IN PARTNERSHIP WITH:
CNRS

Université Rennes 1

Activity Report 2014

Project-Team SAGE

Simulations and Algorithms on Grids for Environment

IN COLLABORATION WITH: Institut de recherche en informatique et systèmes aléatoires (IRISA)

RESEARCH CENTER
Rennes - Bretagne-Atlantique

THEME
Earth, Environmental and Energy Sciences

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Project-Team SAGE

Keywords: Scientific Computation, Stochastic Models, Numerical Software Platform, High Performance Computing, Environment

Creation of the Project-Team: 2004 December 06.

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2. Overall Objectives

2.1. Main research areas

Numerical models are very useful for environmental applications. Several difficulties must be handled simultaneously, in a multidisciplinary context. For example, in geophysics, media are highly heterogeneous and only few data are available. Stochastic models are thus necessary. Some computational domains are complex 3D geometries, requiring adapted space discretization. Equations modeling flow and transport are transient, requiring also adapted time discretization. Moreover, these equations can be coupled together or with other equations in a global nonlinear system. These large-scale models are very time and memory consuming. High performance computing is thus required to run these types of scientific simulations. Supercomputers and clusters are quite powerful, provided that the numerical models are written with a parallel paradigm.

The team SAGE undertakes research on environmental applications and high performance computing and deals with two subjects:

1. numerical algorithms, involving parallel and grid computing,
2. numerical models applied to hydrogeology and physics.

These two subjects are highly interconnected: the first topic aims at designing numerical algorithms, which lead to high efficiency on parallel and grid architectures; these algorithms are applied to geophysical models.

Moreover, the team SAGE, in collaboration with other partners, develops the software platform H2OLab for groundwater numerical simulations in heterogeneous subsurface.

3. Research Program

3.1. Numerical algorithms and high performance computing

Linear algebra is at the kernel of most scientific applications, in particular in physical or chemical engineering. For example, steady-state flow simulations in porous media are discretized in space and lead to a large sparse linear system. The target size is 10^7 in 2D and 10^{10} in 3D. For transient models such as diffusion, the objective is to solve about 10^4 linear systems for each simulation. Memory requirements are of the order of Giga-bytes in 2D and Tera-bytes in 3D. CPU times are of the order of several hours to several days. Several methods and solvers exist for large sparse linear systems. They can be divided into three classes: direct, iterative or semi-iterative. Direct methods are highly efficient but require a large memory space and a rapidly increasing computational time. Iterative methods of Krylov type require less memory but need a scalable preconditioner to remain competitive. Iterative methods of multigrid type are efficient and scalable, used by themselves or as preconditioners, with a linear complexity for elliptic or parabolic problems but they are not so efficient for hyperbolic problems. Semi-iterative methods such as subdomain methods are hybrid direct/iterative methods which can be good tradeoffs. The convergence of iterative and semi-iterative methods and the accuracy of the results depend on the condition number which can blow up at large scale. The objectives are to analyze the complexity of these different methods, to accelerate convergence of iterative methods, to measure and improve the efficiency on parallel architectures, to define criteria of choice.

In geophysics, a main concern is to solve inverse problems in order to fit the measured data with the model. Generally, this amounts to solve a linear or nonlinear least-squares problem. Complex models are in general coupled multi-physics models. For example, reactive transport couples advection-diffusion with chemistry. Here, the mathematical model is a set of nonlinear Partial Differential Algebraic Equations. At each timestep of an implicit scheme, a large nonlinear system of equations arise. The challenge is to solve efficiently and accurately these large nonlinear systems.

Approximation in Krylov subspace is in the core of the team activity since it provides efficient iterative solvers for linear systems and eigenvalue problems as well. The later are encountered in many fields and they include the singular value problem which is especially useful when solving ill posed inverse problems.

