInria

Participants: Benoît Bleuzé, Florian Vichot, Hakim Fadil, Loic Cadour, Agata Krason, Maxime Sermesant [correspondant], Nicolas Toussaint.

MedInria is a free collection of softwares developed by the Asclepios research project in collaboration with the Athena, Parietal and Visages Inria research projects. It aims at providing to clinicians 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. MedInria is available for Microsoft windows XP/Vista/7, Linux Fedora Core, MacOSX, and is fully multithreaded.

The first release of Medinria 2.0 was done in April 2012.

See also the web page http://med.inria.fr.

- Version: 2.0
- Keywords: Medical Image Processing
- License: Proprietary Licence
- Type of human computer interaction: QT
- OS/Middleware: Windows - Linux - MacOSX
- Required library or software: DTI Track (Proprietary), vtkInria3D (CeCillB), Baladin (Proprietary)
- Programming language: C++

ATHENA Project-Team

5. Software

5.1. OpenMEEG

Participants: Théodore Papadopoulo, Maureen Clerc, Alexandre Gramfort [Telecom ParisTech].

OpenMEEG provides state-of-the art tools for low-frequency bio-electromagnetism, notably solving forward problems related to EEG and MEG [5]. It implements the symmetric BEM which provides excellent accuracy and versatility OpenMEEG is a free open software written in C++. It can be accessed either through a command line interface or through Python/Matlab interfaces.

OpenMEEG is multiplatform (Linux, MacOS, Windows) and it is distributed under the French opensource license CeCILL-B. See also the web page http://www-sop.inria.fr/athena/software/OpenMEEG/.

5.2. Diffusion MRI

Participants: Aurobrata Ghosh, Rachid Deriche.

The algorithms previously developed within the ODYSSÉE Project team and related to the Diffusion Tensor and Q-Ball imaging are available upon request from the Inria source forge (https://gforge.inria.fr). One can use all the estimation and visualization tools developed, ranging from estimation, regularization, segmentation to Q-ball estimation, fiber ODF estimation and tractography algorithms. New visualization tools for Q-Ball images represented by spherical harmonic decomposition have also been developed.

The software library comprises geometric and variational methods devised to estimate, regularize, segment and perform tractography in DT (Diffusion Tensor) and HARDI (High Angular Resolution) MRI images. The library is multi-platform (Linux, Windows and OS X) ans is embedded into two open-source high level languages, TCL and Python.

5.3. medInria

Participants: Jaime Garcia Guevara, Théodore Papadopoulo.

The Athena team is involved along with the research teams Asclepios, Parietal and Visages in the development of medInris a free software platform dedicated to medical data visualization and processing.

It aims at providing to clinicians and researchers state-of-the-art algorithms developed at Inria and elsewhere (for the future), through an intuitive user interface. medInria offers from standard to cutting-edge processing functionalities for medical images such as 2D/3D/4D image visualization, image registration, diffusion MR processing and tractography.

Athena contribution so far consists in various improvements on the core application as well as several plugins which will be available in the next version: advanced dMRI visualization and processing (integration of the Diffusion MRI library depicted in the previous section), M/EEG signal visualisation (by integrating code from the software AnyWave developed at by Bruno Colombet and J.-M. Badier Inserm UMR 1106 and Aix-Marseille University).

See also the web page http://med.inria.fr.

- Version: 2.0.1
- Keywords: Medical Image Processing and Visualization
- License: Proprietary Licence (soon open source for the core application)
- Multiplatform: Windows - Linux - MacOSX
- Programming language: C++

CORTEX Project-Team

5. Software

5.1. Spiking neural networks simulation

Participants: Dominique Martinez, Yann Boniface.

A spiking neuron is usually modeled as a differential equation describing the evolution over time of its membrane potential. Each time the voltage reaches a given threshold, a spike is sent to other neurons depending on the connectivity. A spiking neural network is then described as a system of coupled differential equations. For the simulation of such a network we have written two simulation engines : (i) Mvaspike based on an event-driven approach and (ii) sirene based on a time-driven approach.

- Mvaspike : The event-driven simulation engine was developed in C++ and is available on http://mvaspike.gforge.inria.fr. Mvaspike is a general event-driven purpose tool aimed at modeling and simulating large, complex networks of biological neural networks. It allows to achieve good performance in the simulation phase while maintaining a high level of flexibility and programmability in the modeling phase. A large class of spiking neurons can be used ranging from standard leaky integrate-and-fire neurons to more abstract neurons, e.g. defined as complex finite state machines.
- Sirene : The time-driven simulator engine was written in C and is available on http://sirene.gforge.inria.fr. It has been developed for the simulation of biologically detailed models of neurons —such as conductance-based neurons— and synapses. Its high flexibility allows the user to implement easily any type of neuronal or synaptic model and use the appropriate numerical integration routine (e.g. Runge-Kutta at given order).

5.2. DANA: Implementation of computational neuroscience mechanisms

Participants: Nicolas Rougier, Mathieu Lefort, Wahiba Taouali.

Computational neuroscience is a vast domain of research going from the very precise modeling of a single spiking neuron, taking into account ion channels and/or dendrites spatial geometry up to the modeling of very large assemblies of simplified neurons that are able to give account of complex cognitive functions. DANA attempts to address this latter modeling activity by offering a Python computing framework for the design of very large assemblies of neurons using numerical and distributed computations. However, there does not exist something as a unified model of neuron: if the formal neuron has been established some sixty years ago, there exists today a myriad of different neuron models that can be used within an architecture. Some of them are very close to the original definition while some others tend to refine it by providing extra parameters or variables to the model in order to take into account the great variability of biological neurons. DANA makes the assumption that a neuron is essentially a set of numerical values that can vary over time due to the influence of other neurons and learning. DANA aims at providing a constrained and consistent Python framework that guarantee this definition to be enforced anywhere in the model, i.e., no symbol, no homonculus, no central executive.

5.3. ENAS: Event Neural Assembly Simulation

Participants: Frédéric Alexandre, Axel Hutt, Nicolas Rougier, Thierry Viéville.

EnaS (that stands for “Event Neural Assembly Simulation”) is a middleware implementing our last numerical and theoretical developments, allowing to simulate and analyze so called "event neural assemblies". The recent achievements include (in collaboration with the Neuromathcomp EPI): spike trains statistical analysis via Gibbs distributions, spiking network programing for exact event’s sequence restitution, discrete neural field parameters algorithmic adjustments and time-constrained event-based network simulation reconciling clock and event based simulation methods. It has been designed as plug-in for our simulators (e.g. DANA or Mvaspike) as other existing simulators (via the NeuralEnsemble meta-simulation platform) and additional modules for computations with neural unit assembly on standard platforms (e.g. Python or the Scilab platform).

5.4. OpenViBE

Participants: Laurent Bougrain, Octave Boussaton.

OpenViBE is a C++ open-source software devoted to the design, test and use of Brain-Computer Interfaces. The OpenViBE platform consists of a set of software modules that can be integrated easily and efficiently to design BCI applications. Key features of the platform are its modularity, its high-performance, its portability, its multiple-users facilities and its connection with high-end/Virtual Reality displays. The "designer" of the platform enables to build complete scenarios based on existing software modules using a dedicated graphical language and a simple Graphical User Interface (GUI). This software is available on the Inria Forge under the terms of the LGPL-V2 license.The development of OpenVibe is done in association with the Inria research team BUNRAKU for the national Inria project: ADT LOIC (*cf.* § 7.2).

5.5. CLONES: Closed-Loop Neural Simulations

Participant: Thomas Voegtlin.

The goal of this work is to provide an easy-to-use framework for closed-loop simulations, where interactions between the brain and body of an agent are simulated.

We developed an interface between the Sofa physics engine, (http://www.sofa-framework.org) and the Brian neural simulator (http://www.briansimulator.org). The interface consists in a Sofa plugin and a Python module for Brian. Sofa and Brian use different system processes, and communicate via shared memory. Synchronization between processes is achieved through semaphores.

As a demonstration of this interface, a physical model of undulatory locomotion in the nematode *c. elegans* was implemented, based on the PhD work of Jordan H. Boyle.

5.6. GINNet-DynNet: Decision-making platform

Participant: Marie Tonnelier.

GINNet (Graphical Interface for Neural Networks) is a decision-aid platform written in Java, intended to make neural network teaching, use and evaluation easier, by offering various parametrizations and several data pre-treatments. GINNet is based upon a local library for dynamic neural network developments called DynNet. DynNet (Dynamic Networks) is an object-oriented library, written in Java and containing base elements to build neural networks with dynamic architecture such as Optimal Cell Damage and Growing Neural Gas. Classical models are also already available (multi-layer Perceptron, Kohonen self-organizing maps, ...). Variable selection methods and aggregation methods (bagging, boosting, arcing) are implemented too.

The characteristics of GINNet are the following: Portable (100% Java), accessible (model creation in few clicks), complete platform (data importation and pre-treatments, parametrization of every models, result and performance visualization). The characteristics of DynNet are the following: Portable (100% Java), extensible (generic), independent from GINNet, persistent (results are saved in HML), rich (several models are already implemented), documented.

This platform is composed of several parts:

1. Data manipulation: Selection (variables, patterns), descriptive analysis (stat., PCA..), detection of missing, redundant data.
2. Corpus manipulation: Variable recoding, permutation, splitting (learning, validation, test sets).
3. Supervised networks: Simple and multi-layer perceptron.
4. Competitive networks: Kohonen maps, Neural Gas, Growing Neural Gas.
5. Metalearning: Arcing, bagging, boosting.
6. Results: Error curves, confusion matrix, confidence interval.

DynNet and GINNet are free softwares, registrated to the APP and distributed under CeCILL license, Java 1.4 compatible (http://ginnet.gforge.inria.fr). GINNet is available as an applet. For further information, see http://gforge.inria.fr/projects/ginnet (news, documentations, forums, bug tracking, feature requests, new releases...)

DEMAR Project-Team

5. Software

5.1. Software

5.1.1. RdP to VHDL tool

Participants: Gregory Angles, David Andreu, Thierry Gil.

Our SENIS (Stimulation Electrique Neurale dIStribuee) based FES architecture relies on distributed stimulation units (DSU) which are interconnected by means of a 2-wire based network. A DSU is a complex digital system since its embeds among others a dedicated processor (micro-machine with a specific reduced instruction set), a monitoring module and a 3-layer protocol stack. To face the complexity of the unit's 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, a set of functions whose execution is controlled by the PN, and a set of variables and signals. Its interface contains places and transitions from which its PN model can be inter-connected as well as signals it exports or imports. The interconnection of those components, from a behavioral point out view, consists in the interconnection of places and/or transitions according to well-defined mechanisms: interconnection by means of oriented arcs or by means of the "merging" operator (existing for both places and transitions).

GALS (Globally Asynchronous Locally Synchronous) systems can be specified, connecting different clocks to HILECOP components, and interconnecting them by means of asynchronous signals.

Undergoing work includes the modification of the formalism in order to allow behavior agregation as well as exception handling.

The Eclipse-based version of HILECOP is regulary updated. The last version of HILECOP (registered at the french Agence de Protection des Programmes (APP)) is accessible to the academic community (http://www.lirmm.fr/ gil/Temp/).

5.1.2. SENISManager

Participants: Robin Passama, David Andreu.

We developed a specific software environment called SENISManager 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.