3.2. Numerical models applied to hydrogeology and physics

The team Sage is strongly involved in numerical models for hydrogeology and physics. There are many scientific challenges in the area of groundwater simulations. This interdisciplinary research is very fruitful with cross-fertilizing subjects. For example, high performance simulations were very helpful for finding out the asymptotic behaviour of the plume of solute transported by advection-dispersion. Numerical models are necessary to understand flow transfer in fractured media.

The team develops stochastic models for groundware simulations. Numerical models must then include Uncertainty Quantification methods, spatial and time discretization. Then, the discrete problems must be solved with efficient algorithms. The team develops parallel algorithms for complex numerical simulations and conducts performance analysis. Another challenge is to run multiparametric simulations. They can be multiple samples of a non intrusive Uncertainty Quantification method, or multiple samples of a stochastic method for inverse problems, or multiple samples for studying the sensitivity to a given model parameter. Thus these simulations are more or less independent and are well-suited to grid computing but each simulation requires powerful CPU and memory resources.

A strong commitment of the team is to develop the scientific software platform H2OLab for numerical simulations in heterogeneous hydrogeology.

4. Application Domains

4.1. Geophysics

The team has chosen a particular domain of application, which is geophysics. In this domain, many problems require solving large scale systems of equations, arising from the discretization of coupled models. Emphasis is put on hydrogeology, but the team also investigates geodesy, heat and mass transfer in soil, and granular materials. One of the objectives is to use high performance computing in order to tackle 3D large scale computational domains with complex physical models.

4.2. Hydrogeology

This is joint work with Geosciences Rennes at OSUR, Pprime at University of Poitiers and CDCSP at University of Lyon. It is also done in the context of the group Momas and previous Andra grants.

Many environmental studies rely on modelling geo-chemical and hydrodynamic processes. Some issues concern water resources, aquifer contamination, underground waste disposal, clean-up of former waste deposits, acid mine drainage remediation. Other issues, also related to energy, concern geothermy, unconventional gas, enhanced oil recovery, underground storage of CO2, underground storage of nuclear waste.

Simulation of contaminant transport in groundwater is a highly complex problem, governed by coupled linear or nonlinear PDAEs. Moreover, due to the lack of experimental data, stochastic models are used for dealing with heterogeneity. The main objective of the team is to design and to implement efficient and robust numerical models, including Uncertainty Quantification methods.

Recent research showed that rock solid masses are in general fractured and that fluids can percolate through networks of inter-connected fractures. Fractured media are by nature very heterogeneous and multi-scale, so that homogenisation approaches are not relevant. The team develops a numerical model for fluid flow and contaminant transport in three-dimensional porous fractured media.

An important output is the parallel scientific platform H2OLab, running on clusters, grids and machines available in supercomputing centers.

5. New Software and Platforms

5.1. Platforms

5.1.1. Platform H2OLab

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel [correspondant], Grégoire Lecourt, 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 7.2.1). 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. Hydrogeology

5.2.1. GRT3D

Participants: Édouard Canot, Jocelyne Erhel [correspondant].

- Version: version 2.0, April 2014
- APP: registered
- Programming language: C
- Abstract: Reactive transport modeling has become an essential tool for understanding complex environmental problems. It is an important issue for MoMaS and C2S@EXA partners (see sections 7.2.5, 7.2.3), in particular Andra. We have developed a method coupling transport and chemistry, based on a method of lines such that spatial discretization leads to a semi-discrete system of algebraic differential equations (DAE system). The main advantage is to use a complex DAE solver, which controls simultaneously the timestep and the convergence of Newton algorithm. The approach SIA uses a fixed-point method to solve the nonlinear system at each timestep, whereas the approach SNIA uses an explicit scheme.

  The software suite GRT3D has four executable modules:

  – SIA1D: Sequential Iterative Approach for 1D domains;
  – GDAE1D: Global DAE approach for 1D domains;
  – SNIA3D: Sequential Non Iterative Approach for 1D, 2D or 3D domains.
  – GDAE3D: Global DAE approach for 1D, 2D or 3D domains. This module has three variants: the original one with logarithms, an optimized one still with logarithms, an optimized one which does not use logarithms.
- Current work: extension of the chemistry module and parallelization.