A new version of SENISManager is under development according to an Eclipse-based design. This new version should be available in 2013.

GALEN Team

5. Software

5.1. Deformable Registration Software

Participant: Nikos Paragios [Correspondant].

deformable image and volume registration, is a deformable registration platform in C++ for the medical imaging community (publicly available at http://www.mrf-registration.net) developed mainly at Ecole Centrale, Technical University of Munich and University of Crete. 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.

5.2. Dense image and surface descriptors

Participant: Iasonas Kokkinos [Correspondant].

Scale-Invariant Descriptor, Scale-Invariant Heat Kernel Signatures DISD (publicly available at http://vision.mas.ecp.fr/Personnel/iasonas/descriptors.html) 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.

5.3. Dissimilarity Coefficient learning

Participant: Pawan Kumar [Correspondant].

weakly supervised learning, dissimilarity coefficient, structured prediction DISC (publicly available at http://www.centrale-ponts.fr/personnel/pawan/code/DISCAPI.zip) software provides a convenient API for dissimilarity coefficient (DISC) based learning. DISC allows the use of weakly supervised datasets (with missing information) by jointly learning a structured prediction classifier and a conditional probability distribution of the missing information. The parameters of the classifier and the distribution are learned by minimizing a user-specified dissimilarity coefficient between them.

5.4. Efficient bounding-based object detection

Participant: Iasonas Kokkinos [Correspondant].

branch-and-bound, parts detection, segmentation, DPMS implements branch-and-bound object detection, cutting down the complexity of detection from linear in the number of pixels to logarithmic (publicly available at http://vision.mas.ecp.fr/Personnel/iasonas/dpms.html). The results delivered are identical to those of the standard deformable part model detector, but are available in 5 to 20 times less time. This website has been visited 1500 times in 10 months.

5.5. Fast Primal Dual Strategies for Optimization of Markov Random Fields

Participant: Nikos Komodakis [Correspondant].

discrete optimization, Markov random field, duality, graph cuts, FASTPD is an optimization platform in C++ for the computer vision and medical imaging community (publicly available at http://www.csd.uoc.gr/~komod/FastPD/) developed mainly at Ecole Centrale and University of Crete. This is the most efficient publicly available platform in terms of a compromise of computational efficiency and ability to converge to a good minimum for the optimization of generic MRFs. The platform is used from approximately 1,500 users worldwide.

5.6. imaGe-based Procedural Modeling Using Shape Grammars

Participant: Iasonas Kokkinos [Correspondant].

procedural modeling, image-based building reconstruction, shape grammars GRAPES is a generic image parsing library based on re-inforcement learning (publicly available at http://cvc.centrale-ponts.fr/). It can handle grammars (binary-split, four-color, Hausmannian) and image-based rewards (Gaussian mixtures, Randomized Forests) of varying complexity while being modular and computationally efficient both in terms of grammar and image rewards. The platform is used from approximately 500 users worldwide.

5.7. Learning-based symmetry detection

Participant: Stavros Tsogkas [Correspondant].

Scale-Invariant Descriptor, Scale-Invariant Heat Kernel Signatures LBSD (publicly available at http://www.centrale-ponts.fr/personnel/tsogkas/code.html implements the learning-based approach to symmetry detection published in [32]. 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.

5.8. Texture Analysis Using Modulation Features and Generative Models

Participant: Iasonas Kokkinos [Correspondant].

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 (publicly available at http://cvsp.cs.ntua.gr/software/texture/). 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. The platform is used from approximately 250 users worldwide.

5.9. Sparse Prediction

Participant: Andreas Argyriou [Correspondant].

Sparse prediction, K-support norm, SPARSE_K is a sparse prediction code (publicly available at http://www.centrale-ponts.fr/personnel/andreas/code/sparse_k/sparse_k.tar) using regularization with the k-support norm, which we have introduced [36]. The algorithm uses an accelerated first-order method similar to Nesterov's method.

MNEMOSYNE Team

5. Software

5.1. Positioning

Our previous works in the domain of well-defined distributed asynchronous adaptive computations [32], [29], [34] have already made us define a library (DANA [3]), 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 organized into layers, maps and network.

More generally, we gather in the middleware EnaS (that stands for *Event Neural Assembly Simulation*; cf. http://gforge.inria.fr/projects/enas) our numerical and theoretical developments, allowing to simulate and analyze so called "event neural assemblies". Enas has been designed as a plug-in for our simulators (e.g. DANA or MVASpike) as other existing simulators (via the NeuralEnsemble meta-simulation platform) and additional modules for computations with neural unit assembly on standard platforms (e.g. Python or the Scilab platform).

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 [19], 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).

5.2. Dana

Participant: Nicolas Rougier.

DANA [28] is a python framework (http://dana.loria.fr) 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 evolution 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.).

5.3. ENAS: Event Neural Assembly Simulation

Participants: Frédéric Alexandre, Nicolas Rougier, Thierry Viéville.

EnaS (that stands for “Event Neural Assembly Simulation”) is a middleware implementing our last numerical and theoretical developments, allowing to simulate and analyze so called "event neural assemblies". The recent achievements include (in collaboration with the Neuromathcomp EPI): spike trains statistical analysis via Gibbs distributions, spiking network programing for exact event’s sequence restitution, discrete neural field parameters algorithmic adjustments and time-constrained event-based network simulation reconciling clock and event based simulation methods. It has been designed as plug-in for our simulators (e.g. DANA or Mvaspike) as other existing simulators (via the NeuralEnsemble meta-simulation platform) and additional modules for computations with neural unit assembly on standard platforms (e.g. Python or the Scilab platform).

5.4. Virtual Enaction

Participants: Frédéric Alexandre, André Garenne, Nicolas Rougier, Thierry Viéville.

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 are going to 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 will consist of a platform associated to a scenario that would be the closest possible to a survival situation (foraging, predator-prey relationship, partner approach to reproduction) and in which it would be 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 will be slowed down enough to be able to run non trivial brainy-bot implementations.

NEUROMATHCOMP Project-Team

4. Software

4.1. Virtual Retina: A Large-Scale Simulator of Biological Retina

Participants: Bruno Cessac, Maria-Jose Escobar [Universidad Técnica Federico Santa María, Valparaiso, Chile], Christobal Nettle [Universidad Técnica Federico Santa María, Valparaiso, Chile], Pierre Kornprobst [correspondent], Adrien Wohrer [Group for Neural Theory - ENS, Paris, France].

Virtual Retina is a simulation software developped by Adrien Wohrer during his PhD [79], [78] that allows large-scale simulations of biologically-plausible retinas.

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

Virtual Retina is under Inria CeCill C open-source licence, so that one can download it, install it and run it on one's own sequences. Virtual Retina also offers a web service (v 2.1), so that users may test directly the main software on their own data, without any installation. This webservice was developed in collaboration with Nicolas Debeissat (engineer, 2002).

We are now interested in the analysis of the collective behavior of ganglion cells responses. To take this collective behavior into account, Virtual Retina needs to be extended since in its current version, ganglion cells are independent. Other evolutions of Virtual Retina are also investigated by external partners like the role/implementation of starbust amacrine cells involved in direction selectivity (collaboration with Universidad Técnica Federico Santa María, Valparaiso, Chile, and Centro de urociencia de Valaparaiso) (see also e.g., [70]).

- IDDN number: IDDN.FR.001.210034.000.S.P.2007.000.31235
- Version: v 2.2.2 (September 2011)
- Link: http://www-sop.inria.fr/neuromathcomp/public/software/virtualretina

4.2. Event Neural Assembly Simulation

Participants: Bruno Cessac [correspondent], Sélim Kraria [Inria DREAM], Olivier Marre [Institut de la vision, Paris], Hassan Nasser, Thierry Viéville [Inria Mnemosyne Bordeaux].

Enas is a library providing numerical tools for the simulation of neural networks and the analysis of spike trains either coming from neural simulators or from biological experiments.

It is designed mainly as

- An existing simulator plug-in (e.g. MVASpike or other simulators via the NeuralEnsemble meta-simulation platform),
- Additional modules for computations with neural unit assembly on standard platforms (e.g. Python, Matlab or the Scilab platform).
- Original modules for the analysis of spike train statistics intended to be used by the neuroscientists community.

Achievements include:

- Spike trains statistical analysis via Gibbs distributions. They are based on the estimation of a parametric Gibbs potential optimaly 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 and statistical entropy 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: are correlations (or time synchrony or a given set of spike patterns,. . .) significant with respect to rate coding?
- Spiking network programing for exact event's sequence restitution;
- Discrete neural field parameters algorithmic adjustments and time-constrained event-based network simulation reconciling clock and event based simulation methods.

Compared to existing libraries Enas offers new computational methods taking into account time constraints in neural networks (such as memory effects), based on theoretical methods rooted in statistical physics and applied mathematics. The algorithms used are based on linear programming, nonlinear parameter estimations, statistical methods. The C/C++ code has been organized as "bean java" to ease its use by programmers non specialized in advanced object programming. As a consequence the code is distributed in the form of an include source for the lightest and the most universal integration into users codes. The standard algorithms are based on the best free libraries in the domain such as gsl http://www.gnu.org/software/gsl.

Event neural assembly simulation is developed in gForge. It is under CeCILL C licence
APP logiciel Enas: IDDN.FR.OO1.360008.000.S.P.2009.000.10600.

Its development as a friendly software designed for the neuroscience community is our present purpose. This is done with the support of an ADT Inria.

Website: `http://enas.gforge.inria.fr/`

PARIETAL Project-Team

5. Software

5.1. Mayavi

Participant: Gaël Varoquaux [Correspondant].

Mayavi is the most used scientific 3D visualization Python software (http://mayavi.sourceforge.net/). It has been developed by Prabhu Ramachandran (IIT Bombay) and Gaël Varoquaux (PARIETAL, Inria Saclay). 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 (http://pyrx.scripps.edu) and brain connectivity analysis tools (connectomeViewer).

See also the web page http://mayavi.sourceforge.net/ and the following paper http://hal.inria.fr/inria-00528985/en.

- Version: 3.4.0

5.2. Nipy

Participants: Bertrand Thirion [correspondant], Virgile Fritsch, Elvis Dohmatob, Gaël Varoquaux.

Nipy is an open-source Python library for neuroimaging data analysis, developed mainly at Berkeley, Stanford, MIT and Neurospin. It is open to any contributors and aims at developing code and tools sharing. Some parts of the library are completely developed by Parietal and LNAO (CEA, DSV, Neurospin). It is devoted to algorithmic solutions for various issues in neuroimaging data analysis. All the nipy project is freely available, under BSD license. It is available in NeuroDebian.

See also the web page http://nipy.org.

- Version: 0.3

5.3. MedInria

Participants: Pierre Fillard [correspondant], Sergio Medina, Viviana Siless.

MedInria is a free collection of softwares developed within the ASCLEPIOS, ATHENA and VISAGES research projects. It aims at providing to clinicians 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. MedInria is available for Microsoft windows XP/Vista, Linux Fedora Core, MacOSX, and is fully multi-threaded.
See also the web page http://med.inria.fr/.

- Version: 2.0

5.4. Scikit learn

Participants: Bertrand Thirion, Gaël Varoquaux [correspondant], Jaques Grobler, Alexandre Gramfort, Fabian Pedregosa, Virgile Fritsch.