5.2.2. SBM

Participant: Géraldine Pichot [correspondant].

- Version: version 1.0, November 2013
- Programming language: C
- Abstract: SBM (Skew Brownian Motion) is a code developed with A. Lejay (Inria, Nancy). This code allows exact or approximated simulations of the Skew Brownian Motion. This code is used for the simulation, with a Monte-Carlo approach, of a 1D diffusion process with a discontinuous diffusion coefficient. Several benchmark tests are also implemented.
- Current work: paper about benchmarking results 5.2.2.

5.2.3. GENFIELD

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel, Grégoire Lecourt, Géraldine Pichot [correspondant].

- Version: version 1.0, December 2014
- Programming language: C++
- Abstract: GENFIELD allows the generation of log-normal correlated fields. It is based on a spectral method and uses the FFTW library. Parallelism is implemented using MPI communications. GENFIELD is used in hydrogeology to model natural fields, like hydraulic conductivity or porosity fields.
- Current work: paper about algorithms 6.4.7.

5.3. High Performance Scientific Computing

5.3.1. PALMTREE

Participants: Lionel Lenôtre [correspondant], Géraldine Pichot.

- Version: version 1.0, November 2013
- Programming language: C++
- Abstract: We present an easy-to-use package for the parallelization of Lagrangian methods for partial differential equations. In addition to the reduction of computation time, the code aims at satisfying three properties:
  - simplicity: the user just has to add the algorithm governing the behaviour of the particles.
  - portability: the possibility to use the package with any compiler and OS.
  - action-replay: the ability of the package to replay a selected batch of particles.

  The last property allows the user to replay and capture the whole sample path for selected particles of a batch. This feature is very useful for debugging and catching some relevant information.
- Current work: paper about performance results.

5.3.2. MUESLI

Participant: Édouard Canot [corresponding author].

Muesli is a library designed to help in coding scientific problems in Fortran using a vector-oriented syntax like Matlab. One of its aims is therefore to speed-up the development process. It contains all the necessary materials to work numerically with a dynamic array (dynamic in size, shape, type, and storage structure), called mfArray. Muesli includes all or some parts of the following numerical libraries: Blas and Lapack, Arpack, Minpack, Slatec, Sparskit, SuiteSparse, Metis, Triangle, RngStreams, and other routines based on ACM algorithms.

The key points of Muesli is to efficiently solve large ODE/DAE systems (which come from, e.g., PDE problems after using the method of lines) or large non-linear minimization problems (where Jacobian matrices can be provided in a sparse format). The user can easily monitor the whole integration process and have access to tools to fix the singularity of the system of equations.

The lastest version of Muesli is 2.9.5 (2014-10-03). More information can be found at: http://people.irisa.fr/Edouard.Canot/muesli.

5.3.3. Zohour

Participant: Édouard Canot [correspondant].

Zohour is a node-based adaptive 2D mesh algorithm, written in Fortran 2003. A basic rectangular, regular set of nodes is recursively refined. Then the cells come from the Voronoi tessellation. While the domain is currently limited to a rectangular shape, its strength is three-fold:

- first, computing the flux via a Finite Element or Finite Volume method is both simple and accurate because each cell-side of cells is the bisection of two nodes;
- second, the transition between zones of different levels of refinement is more progressive than other methods, leading to a smaller number of nodes for the whole mesh;
- third, during successive refinements when dealing with a transient problem, interpolation is needed only by the new nodes, limiting the numerical errors.

It is planned for use in the HeMaTiS code (5.4.1) in order to get a refined mesh zone around the phase change surface.

See also the web page http://people.irisa.fr/Edouard.Canot/zohour.

5.4. Heat diffusion in soils

5.4.1. HeMaTiS

Participants: Édouard Canot [correspondant], Salwa Mansour.