Scikit-learn is an open-source machine learning toolkit written in Python/C that provides generic tools to learn information for the classification of various kinds of data, such as images or texts. It is tightly associated to the scientific Python software suite (numpy/scipy) for which it aims at providing a complementary toolkit for machine learning (classification, clustering, dimension reduction, regression). There is an important focus on code quality (API consistency, code readability, tests, documentation and examples), and on efficiency, as the scikit-learn compares favorably to state-of-the-art modules developed in R in terms of computation time or memory requirements. Scikit-learn is currently developed by more than 60 contributors, but the core developer team has been with the Parietal Inria team at Saclay-Île-de-France since January 2010. The scikit-learn has recently become the reference machine learning library in Python.

- Version: 0.12
- Programming language: Python, C/Cython

SHACRA Project-Team

5. Software

5.1. SOFA

SOFA, the Simulation Open Framework Architecture, is an international, multi-institution, collaborative initiative, aimed at developing a flexible and open source framework for interactive simulations. This will eventually establish new grounds for a widely usable standard system for long-term research and product prototyping, ultimately shared by many academic and industrial sites. Over the last two years, the SOFA framework has evolved from an informal collaborative work between the Sim Group at CIMIT, the Alcove, Asclepios and Evasion teams at Inria into a more structured development project. By proposing a unique architecture allowing the integration of the multiple competencies required for the development of a medical training system, we believe it will be possible to accelerate and foster research activities in the field of interactive medical simulation. The main objectives of the SOFA framework are:

- Simplify the development of medical simulation systems by improving interoperability
- Evaluate and validate new algorithms
- Accelerate the prototyping of simulation systems by promoting component reusability
- Promote collaboration between research groups
- Facilitate technology transfer between research and industry

Our activities around the SOFA framework will be twofold. We will remain one of the leading teams contributing to the design of SOFA, the development of its architecture and its distribution to research groups and industrial partners. In addition, we will use SOFA as a core element of most of our simulations, as a mean to facilitate the integration of results from partners of the national initiative, and to simplify the development of prototypes of simulation systems. For the past few years, there have been a few attempts at designing software toolkits for medical simulation. Examples include [36], GiPSi [25], SPORE [35] or SSTML [22]. These different solutions aim at the same goal: providing an answer (usually Open Source) to the various challenges of medical simulation research and development. Although our aim is similar, we propose a different approach, through a very modular and flexible software framework, while minimizing the impact of this flexibility on the computation overhead. To achieve these objectives, we have developed a new architecture that implements a series of innovative concepts. Also, by developing the SOFA framework collaboratively with scientific experts in the different areas of medical simulation, we believe we can provide state-of-the-art solutions that are generically applicable, yet computationally efficient. The following sections describe in more details our approach to the development of this framework, from a technical standpoint and from the perspective of a collaborative work.

5.1.1. SOFA architecture

Medical simulation relies on a variety of interacting physics-based models, such as rigid structures (e.g. bones), deformable structures (e.g. soft-tissues) and fluids. It also involves anatomical representations through geometrical models, used for visual rendering, collision detection or meshes that will support various computational models. Finally, interactions between these different models need to be efficient, accurate and capable of handling a variety of representations. In some instances, a hierarchy also exists between the various anatomical structures, and needs to be taken into account in the description of the simulated environment. The design of the SOFA architecture, by supporting these various requirements, brings the flexibility needed for academic research. Yet, its very efficient implementation makes it also suitable for professional applications and potentially for product development. This architecture relies on several innovative concepts, in particular the notion of multi-model representation. In SOFA, most simulation components (deformable models, collision models, medical devices, etc.) can have several representations, connected through a mechanism called mapping. Each representation is optimized for a particular task (e.g. collision detection, visualization) while at the same time

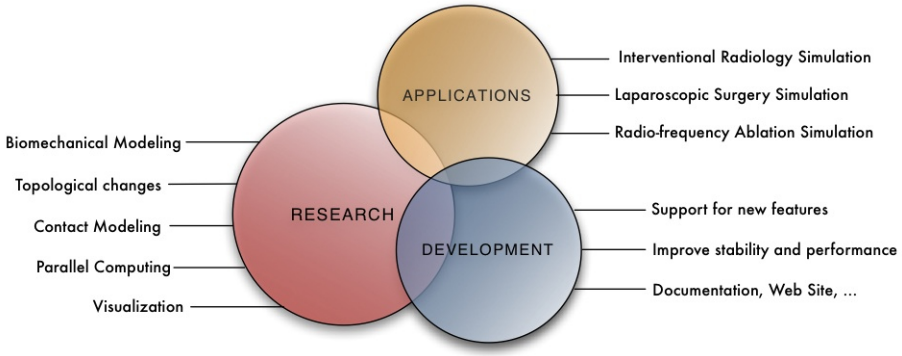


Figure 3. Multidisciplinary research and development of the SOFA framework need to take place simultaneously to quickly advance research in the field of computer-based interactive medical simulation

improving interoperability by creating a clear separation between the functional aspects of the simulation components. As a consequence, it is possible to have models of very different nature interact together, for instance rigid bodies, deformable objects, and fluids. This is an essential aspect of SOFA, as it will help the integration of new research components. This modular design also facilitates the rapid prototyping of simulation systems, allowing various combinations of algorithms to be tested and compared against each other. At a finer level of granularity, we also propose a decomposition of physical models (i.e. any model that behaves according to the laws of physics) into a set of basic components. In the case of (bio)mechanical models, which are computationally expensive, many strategies have been used to improve computation times or to reduce the complexity of the original model: linear elastic models have often been used instead of more complex non-linear representations, mass-spring methods as an alternative to finite element methods, etc. Each of these simplifications induces drawbacks, yet the importance of these drawbacks depends largely on the context in which they are applied. It becomes then very difficult to choose which particular method is most likely to provide the best results for a given simulation. To address this issue in SOFA we have introduced a finer level of granularity which permits to independently test and compare each component, such as time integration schemes, to see the change in performance or robustness of the simulation, or to test different constitutive models. These changes can be made in a matter of seconds, without having to recompile any of the code, by simply editing an XML file.

5.1.2. Current Results

Version 1.0 RC1 of SOFA was released in December 2011 but since October 2012, SOFA is now available through a public and anonymous SVN. More than 137,000 downloads of SOFA have been counted as of November 2012. More than 70 researchers, students, engineers have contributed at various degrees to SOFA, for a total of about 1,200,000 lines of code. Currently, thanks to its advanced architecture, SOFA allows to:

- Create complex and evolving simulations by combining new algorithms with existing algorithms
- Modify most parameters of the simulation by simply editing a XML file
- Build complex models from simpler ones using a scene-graph description
- Efficiently simulate the dynamics of interacting objects using abstract equation solvers
- Reuse and easily compare a variety of available methods
- Transparently parallelize complex computations using semantics based on data dependencies
- Use new generations of GPUs through the CUDA API to greatly improve computation times
- Use embedded Python environment to create interactive and parametric scenes, and interact with 3rd party software

Various results and information can be obtained on the SOFA website at http://www.sofa-framework.org. Most of the current results are generic and only aim at validating the different aspects of the SOFA framework. Developments of complex medical simulations have recently started, in particular in the areas of ophthalmic surgery and interventional radiology. We have also started a collaboration with a few companies (Digital Trainers, Didhaptics, B.K.) which are in the process of developing medical applications based on SOFA.

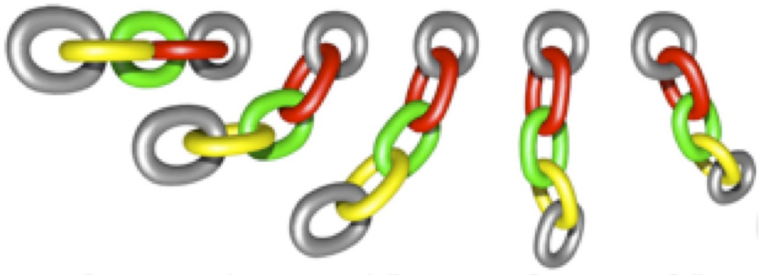


Figure 4. Animation of a chain combining a FEM model, a mass-spring model, a FFD grid, and a rigid body. This example is a perfect illustration of the flexibility of SOFA. Not only several algorithms for rigid or deformable bodies can be part of the same simulation, but they can also interact in a physically correct manner. No constraints between links were pre-defined, instead we relied on collision detection and stiff contact forces to handle the contacts. Using implicit integrator handling dynamically-created groups of interacting objects resulted in a stable simulation

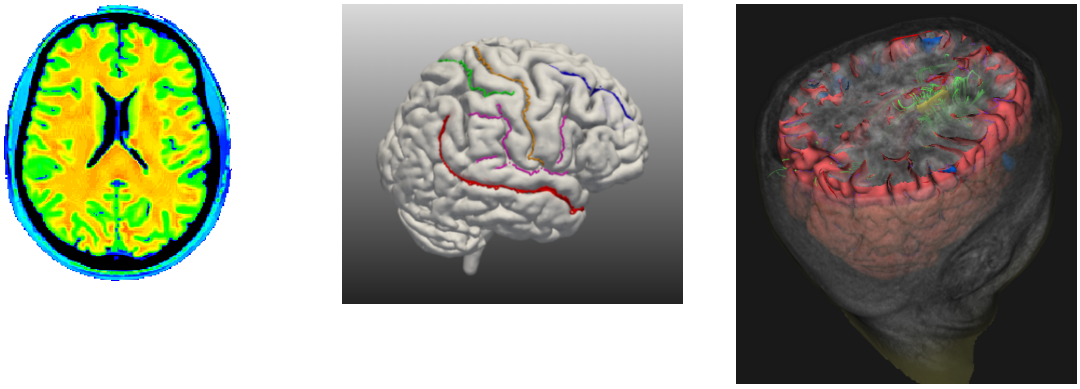
VISAGES Project-Team

5. Software

5.1. Vistal

Participants: Olivier Commowick, Clément Philipot.

VistaL is a software platform of 3D and 3D+t image analysis allowing the development of generic algorithms used in different contexts (rigid and non-rigid registration, segmentation, statistical modelling, calibration of free-hand 3D ultrasound system and so on, diffusion tensor image processing, tractography). This software platform is composed of generic C++ template classes (Image3D, Image4D, Lattice and so on) and a set of 3D/3D+t image processing libraries. VistaL is a multi-operating system environment (Windows, Linux/Unix...). A web site presenting the project has been developped, precompiled packages and the SDK are now available. VistaL APP registration number is:IDDN.FR.001.200014.S.P.2000.000.21000.
See also the web page http://vistal.gforge.inria.fr.



(a) (b) (c)

Figure 2. Some ViSTAL results screenshots: a) The ViSTAL Logo, b) ViSTAL Brain surface and sulci modelisation, c) The ROI3D Extraction view

- Keywords: medical image processing, image analysis, registration, segmentation, denoising
- Software benefit: New methodological image processing, some GPU based algorithms, easy to use C++ library
- APP: IDDN.FR.001.200014.S.P.2000.000.21000
- License: Licence Propriétaire
- Type of human computer interaction: C++ API and less complete Python API
- OS/Middleware: Windows, Mac et Linux.
- Required library or software: CMake (GPL) - ITK (BSD) - VTK (BSD) - Boost (BSD) - Libxml++ (LGPL) - CppUnit (LGPL)
- Programming language: C/C++, Python
- Documentation: Documentation Doxygen, documentation utilisateur.

5.2. CLARCS: C++ Library for Automated Registration and Comparison of Surfaces

Participants: Juan Francisco Garamendi, Sylvain Prima.

In collaboration with Benoit Combès (Géosciences Rennes, UMR 6118) and Alexandre Abadie (Inria Saclay Île-de-France), within the 3D-MORPHINE ARC project (http://3dmorphine.inria.fr), we conceived and implemented a C++ library (named CLARCS) for the automated analysis and comparison of surfaces. One of the primary goal of this library is to allow the assessment and quantification of morphological differences of free-form surfaces from medical or paleoanthropological data.

- APP: IDDN.FR.001.130002.000.S.P.2011.000.21000
- Programming language: CC++

CLARCS was presented at the MeshMed MICCAI workshop (http://www2.imm.dtu.dk/projects/MeshMed/2011/index.html) [49] and is to be distributed through a dedicated website (http://clarcs.inria.fr).

We also developed a surface viewer (named 'Surface').

- APP: IDDN.FR.001.110019.000.S.P.2011.000.21000
- Programming language: C++, Python

5.3. SUBANA: SUrface-BAsed Neuronavigation on Atlas for TMS

Participant: Sylvain Prima.

In collaboration with Charles Garraud (Syneika), Benoit Combès (Géosciences Rennes, UMR 6118) and Pierre Hellier (Technicolor), we developed a software for i) the automated surface reconstruction of the face and skull cap from sparsely acquired points and ii) the automated nonlinear registration of free-form surfaces. The latter step is implemented using the CLARCS library (http://clarcs.inria.fr). The primary goal of this software is the surface-based neuronavigation for transcranial magnetic stimulation. The method was presented at the MeshMed MICCAI workshop (http://www2.imm.dtu.dk/projects/MeshMed/2011/index.html) [50].

- APP: IDDN.FR.001.440010.000.S.P.2010.000.31230
- Patent: was granted, but the reference number is unknown
- Programming language: C++

5.4. Shanoir

Participants: Guillaume Renard, Justine Guillaumont, Christian Barillot.

Shanoir (Sharing NeurOImaging Resources) is an open source neuroinformatics platform designed to share, archive, search and visualize neuroimaging data. It provides a user-friendly secure web access and offers an intuitive workflow to facilitate the collecting and retrieving of neuroimaging data from multiple sources and a wizzard to make the completion of metadata easy. Shanoir comes along many features such as anonymization of data, support for multi-centres clinical studies on subjects or group of subjects.

Shanoir APP registration number is : IDDN.FR.001.520021.000.S.P.2008.000.31230

See also the web page http://www.shanoir.org

- Keywords: neuroimaging, ontology, sharing neuroimage
- Software benefit: full featured neuroimaging management system with additionnal web services
- APP: IDDN.FR.001.200014.S.P.2000.000.21000
- License: Licence QPL
- Type of human computer interaction: Online web application, web service (SOAP messages based)
- OS/Middelware: Windows, Mac et Linux.
- Required library or software : Java 1.6, JBoss server, JBoss Seam, JSF, JPA Hibernate, EJB, Richfaces, Faceless, Ajax4JSF, Dcmtk, Dcm4chee.
- Programming language: Java
- Documentation : see the website

5.5. QtShanoir

Participants: Olivier Commowick, Guillaume Renard.

QtShanoir is a C++ Qt based library for querying data from a Shanoir server. For those who don't know what is shanoir, see the shanoir website at http://shanoir.org. QtShanoir uses the soap based webservices provided by a shanoir server to get and display studies, patients, data with their associated metadata. In QtShanoir, you will find a set of Qt widgets (inherited from a QWidget object) that you can embed in your Qt application.

An APP registration is in progress and the library has been release in october under the LGPL license. See http://qtshanoir.gforge.inria.fr.

- Keywords : medical imaging, dicom
- Software benefit: offers a great solution to query a Shanoir server. Can be easily re used in larger Qt applications
- License: no defined licence for the moment
- Type of human computer interaction: C++ library
- OS/Middelware: Linux, Windows and Mac
- Required library or software : Qt
- Programming language: C++
- Documentation : http://qtshanoir.gforge.inria.fr

5.6. AutoMRI

Participants: Camille Maumet, Isabelle Corouge, Elise Bannier.

AutoMRI is an SPM-based set of tools to study structural and functional MRI data. This software is currently made up of 9 modules : autofMRI, autoVBM, automorpho, autoASL, autoFASL, autoROI, autoasltemplate, autofmriacontrario and autoNCEMRA. AutofMRI produces statistical maps of activations and deactivations at the group or the subject level based on functional MRI data. It can deal with block or event-related designs and is highly configurable in order to fit to a wide range of needs. autoVBM performs between-group voxel-based morphometric analysis in order to outline regions of grey (or white) matter volume reduction and increase. To further study a morphometric or a functional analysis, regions of interest analysis can be performed with autoROI. This module also provides the user with laterality indexes. Automorpho performs one-versus-many group analysis on anatomical data in order to outline pathological dysplasia or heterotopia. AutoFASL (collaboration with Rémi Dubujet) produces statistical maps of activations and deactivations at the group or the subject level based on functional Arterial Spin Labeling data. AutoASL performs between-group voxel-based morphometric analysis in order to outline regions of reduced (or increased) perfusion. Autoasltemplate focus on patient-specific detection of perfusion abnormalities with a standard massively univariate General Linear Model or with an a contrario approach. Autofmriacontrario provides an alternative to autofmri to produce statistical maps of activations and deactivations at the subject level using an a contrario approach. autoNCEMRA enables automatic processing of 4D MRA data to remove unwanted signal from the skull, using a mask based on 3D T1w segmentation of grey matter, white matter and CSF. Thus, denoised maximum intensity projections in axial, coronal and sagittal planes can be calculated to enable accurate assessment of hemodynamic patterns, from arterial input to venous drainage (in particular in patients presenting arteriovenous malformations).

- Keywords : fMRI, MRI, ASL, fASL, SPM, automation
- Software benefit: Automatic MRI data analysis based on SPM. Once the parameters are set, the analysis is performed without human interaction.
- APP: Part in IDDN.FR.001.130017.000.S.A.2012.000.31230
- Type of human computer interaction: Matlab function (script, no GUI)
- OS/Middleware: Linux/Windows
- Required library or software : Matlab, SPM, SPM toolboxes : Marsbar, LI-toolbox, NS
- Programming language: Matlab
- Documentation : Available

5.7. Medinria

Participants: René-Paul Debroize, Clément Philipot, Guillaume Pasquier, Olivier Commowick.

Medinria is a national Inria project shared between 4 Inria teams (Asclepios, Athena, Parietal and Visages). 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 for two years 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. Medinria 2.0.1 has been released in April 2012 for the main distribution platforms. Development of an SDK and of a new verions is underway and should be released in June 2013.

See also the web page http://med.inria.fr

- Keywords: medical imaging, diffusion imaging, registration, filtering, user-friendly interface
- Software benefit: user-friendly interface to cutting-edge research tools for research clinicians. Straightforward to add functionalities through plugins.
- License: core: BSD, plugins: choice of each team.
- Type of human computer interaction: Qt-based GUI
- OS/Middelware: Windows, Mac et Linux.
- Required library or software : Qt, DTK, ITK, VTK.
- Programming language: C++

5.8. USGraphCut

Participant: Christian Barillot.

This software has been developed in collaboration with Jan Petr and Alexandre Krupa during the ANR USComp project. It concerns the segmentation of echographic data by using the graph cut algorithm. It allows the segmentation and the tracking of evolving objects in 2D/3G echographic data in real time thanks to a specific CUDA framework.

5.9. CtrlQ - MR Quality Assurance

Participants: René-Paul Debroize, Isabelle Corouge, Elise Bannier.

As part of the monitoring of the 3Tesla MR equipment, a quality control consistent with the one recommended by the American College Of Radiology (ACR) is performed weekly. As part of its MRI accreditation program, the ACR standardized a procedure for monitoring quality consisting of a series of measurements performed on a standardized imaging protocol on a test object with known geometry. A robust and intuitive software was developed, with a graphical interface, to ensure the automation of the measurements necessary to the control. The application was developed in C++ using the Qt, ITK, and DCMTK libraries.

5.10. SimuBloch

Participants: Fang Cao, Olivier Commowick, Elise Bannier, Christian Barillot.

We developed a simulator package *SimuBloch*, which is made for a fast simulation of image sequences based on Bloch equations, which can be run directly from VIP Portal: http://vip.creatis.insa-lyon.fr. The current version is v0.3. The simulator allows to construct 6 different MR pulse sequences:

1. *SimuBlochSE*: Simulation of spin echo sequences.
2. *SimuBlochGRE*: Simulation of gradient echo sequences.
3. *SimuBlochIR-SE*: Simulation of inversion recovery spin echo sequences.
4. *SimuBlochIR-GRE*: Simulation of inversion recovery gradient echo sequences.
5. *SimuBlochSP-GRE*: Simulation of spoiled gradient echo sequences.
6. *SimuBlochCoherentGRE*: Simulation of coherent gradient echo sequences.

CLIME Project-Team

5. Software

5.1. Polyphemus

Participants: Vivien Mallet, Anne Tilloy.

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 forecast and daily forecasts. Its completeness makes it suitable for use in many applications: photochemistry, aerosols, radionuclides, *etc*. It is able to handle simulations from local to continental scales, with several physical models. It is divided into three main parts:

- libraries that gather data processing tools (SeldonData), physical parameterizations (AtmoData) and postprocessing abilities (AtmoPy);
- programs for physical preprocessing and chemistry-transport models (Polair3D, Castor, two Gaussian models, a Lagrangian model);
- drivers on top of the models in order to implement advanced simulation methods such as data assimilation algorithms.

Figure 1 depicts a typical result produced by Polyphemus. Clime is involved in the overall design of the system and in the development of advanced methods in model coupling, data assimilation and ensemble forecast (through drivers and post-processing).

In 2012, Polyphemus received several physical developments on secondary organic aerosols, modeling of pollution due to traffic emissions and coupling of local and regional scale models. Further integration with the data assimilation library Verdandi has been carried out. A Python interface to the Eulerian model Polair3D has been introduced.

5.2. Data assimilation library: Verdandi

Participants: Kévin Charpentier, Marc Fragu [MACS], Vivien Mallet, Dominique Chapelle [MACS], Philippe Moireau [MACS], Sergiy Zhuk, Anne Tilloy.

The leading idea is to develop a data assimilation library 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 2012, versions 1.2, 1.3 and 1.4 were released. The design of the library has been improved for optimal performance and is now stable. It is possible to write models and observation managers in Python. Efficient support for parallel computations has been introduced. The documentation has been improved.

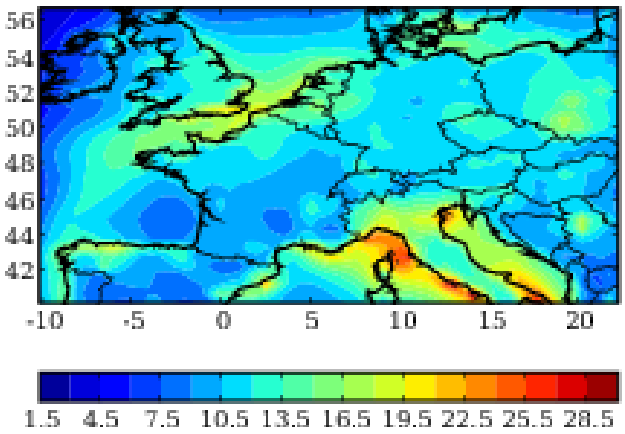


Figure 1. Map of the relative standard deviation (or spread, %) of an ensemble built with Polyphemus (ozone simulations, $\mu g\ m^{-3}$). The standard deviations are averaged over the summer of 2001. They provide an estimation of the simulation uncertainties.

5.3. Urban air quality analysis

Participants: Anne Tilloy, Vivien Mallet.

"Urban Air Quality Analysis" carries out data assimilation at urban scale. It merges the outputs of a numerical model (maps of pollutant concentrations) with observations from an air quality monitoring network, in order to produce the so-called analyses, that is, corrected concentration maps. The data assimilation computes the Best Linear Unbiased Estimator (BLUE), with a call to the data assimilation library Verdandi. The error covariance matrices are parameterized for both model simulations and observations. For the model state error covariances, the parameterization primarily relies on the road network. The software handles ADMS Urban output files, for a posteriori analyses or in an operational context.

FLUMINANCE Project-Team

5. Software

5.1. DenseMotion software - Estimation of 2D dense motion fields

Participants: Thomas Corpetti, Patrick Héas, Etienne Mémin.

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 model and different regularization functional depending on the targeted application. Generic motion estimator for video sequences or dedicated motion estimator for fluid flows can be specified. This estimator 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 end Remote Sensing. The binary of this code can be freely downloaded on the FLUID web site http://fluid.irisa.fr.

5.2. 2DLayeredMotion software - Estimation of 2D independent mesoscale layered atmospheric motion fields

Participants: Patrick Héas, Etienne Mémin.

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. This code corresponds to research studies published in IEEE transaction on Geo-Science and Remote Sensing. It can be freely downloaded on the FLUID web site http://fluid.irisa.fr.

5.3. 3DLayeredMotion software - Estimation of 3D interconnected layered atmospheric motion fields

Participants: Patrick Héas, Etienne Mémin.

This software extends the previous 2D version. It allows (for the first time to our knowledge) the recovery of 3D wind fields from satellite image sequences. As with the previous techniques, the atmosphere is decomposed into a stack of pressure layers. The estimation relies also on pressure data and classification clouds maps and top of clouds pressure maps. In order to recover the 3D missing velocity information, physical knowledge on 3D mass exchanges between layers has been introduced in the data model. The corresponding data model appears to be a generalization of the previous data model constructed from a vertical integration of the continuity equation. This research study has been recently accepted for publication in IEEE trans. on Geo-Science and Remote Sensing. A detailed description of the technique can be found in an Inria research report. The binary of this code can be freely downloaded on the FLUID web site http://fluid.irisa.fr.

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

Participants: Anne Cuzol, Etienne Mémin.

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 obtained 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. Different versions of this estimation are available. The code which includes a Matlab user interface can be downloaded on the FLUID web site http://fluid.irisa.fr. This program corresponds to a research study that has been published in the International Journal on computer Vision.

MAGIQUE-3D Project-Team

5. Software

5.1. Hou10ni

This software, written in FORTRAN 90, simulates the propagation of acoustic waves in heterogeneous 2D and 3D media. It is based on an Interior Penalty Discontinuous Galerkin Method (IPDGM). The 2D version of the code has been implemented in the Reverse Time Migration (RTM) software of TOTAL in the framework of the Ph.D thesis of Caroline Baldassari. The 2D code allows for the use of meshes composed of cells of various order (p-adaptivity in space). For the time discretization, we used the local time stepping strategy described at section 3.2 , item **High-Order Schemes in Space and Time** which permits not only the use of different time-step, but also to adapt the order of the time-discretization to the order of each cells (hp-adaptivity in time).

The main competitors of Hou10ni are codes based on Finite Differences, Spectral Element Method or other Discontinuous Galerkin Methods (such as the ADER schemes). During her Ph.D thesis, Caroline Baldassari compared the solution obtained by Hou10ni to the solution obtained by a Finite Difference Method and by a Spectral Element Method (SPECFEM). To evaluate the accuracy of the solutions, we have compared them to analytical solutions provided by the codes Gar6more (see below). The results of these comparisons is: a) that Hou10ni outperforms the Finite Difference Methods both in terms of accuracy and of computational burden and b) that its performances are similar to Spectral Element Methods. Since Hou10ni allows for the use of meshes based on tetraedrons, which are more appropriate to mesh complex topographies, and for the p-adaptivity, we decided to implement it in the RTM code of TOTAL. Of course, we also used these comparisons to validate the code. Now, it remains to compare the performances of Hou10ni to the ADER schemes.

Recently, we have extended the 2D version of Hou10ni for computing the solution of the harmonic wave equation (Helmholtz). This new version is able to deal with both acoustic and elastodynamic media, but also to model elastoacoustic problems. The surfaces between the different media can be approximated by curved elements. We can use up to P^{15} elements when dealing with curved elements and element of arbitrary order (with of course a limitation depending on the machine precision) when dealing with non-curved elements.

5.2. Gar6more3D

Participant: Julien Diaz [correspondant].

This code computes the analytical solution of problems of waves propagation in two layered 3D media such as- acoustic/acoustic- acoustic/elastodynamic- acoustic/porous- porous/porous, based on the Cagniard-de Hoop method.
See also the web page http://web.univ-pau.fr/~jdiaz1/software.html.

The main objective of this code is to provide reference solutions in order to validate numerical codes. They have been already used by J. Tromp and C. Morency to validate their code of poroelastic wave propagation [87]. They are freely distributed under a CECILL licence and can be downloaded on the website http://web.univ-pau.fr/~jdiaz1/software.html. As far as we know, the main competitor of this code is EX2DELDEL (available on http://www.spice-rtn.org), but this code only deals with 2D acoustic or elastic media. Our codes seem to be the only one able to deal with bilayered poroelastic media and to handle the three dimensional cases.

- ACM: J.2
- AMS: 34B27 35L05 35L15 74F10 74J05
- Programming language: Fortran 90

MOISE Project-Team

5. Software

5.1. Adaptive Grid Refinement

Participants: Laurent Debreu, Marc Honnorat.

AGRIF (Adaptive Grid Refinement In Fortran, [80],[6]) 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. As an example, AGRIF is currently used in the following ocean models: MARS (a coastal model developed at IFREMER-France), ROMS (a regional model developed jointly at Rutgers and UCLA universities), OPA-NEMO ocean modelling system (a general circulation model used by the French and European scientific community) and HYCOM (a regional model developed jointly by University of Miami and the French Navy).
In 2012, a new contract has been signed with IFREMER to optimize parallel capabilities of the software. The software will be used operationally to attain a resolution of 500meters along the French coasts. (http://www.previmer.org) AGRIF is licensed under a GNU (GPL) license and can be downloaded at its web site (http://ljk.imag.fr/MOISE/AGRIF/index.html).

5.2. NEMOVAR

Participants: Arthur Vidard, Pierre-Antoine Bouttier, Bénédicte Lemieux-Dudon.

NEMOVAR is a state-of-the-art multi-incremental variational data assimilation system dedicated to the european ocean modelling platform NEMO for research and operational applications. It is co-developed by MOISE, CERFACS (FR), ECMWF (EU) and MetOffice (UK) under the CeCILL license, written in fortran and python. It is now in use in both ECMWF and MetOffice for their operational oceanic forecasting systems. It has also been used for specific studies in collaboration with Mercator-Ocean, LPO, LOCEAN and LEGI in France and University of Namur in Belgium. It is also a likely candidate for becoming the future Black-Sea forecasting system of the Marine Hydrographical Institute of Ukraine with whom we collaborate actively. Previously part of NEMOVAR, NEMO-TAM (Tangent and adjoint models for NEMO) that have been developed by the MOISE team will be now distributed directly by the NEMO consortium. The first official tagged release including NEMO-TAM will be published early 2013.

5.3. DatIce

Participants: Bénédicte Lemieux-Dudon, Habib Toye Mahamadou Kele.

Antarctic and Greenland ice cores provide a mean to study the phase relationships of climate changes in both hemispheres. They also enable to study the timing between climate, and greenhouse gases or orbital forcings. One key step for such studies is to improve the absolute and relative precisions of ice core age scales (for ice and trapped gas), and beyond that, to try to reach the best consistency between chronologies of paleo-records of any kind.

The DatIce tool is designed to increase the consistency between pre-existing core chronologies (also called background). It formulates a variational inverse problem which aims at correcting three key quantities that uniquely define the core age scales: the accumulation rate, the total thinning function, and the close-off depth. For that purpose, it integrates paleo-data constraints of many types among which age markers (with for instance documented volcanoes eruptions), and stratigraphic links (with for instance abrupt changes in methane concentration). A cost function is built that enables to calculate new chronologies by making a trade-off between all the constraints (background chronologies and paleo-data).

DatIce enables to circumvent the limits encountered with other dating approaches, in particular because it controls the model errors, which are still large despite efforts to better describe the firn densification, the ice flow and the forcing fields (ice sheet elevation, temperature and accumulation rate histories). Controlling the model error makes it possible to assimilate large set of observations, to constrain both the gas and ice age scales, and to apply the process on several cores at the same time by including stratigraphic links between cores. This approach greatly improves the consistency of ice cores age scales.

The method presented in ([84], [85]) has already been applied simultaneously to EPICA EDML and EDC, Vostok and NGRIP drillings. The DatIce tool has aroused some interest in the glaciological and paleo-community since 2009.

The code has been recently applied in two publications [2] and [22] which aimed at the construction of a unified chronology for Antarctic ice cores. LGGE, LSCE and MOISE are partners to extend the code to marine and terrestrial cores. On going development efforts are made to ensure the robustness of the dating solution (diagnostics on the assimilation system, calibration of the background error covariance matrices).

5.4. SDM toolbox

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, we develop a new method based on the combination of an existing numerical weather prediction model providing a coarse prediction, and a Lagrangian Stochastic Model adapted from a pdf method introduced by S.B. Pope for turbulent flows. This Stochastic Downscaling Method (SDMhttp://sdm.gforge.inria.fr/) is thus aimed to be used as a refinement toolbox of large-scale numerical models. SDM requires a specific modelling of the turbulence closure, and involves various simulation techniques whose combination is totally new (such as Poisson solvers, optimal transportation mass algorithm, original Euler scheme for confined Langevin stochastic processes, and stochastic particle methods). Since 2011, we work on the comparison of the SDM model (endowed with a physical geostrophic forcing and a wall log law) with simulations obtained with a LES method (Méso-NH code) for the atmospheric boundary layer (from 0 to 750 meters in the vertical direction), in the neutral case.

5.5. CompModSA package

Alexandre Janon is a contributor of the packages CompModSA - Sensitivity Analysis for Complex Computer Models (see http://cran.r-project.org/web/packages/CompModSA/index.html), and sensitivity (see http://cran.r-project.org/web/packages/sensitivity/index.html). These packages are useful for conducting sensitivity analysis of complex computer codes.

POMDAPI Project-Team

3. Software

3.1. LifeV

Participant: Michel Kern.

LifeV is a finite element (FE) library providing implementations of state of the art mathematical and numerical methods. It serves both as a research and production library. It has been used already in medical and industrial context to simulate fluid structure interaction and mass transport. LifeV is the joint collaboration between four institutions: École Polytechnique Fédérale de Lausanne (CMCS) in Switzerland, Politecnico di Milano (MOX) in Italy, Inria (Pomdapi) in France and Emory University (Sc. Comp) in the U.S.A.

- Version 3.1.1
- Programming language: C++
- http://www.lifev.org/

3.2. M1cg1

– Participant: J. Ch. Gilbert.
– Version: 1.2.
– Programming language: Fortran 77.
– Solves a convex quadratic optimization problem and builds a preconditioning matrix, 8 downloads in 2012.
– https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/m1cg1/m1cg1.html.

3.3. M1qn3

– Participants: J. Ch. Gilbert, Cl. Lemaréchal.
– Version: 3.3.
– Programming language: Fortran 77.
– Solves a very large scale differentiable optimization problem, 34 downloads in 2012.
– https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/m1qn3/m1qn3.html.

3.4. Sklml

Participants: François Clément, Pierre Weis.

Easy coarse grain parallelization.

See also the web page http://sklml.inria.fr/.

- Version: 1.0+pl1
- Programming language: OCaml

3.5. SQPlab

– Participant: J. Ch. Gilbert.
– Version: 0.4.5.
– Programming language: Matlab.
– Solves a constrained differentiable optimization problem, 211 downloads in 2012.
– https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/sqplab/sqplab.html.

SAGE Project-Team

5. Software

5.1. H2OLab

Participants: Thomas Dufaud, Jocelyne Erhel [correspondant], Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot.

The software platform H2OLab is devoted to stochastic simulations of groundwater flow and contaminant transport in highly heterogeneous porous and fractured geological media. It contains a database which is interfaced through the web portal H2OWeb. It contains also software modules which can be used through the interface H2OGuilde. The platform H2OLab is an essential tool for the dissemination of scientific results. Currently, software and database are shared by the partners of the h2mno4 project (see 8.1.1). Software integrated in the platform and registered at APP are GW-UTIL, GW-NUM, PARADIS, MP-FRAC.

See also the web page http://h2olab.inria.fr.

5.2. GW-UTIL

Participants: Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr.
- Abstract: The software GW-UTIL allows to discretize PDE for flow and transport in aquifers and to deal with stochastic models. It contains a set of utilitary modules for geometry, input, output, random numbers, visualization, parallel computing, numerical algorithms, etc. A package is devoted to launch applications.
- Current work: refactoring.

5.3. GW-NUM

Participants: Thomas Dufaud, Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr.
- Abstract: The software GW-NUM is a set of generic modules to discretize PDE of flow and transport in 2D computational domains in order to deal with stochastic models. Methods for flow simulations are either Finite Volume on structured meshes or Mixed Finite Element with unstructured meshes. Method for transport simulations is a particle tracker for advection and a random walker for diffusion. Uncertainty Quantification method is Monte-Carlo. For flow computations, the involved linear system is solved by external software devoted to sparse matrices.
- Current work: refactoring.

5.4. MP-FRAC

Participants: Thomas Dufaud, Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr.
- Abstract: The software MP-FRAC aims at modelling and simulating numerically flow in a fractured aquifer. The physical domain is a network of fractures, either deterministic or stochastic, with a permeability field either deterministic or stochastic. The software computes the velocity field in the aquifer, by assuming that the medium is saturated and that flow is steady-state. Physical equations are stochastic PDEs, handled by a Monte-Carlo method. This non intrusive approach generates a set of random samples, which are used for simulations. Then, the software analyzes statistically the flow in the stochastic case. The objective is to characterize hydraulic properties in Discrete Fracture Networks. The software MP-FRAC handles a simulation corresponding to one sample, whereas Monte-Carlo method is implemented in a generic way by the software GW-NUM. The software is specific of the physical model (Discrete Fracture Network) and of the application (steady-state flow). Generic numerical methods to discretize PDE are implemented in the software GW-NUM.
- Current work: refactoring and design of libraries.

5.5. PARADIS

Participants: Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr/.
- Abstract: The software PARADIS aims at modelling and simulating numerically flow in a porous aquifer and transport by convection-diffusion of an inert solute. The porous medium is heterogeneous, with a stochastic or deterministic permeability field. A first step computes the velocity filed in the aquifer, by assuming that the medium is saturated and that flow is steady-state. A second step computes the distribution of solute concentration, by assuming a transport by convection and by molecular diffusion. Physical equations are stochastic PDEs, handled by a Monte-Carlo method and discretized by numerical methods. This non intrusive approach generates a set of random samples, which are used for simulations. Then, the software analyzes statistically the flow in the stochastic case. The objectives are to determine asymptotic laws of transport, to characterize pre-asymptotic behavior and to define global laws.

  The software PARADIS handles a simulation corresponding to one sample, whereas Monte-Carlo method is implemented in a generic way by the software GW-NUM. The software is specific of the physical model (heterogeneous porous medium) and of the application (steady-state flow then transport with macro-dispersion). Generic numerical methods to discretize PDE are implemented in the software GW-NUM.
- Current work: refactoring and design of libraries.

5.6. GRT3D

Participants: Édouard Canot, Jocelyne Erhel [correspondant], Souhila Sabit.

- Version: version 1.0, April 2011
- APP: registered
- Programming language: C
- Abstract: Reactive transport modeling has become an essential tool for understanding complex environmental problems. It is an important issue for MoMaS partners (see section 8.1.7), in particular Andra (see section 7.1). 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. Another approach, called SIA, is to use a fixed-point method to solve the nonlinear system at each timestep.

  The software suite GRT3D has four executable modules:
  - SIA1D: Sequential Iterative Approach for 1D domains;
  - GDAE1D: Global DAE approach for 1D domains;
  - SNIA3D: Sequential Non Iterative Approach for 1D, 2D or 3D domains.
  - GDAE3D: Global DAE approach for 1D, 2D or 3D domains.
- Current work: extension of the chemistry module and reduction of CPU time.

5.7. GPREMS

Participants: Édouard Canot, Jocelyne Erhel [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://www.irisa.fr/sage/.
- Abstract: GPREMS implements a robust hybrid solver for large sparse linear systems that combines a Krylov subspace method as accelerator with a Schwarz-based preconditioner. This preconditioner uses an explicit formulation associated to one iteration of the multiplicative Schwarz method. The Newton-basis GMRES, which aims at expressing a good data parallelism between subdomains is used as accelerator.

5.8. DGMRES

Participant: Jocelyne Erhel [correspondant].

- Version: version 1.0, June 2011
- APP: distributed with the free software PETSC
- Programming language: C
- See also: http://www.irisa.fr/sage/.
- Abstract: DGMRES implements a preconditioner based on adaptive deflation, which can be used with any preconditioner for the GMRES algorithm.

5.9. AGMRES

Participant: Jocelyne Erhel [correspondant].

- Version: version 1.0, November 2011
- APP: distributed with the free software PETSC
- Programming language: C
- See also: http://www.irisa.fr/sage/.
- Abstract: AGMRES implements an augmented subspace approach, based on adaptive deflation, which can be used with any preconditioner for the GMRES algorithm. It also implements a Newton basis for enhancing parallelism.

5.10. PPAT: pseudo-spectrum

Participants: Édouard Canot [corresponding author], Bernard Philippe.

PPAT (Parallel PATh following software) is a parallel code, developed by D. Mezher, W. Najem (University of Saint-Joseph, Beirut, Lebanon) and B. Philippe. This tool can follow the contours of a functional from $\mathbb{C}$ to $\mathbb{R}^+$. The present version is adapted for determining the level curves of the function $f(z) = \sigma_{\min}(A - zI)$ which gives the pseudospectrum of matrix A.

The algorithm is reliable: it does not assume that the curve has a derivative everywhere. The process is proved to terminate even when taking into account roundoff errors. The structure of the code spawns many independent tasks which provide a good efficiency in the parallel runs.

The software can be downloaded under the GPL licence from: http://sourceforge.net/projects/ppat.

5.11. MUESLI: Scientific computing

Participant: Édouard Canot [corresponding author].

Doing linear algebra with sparse and dense matrices is somehow difficult in scientific computing. Specific libraries do exist to deal with this area (*e.g.* BLAS and LAPACK for dense matrices, SPARSKIT for sparse ones) but their use is often awful and tedious, mainly because of the large number of arguments which must be used. Moreover, classical libraries do not provide dynamic allocation. Lastly, the two types of storage (sparse and dense) are so different that the user must know in advance the storage used in order to declare correctly the corresponding numerical arrays.

MUESLI is designed to help in dealing with such structures and it provides the convenience of coding in Fortran with a matrix-oriented syntax; its aim is therefore to speed-up development process and to enhance portability. It is a Fortran 95 library split in two modules: (i) FML (Fortran Muesli Library) contains all necessary material to numerically work with a dynamic array (dynamic in size, type and structure), called `mfArray`; (ii) FGL (Fortran Graphics Library) contains graphical routines (some are interactive) which use the `mfArray` objects.

MUESLI includes some parts of the following numerical libraries: Arpack, Slatec, SuiteSparse, Triangle, BLAS and LAPACK.

Linux is the platform which has been used for developing and testing MUESLI. Whereas the FML part (numerical computations) should work on any platform (*e.g.* Win32, Mac OS X, Unix), the FGL part is intended to be used only with X11 (*i.e.* under all UNIXes).

Last version of MUESLI is 2.6.6 (2012-08-29). More information can be found at: http://people.irisa.fr/Edouard.Canot/muesli

5.12. CANARD: BEM for surface flows

Participant: Édouard Canot [corresponding author].

When dealing with non-linear free-surface flows, mixed Eulerian-Lagrangian methods have numerous advantages, because we can follow marker particles distributed on the free-surface and then compute with accuracy the surface position without the need of interpolation over a grid. Besides, if the liquid velocity is large enough, Navier-Stokes equations can be reduced to a Laplace equation, which is numerically solved by a Boundary Element Method (BEM); this latter method is very fast and efficient because computing occur only on the fluid boundary. This method has been applied to the spreading of a liquid drop impacting on a solid wall and to the droplet formation at a nozzle; applications take place, among others, in ink-jet printing processes.

The code used (CANARD) has been developped with Jean-Luc Achard (LEGI, Grenoble) for fifteen years and is used today mainly through collaborations with Carmen Georgescu at UPB (University Polytechnica of Bucarest, Romania), and with Alain Glière (CEA-LETI, Grenoble).

STEEP Exploratory Action

5. Software

5.1. TEOS: Tranus Exploration and Optimization Software

Participants: Anthony Tschirhard, Mathieu Vadon, Elise Arnaud, Emmanuel Prados.

The TEOS software offers a set of tools to help the calibration of the land use and transport integrated model TRANUS. It uses some exploration and optimization procedures of the relevant parameters.

BANG Project-Team

5. Software

5.1. Software

5.1.1. Continuation of M3N

A large part of the software currently in use in the project-team was initiated and developed within former projects (Menusin, M3N).

5.1.2. CellSys

Participants: Dirk Drasdo [correspondent], Stefan Höhme [Research Associate, University of Leipzig], Adrian Friebel [PhD student, University of Leipzig], Tim Johann [Software Engineer, University of Leipzig], Nick Jagiella [PhD student].

Computer simulation software for image analysis of tissue samples at histological scales, as well as individual cell (agent)-based models of tumour and tissue growth solved either by systems of coupled equations of motion for each individual cell or by Kinetic Monte Carlo methods [56].
The software CellSys is currently been completely reorganised to permit easier use by external and internal researchers. The idea is to perspectively go open-source and offer consultancy for potential users.

BIGS Project-Team

5. Software

5.1. Light diffusion into tissues

We are currently considering the possibility to implement our Matlab algorithms concerning light diffusion into tissues into the Matlab toolbox *Contsid*, developed by the System Identification team of the CRAN (http://www.iris.cran.uhp-nancy.fr/contsid/).

5.2. Online data analysis

A R package performing most of the methods of factorial analysis in an online way is under development by R. Bar and J-M. Monnez. Starting from a simulated data flow, the main goal of the program is to perform online factorial analyses (Principal Component Analyses, Canonical Correlation Analysis, Canonical Discriminant Analysis, Correspondence Analysis). Data are supposed to be independent and identically distributed observations of a random vector (whose distribution is a priori unknown). Defining stochastic approximation processes, the procedure is adaptative in the sense that the results of the analyses are updated recursively each time that a new data is taken into account.

From a theoretical point of view, the i.i.d case has been recently extended to the case of an expectation and/or covariance matrix of the random vector varying with time. We plan to include these improvements into our software.

5.3. Socio-economic index

A R package called SesIndexCreatoR has been written by B. Lalloué and J-M. Monnez in order to implement our socio-economic index for health inequalities. The version 1.0 of this package is currently freely available on the website of the Equit'Area project: http://www.equitarea.org/documents/packages_1.0-0/. It contains the functions needed to run the procedure (either integrally or partially) and obtain the corresponding SES index. The user may also create categories of this index with different methods (hierarchical clustering with or without k-nearest neighbors, quantiles, or intervals) and generate automatic reports of the results. Visualization and plotting functions are provided in the package.

BIOCORE Project-Team

5. Software

5.1. Supervision software

We are developing a software for the supervision of bioreactors: this platform, named ODIN, has been built for the smart management of bioreactors (data acquisition, fault diagnosis, automatic control algorithm,...). This software was developed in C++ and uses a Scilab engine to run the advanced algorithms developed within BIOCORE. It has been implemented and validated with four different applications.

CARMEN Team (section vide)

DRACULA Project-Team

5. Software

5.1. CelDyn

Participants: Laurent Pujo-Menjouet, Alen Tosenberger, Vitaly Volpert [correspondant].

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.

MACS Project-Team

5. Software

5.1. FELISCE

Participants: Dominique Chapelle, Sébastien Gilles [correspondant], Philippe Moireau.

FELISCE – standing for "Finite Elements for LIfe SCiences and Engineering" – is a new finite element code which the MACS and REO 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 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. https://gforge.inria.fr/projects/felisce/

5.2. HeartLab

Participants: Matthieu Caruel, Dominique Chapelle, Alexandre Imperiale, Philippe Moireau [correspondant].

The heartLab software is a library written in (64 bits 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 the CardioSense3D community.

The code relies on OpenFEM 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 heart anatomical models compatible with the simulation requirements in terms of mesh quality, fiber direction data defined within each element, and 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 recently 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.

5.3. MITCNL

Participants: Dominique Chapelle [correspondant], Marina Vidrascu [REO team].

The package MITCNL is a set of subroutines that implements the triangular MITC3, MITC6 and quadrilateral MITC4 and MITC9 shell elements for large displacements [2]. We use it as a basis for new developments of shell elements, in particular within Modulef (http://www-rocq.inria.fr/modulef/). It can be easily interfaced with most finite element codes as well. We also license this package to some of our partners for use with their own codes.

5.4. OpenFEM: a Finite Element Toolbox for Matlab and Scilab

Participants: Dominique Chapelle, Philippe Moireau [correspondant].

OpenFEM (http://www.openfem.net) is an *opensource* finite element toolbox for linear and nonlinear structural mechanics within the Matlab and Scilab matrix computing environments. This software is developed in a collaboration between Macs and the SDTools company [1]. Performing finite element analyses within a matrix computing environment is of considerable interest, in particular as regards the ease of new developments, integration of external software, portability, post-processing, etc.

This Library is the core of the finite element computations of HeartLab where a specific version have been developed with the help of Cesare Corrado from Reo.

5.5. SHELDDON

Participants: Dominique Chapelle [correspondant], Marina Vidrascu [REO team].

SHELDDON (SHELls and structural Dynamics with DOmain decomposition in Nonlinear analysis) 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.

5.6. Verdandi

Participants: Dominique Chapelle, Marc Fragu, Vivien Mallet [Clime team], Philippe Moireau [correspondant].

Verdandi is an opensource (LGPL) software library aiming at providing assimilation data methods and related tools. Mainly targeted at large systems arising from the discretization of PDEs, it is intentionally devised as generic, which allows for applications in a wide range of problems (biology and medicine, environment, image processing...). See also the web page http://verdandi.gforge.inria.fr/, with a complete documentation in English. The first stable version (1.0) was released in June 2012 and contains most of the major data assimilation algorithms of both variational and sequential types. The actual version (1.4) contains additional estimation algorithm and parallel capabilities. Note that some specific developments are performed with particular regard to cardiac modeling applications, as Verdandi is partly funded by – and distributed within – the euHeart project and is now referenced in the following peer-reviewed article [15]

- ACM: Mathematical software
- AMS: System theory; control
- Software benefit: Verdandi is the only *generic* data assimilation library
- License: LGPL (2.1 or any later version)
- Type of human computer interaction: Command line and configuration files
- OS/Middelware: Linux, MacOS ou Windows
- Required library or software: Seldon (LGPL, http://seldon.sourceforge.net/)
- Programming language: C++, ISO/IEC 14882: I998(E) Python, version 2.6
- Documentation: Doxygen and utilisation manual in english

[1] http://www.sdtools.com

MASAIE Project-Team (section vide)

MODEMIC Project-Team

5. Software

5.1. VITELBIO

Participants: Jérôme Harmand, Alain Rapaport.

VITELBIO (VIrtual TELluric BIOreactors) is a simulation tool for studying networks of interconnected chemostats with the objective of mimicking microbial activities in soil. The software, developed with the help of ITK Company, is accessible on a server from any web navigator and make use of Flex for the user interface and Octave for the numerical integration. An important effort has been made for obtaining a pleasant and easy interface that is appealing for microbiologists: the network can be drawn graphically on the screen and simulation results can be easily compared between (virtual) experiments, superposing trajectories curves.

This software is used by several researchers, from LBE (INRA Narbonne), UMR Eco & Sols (Montpellier), UREP (Unité de Recherche sur l'Ecosystème Prairial, INRA Theix), Biomeco (Paris-Grignon), UMR EGC (Environnement et grandes cultures, Paris-Grignon)... and also as a teaching support. Viltebio is presented at http://sites.google.com/site/vitelbio/ and it is accessible at http://vitelbio.itkweb.fr.

5.2. SMC DEMOS

Participant: Fabien Campillo.

SMC DEMOS (Sequential Monte Carlo demos) proposes a set of demonstration Matlab procedures for nonlinear filtering approximation via particle filtering (sequential Monte Carlo): bearing-only tracking with obstacles, tracking in digital terrain model, track-before-detect in a sequence of digital picture, mobile phone tracking based on the signal strength to nearby antenna. This software is deposited with the "Agence pour la Protection des Programmes" (APP, 7/7/2009), available at http://www-sop.inria.fr/members/Fabien.Campillo/software/smc-demos/.

NUMED Project-Team

5. Software

5.1. Zebre

Participant: Thierry Dumont [correspondant].

Thierry Dumont is currently developping a toolbox to solve stiff reaction diffusion equations using splitting methods, together with refined numerical schemes for ODEs (RADO 5).

5.2. OptimChemo

Participants: Violaine Louvet [correspondant], Emmanuel Grenier.

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.

REO Project-Team

5. Software

5.1. LiFE-V library

Participants: Miguel Ángel Fernández Varela [correspondant], Jean-Frédéric Gerbeau.

LiFE-V [2] 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.

5.2. Mistral library

Participants: Cristóbal Bertoglio Beltran, Jean-Frédéric Gerbeau [correspondant], Vincent Martin.

Mistral is a finite element library which implements in particular fluid-structure interaction algorithms (ALE and Fictitious domain formulations), fluid surface flow (ALE) and incompressible magnetohydrodynamics equations. Mistral results from a collaboration between Inria and ENPC (CERMICS).

5.3. FELiScE

Participants: Grégory Arbia, Cesare Corrado, Miguel Ángel Fernández Varela, Justine Fouchet-Incaux, David Froger, Jean-Frédéric Gerbeau [correspondant], Damiano Lombardi, Elisa Schenone, Saverio Smaldone, Marina Vidrascu, Irène Vignon-Clementel.

FELiScE – standing for "Finite Elements for Life Sciences and Engineering" – is a new finite element code which the MACS 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 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. https://gforge.inria.fr/projects/felisce/

5.4. SHELDDON

Participant: Marina Vidrascu [correspondant].

SHELDDON (SHELls and structural Dynamics with DOmain decomposition in Nonlinear analysis) 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. (https://gforge.inria.fr/projects/shelddon)

[2] http://www.lifev.org/

SISYPHE Project-Team

4. Software

4.1. The Matlab System Identification ToolBox (SITB)

Participant: Qinghua Zhang.

This development is made in collaboration with Lennart Ljung (Linköping University, Sweden), Anatoli Juditsky (Joseph Fourier University, France) and Peter Lindskog (NIRA Dynamics, Sweden).

The System Identification ToolBox (SITB) is one of the main Matlab toolboxes commercialized by The Mathworks. Inria participates in the development of its extension to the identification of nonlinear systems which is released since 2007. It includes algorithms for both black box and grey box identification of nonlinear dynamic systems. Inria is mainly responsible for the development of black box identification, with nonlinear autoregressive (NLARX) models and block-oriented (Hammerstein-Wiener) models.

4.2. Inverse Scattering for Transmission Lines (ISTL)

Participants: Michel Sorine, Qinghua Zhang.

ISTL is a software for numerical computation of the inverse scattering transform for electrical transmission lines. In addition to the inverse scattering transform, it includes a numerical simulator generating the reflection coefficients of user-specified transmission lines. With the aid of a graphical interface, the user can interactively define the distributed characteristics of a transmission line. This software is mainly for the purpose of demonstrating a numerical solution to the inverse problem of non uniform transmission lines. Its current version is limited to the case of lossless transmission lines. It is registered at Agence pour la Protection des Programmes (APP) under the number IDDN.FR.001.120003.000.S.P.2010.000.30705.

4.3. CGAO: Contrôle Glycémique Assisté par Ordinateur

Participants: Alexandre Guerrini, Michel Sorine.

This development is made in collaboration with Pierre Kalfon (Chartres Hospital) and the small business enterprise LK2.

This software CGAO developed with LK2 and Hospital Louis Pasteur (Chartres) provides efficient monitoring and control tools that will help physicians and nursing staff to avoid hyperglycaemia and hypoglycaemia episodes in Intensive Care Units. It has been used in a large clinical study, CGAO-REA. More than 3500 patients have been included in CGAO-REA. Commercialization is done by LK2. CGAO has been sold to the company Fresenius Kabi.

4.4. DYNPEAK: a user-friendly interface for the analysis of LH (Luteinizing Hormone) secretion rhythms

Participants: Frédérique Clément, Arnaud Ferré, Vincent Ladevèze, Claire Médigue, Serge Steer, Mouhamadoul-Bachir Syll, Alexandre Vidal, Qinghua Zhang.

DYNPEAK is a Webresource interface dedicated to the analysis of the pulsatile rhythm of secretion of the pituitary hormone LH, that aims at providing the final users (experimentalists and clinicians) with a simple-to-use version of the algorithm developed in [54]. DYNPEAK is developed within the PALOMA project devoted to the development of a prototype for a collaborative platform in Biomathematics.

4.5. LARY_CR: Software package for the Analysis of Cardio Vascular and Respiratory Rhythms

Participants: Claire Médigue, Serge Steer.

LARY_CR is a software package dedicated to the study of cardiovascular and respiratory rhythms [97]. It presents signal processing methods, from events detection on raw signals to the variability analysis of the resulting time series. The events detection concerns the heart beat recognition on the electrocardiogram, defining the RR time series, the maxima and minima on the arterial blood pressure defining the systolic and diastolic time series. These detections are followed by the resampling of the time series then their analyse. This analyse uses temporal and time frequency methods: Fourier Transform, spectral gain between the cardiac and blood pressure series, Smooth Pseudo Wigner_Ville Distribution, Complex DeModulation, temporal method of the cardiovascular Sequences. The objective of this software is to provide some tools for studying the autonomic nervous system, acting in particular in the baroreflex loop; its functionning is reflected by the cardiovascular variabilities and their relationships with the other physiological signals, especially the respiratory activity. Today LARY_CR is used internally, in the framework of our clinical collaborations, and the functions devoted to the rhythms analysis are now freely available through the Scilab Cardiovascular toolbox, as an atom module.

VIRTUAL PLANTS Project-Team

4. Software

4.1. V-Plants

Participants: Frédéric Boudon, Christophe Godin [coordinator], Yann Guédon, Christophe Pradal [software architect], Jean-Baptiste Durand, Pascal Ferraro.

Computer algorithms and tools developed by the Virtual Plants team are integrated in a common software suite *V-Plants*, dedicated to the modeling and analysis of plant development at different scales (e.g. cellular tissue, whole plant, stand). The VPlants packages are integrated in OpenAlea as Python components. Several components are distributed and usable through the visual programming environment (see figure 2):

- Multi-scale geometric modeling and visualization. VPlants.PlantGL is a geometric library which provides a set of graphical tools and algorithms for 3D plant modeling at different scales [9]. It is used by many other components to represent the geometry of biological shapes from 3D meristems, plant architectures to plant populations. VPlants.PlantGL is built around a scene-graph data structure and provides efficient algorithms and original geometrical shapes (parametric surfaces, dedicated envelops), that are useful for plant modeling.
- Statistical sequence and tree analysis. Different statistical packages (i.e. VPlants.StatTool, VPlants.SequenceAnalysis, VPlants.TreeMatching and VPlants.TreeAnalysis) are now available in OpenAlea. They provide different models and algorithms for plant architecture analysis and simulation.
- Meristem functioning and development. A first set of components has been created in the last 4-years period to model meristem development in OpenAlea. These tools are currently being integrated thoroughly in the platform so that modelers and biologists can use them, and reuse components easily (for meristem 3D reconstruction, cell tracking, statistical analysis of tissues, creating and manipulating atlases, creating or loading models of growth that can further be run on digitized structures, etc).
- Standard data structure for plants. A new implementation of the MTG formalism for representing and manipulating multiscale plant architecture has been developed. It provides a central data-structure to represent plants in a generic way in OpenAlea. This implementation is available through the packages OpenAlea.MTG. These components make it possible to share plant representations between users and fosters the interoperability of new models.
- Simulation system. The study of plant development requires increasingly powerful modeling tools to help understand and simulate the growth and functioning of plants. In the last decade, the formalism of L-systems has emerged as a major paradigm for modeling plant development. Previous implementations of this formalism were made based on static languages, i.e. languages that require explicit definition of variable types before using them. These languages are often efficient but involve quite a lot of syntactic overhead, thus restricting the flexibility of use for modelers. We developed L-Py an adaptation of L-systems to the Python language (basis of OpenAlea). Thanks to its dynamic typing property, syntax is simple, code execution is made easy and introspection property of the language makes it possible to parameterize and manipulate simply complex models. Independent L-systems can be composed to build-up more complex modular models. MTG structures (that are a common way to represent plants at several scales) can be translated back and forth into L-system data-structure and thus make it easy to reuse in L-systems tools for the analysis of plant architecture based on MTGs. Extensions to integrate multiscale dynamic models are currently being developed in collaboration with P. Prusinkiewicz and his team from the University of Calgary. A paper presenting L-Py [14] has been published to Frontiers in Technical Advances in Plant Sciences.

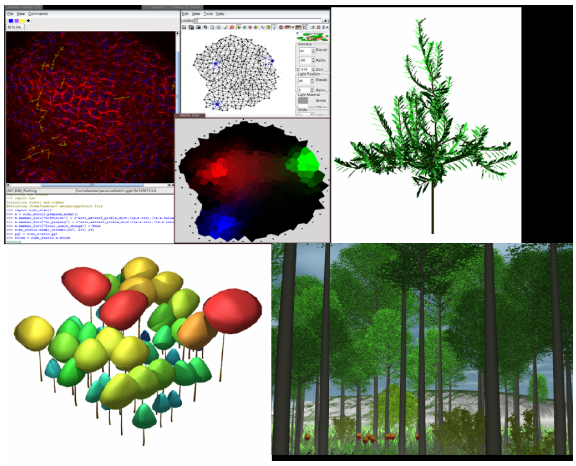


Figure 1. V-Plants components of the OpenAlea platform: simulating plant processes at different scales. Top Left: Reconstruction of a virtual meristem, analysis and simulation of the auxin fluxes inside the meristem. Top Right: Reconstruction of a virtual apple tree from digitized data. Bottom: Simulation of an ecosystem (A beech "Fagus Sylvatica L." trees forest) with a multi level approaches. On the left, explicit representation of the crown volumes that serves as input to generate the detailed representation, on the right.

4.2. OpenAlea

Participants: Frédéric Boudon, Christophe Godin, Yann Guédon, Christophe Pradal [coordinator], Christian Fournier, Julien Coste.

This research theme is supported by the Inria ADT Grant OpenAlea 2.0 and by a Agropolis RTRA Grant named OpenAlea.

OpenAlea [10] is an open source and collaborative software project primarily dedicated to the plant research community. It is designed as a component framework to dynamically glue together models from different plant research labs, and to enhance re-usability of existing models in the plant research community.

The architecture of OpenAlea is based on a component architecture. It provides a set of standard components (OpenAlea.Stdlib), a package manager to dynamically add and retrieve new components, and a port graph data-structure to compose models by interconnecting components into a data-flow.

Visualea provides a visual programming environment, used by scientists to build new model interactively by connecting available components together through an easy-to-use graphical user interface.

In 2012, one major release was done : Openalea 1.0. The following progresses were accomplished:

1. Develop and extend OpenAlea and Visualea:
   - The standard library of components has been extended with useful scientific packages such as a flexible data plotting package (Openalea.Pylab), 2D and 3D image manipulation (Openalea.Image) and linear algebra operations (Openalea.Numpy).
   - Several models of computation have been implemented on the data-flow data-structure to enable discrete event simulation and control flow inside OpenAlea.
2. Animation and diffusion
   - The first OpenAlea Workshop have been held in Montpellier and has been attended by more than 60 scientists. A scientific board has been defined to manage the development and diffusion of OpenAlea. It is composed by 12 scientists.

- StandAlone binary installers have been released on Windows and Mac to ease the installation of a large number of packages without relying on a web server. A Ubuntu repository has been set up on Launchpad.
- A continuous integration server has been set up To test the reliability of all the components after every commit.
- The OpenAlea project is hosted at the Inria gforge (link http://openalea.gforge.inria.fr). The web site is visited by more than 370 unique visitor each month; 650000 web pages have been visited and the different available components of OpenAlea have been downloaded more than 520,000 times during the last two years. OpenAlea is the first project at Inria Gforge in term of number of downloads and of page views.

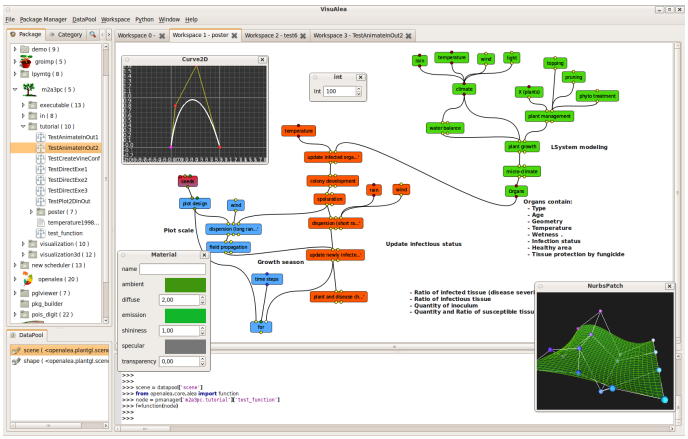


Figure 2. OpenAlea.Visualea: Visual programming interface. The package manager shows the available components. The components can be interconnected on a workspace to form a data-flow. The python interpreter allows low level interaction with the system.

4.3. Alinea

Participants: Christian Fournier, Christophe Pradal, Frédéric Boudon, Christophe Godin.

Other participants : Bruno Andrieu, Michael Chelle, Gaetan Louarn, Benoit de Solan, Mariem Abichou, Liqi Han, Elmer Ccopa-Rivera, Frederic Baret, Rafaele Casa, Youcef Mammeri, Didier Combes, Camille Chambon, Romain Barillot, Pierre Huynh, Jean-Christophe Soulie, Delphine Luquet.

The aim of this Action Ciblée Incitative of INRA is to constitute a consortium of modelers from INRA around the OpenAlea platform, and to integrate various ecophysiological models of simulation in OpenAlea (radiative transfer, interaction between plant and pest, circulation of hydric fluxes, and dispersion). The project includes 3 INRA teams and the Inria Virtual Plants project.

Different components have been integrated into the OpenAlea platform:

- Alinea.Adel is a module to simulate the 3D architectural development of gramineous crops.
- Alinea.Caribu is a modeling suite for lighting 3D virtual scenes, especially designed for the illumination of virtual plant canopies such as virtual crop fields. It uses a special algorithm, the nested radiosity, that allows for a precise estimation of light absorption at the level of small canopy elements.
- Alinea.TopVine is a component to reconstruct grapevine canopy structure.

- Ecomeristem is a crop growth, eco-physiological model that was designed for rice (model plant for cereals) to account for plant morphogenesis and its plasticity depending on genetic potential and sensitivity to the environment (water, temperature, radiation).
- Alinea.Nema is a module used for modeling of nitrogen dynamics between leaves.
- MAppleT is a FSPM model of an apple tree taking into account stochastic models for the topological development, a biomechanical model for branch bending, physiological laws as well as light interception.
- M2A3PC is a generic model to simulate spread of a pathogen on a growing plant like vine/powdery mildew and apple tree/apple scab.

In 2012, a 3D model of gramineous leave has been developped and presented at the PMA conference [28]. This dynamic leaf model is used to simulate different species of annual plants such as rice, wheat and maïze.