HeMaTiS (**He**at and **Ma**ss **T**ransfer **i**n **S**oils) is a set of Finite Volume programs (variants concern different geometrical configurations: 1D, 1D-radial, 2D, 3D-axisymmetric) for computing the transient heat diffusion in soils when there is a phase change of water. Currently, the soil is modelled by a heterogeneous porous medium having constant thermo-physical properties, and the porous medium is saturated with water. The phase change is treated by means of the Apparent Heat Capacity method. In the near future, we plan to use an unsaturated model (but limited to small water content), and an effective thermal conductivity which depends on the local humidity (this latter law may reveal hysteresis behaviour). The software is written in Fortran 95 and is based on the Muesli library (5.3.2). A Computer Algebra System (Maple or Maxima) is used to compute the Jacobian matrix.

5.4.2. TPIP

Participants: Édouard Canot [correspondant], Salwa Mansour.

TPIP (**T**hermal **P**roperties by **I**nverse **P**roblem) is a program which aims at estimating the thermo-physical of a saturated porous medium after a strong heating which leads to the phase change of the water contained in the pores, knowing the experimental heating curves history at few selected points. The least-square criterion is used, in which sensitivity coefficients are the solution of a huge, complex PDE system in order to take into account the phase change of water. These equations for the sensitivity coefficients are therefore obtained via a Computer Algebra System (Maple or Maxima). In many aspects, the forward problem is similar to the HeMaTiS code (5.4.1), and like it, is based on Muesli (5.3.2). Two different minimization algorithms may be used, Damped Gauss-Newton or Levenberg-Marquardt. A special procedure has been applied in order to obtain a robust convergence, by changing some parameters of the forward problem during the iterations.

5.4.3. GLiMuH

Participants: Édouard Canot [correspondant], Salwa Mansour.

The GLiMuH code (**G**rains with **Li**quid **M**eniscus **u**nder **H**eating) is devoted to the understanding of how heat diffuses in an assembly of solid grains separated by air and water. In the pendular regime, the quantity of water is very small, leading to liquid bridges between the grains. In the current approximation, the grains are spherical in shape, and the numerical simulation is done in a 3D axisymmetric coordinate system. The shape of the liquid/gas interface is computed by integrating a differential algebraic system of equations, with a given quantity of water per unit volume of the porous medium, and under the constraint of a given contact angle between the liquid/gas interface and the solid boundaries. The numerical results allow us to estimate the effective thermal conductivity of a real wet granular medium, which is required to establish more realistic models for the HeMaTiS code (5.4.1).

6. New Results

6.1. Highlights of the Year

Lionel Lenôtre and his co-authors revisited in a very efficient way the Hastings-Metropolis Algorithm on Markov Chains for Small-Probability Estimation.

6.2. Numerical algorithms

6.2.1. Hybrid algebraic sparse linear solvers

Participants: Jocelyne Erhel, David Imberti.

Grants and projects: EXA2CT 7.3.1, C2S@EXA 7.2.3

Publications: [17]

Abstract: Sparse linear systems arise in computational science and engineering. The goal is to reduce the memory requirements and the computational cost, by means of high performance computing algorithms. Krylov methods combined with Domain Decomposition are very efficient. Numerical results show the benefits of our methodology.

6.2.2. GMRES and Polynomial Equivalence

Participant: David Imberti.

Grants and projects: EXA2CT 7.3.1, C2S@EXA 7.2.3

Publications: in preparation.

Abstract: We have established a theoretical link between GMRES and the much simpler problem of polynomial evaluation along with some algebraic structures to describe the most important elements of the GMRES algorithm. We use these structures to show the connection between sequential GMRES and Horner's Rule, s-step GMRES and Dorn's rule, and predict future possible GMRES-like algorithms.

6.2.3. Variables s-step GMRES

Participant: David Imberti.

Grants and projects: EXA2CT 7.3.1, C2S@EXA 7.2.3

Publications: in preparation.

Abstract: We introduce a new variation on s-step GMRES in order to improve its stability, reduce the number of iterations necessary to ensure convergence, and thereby improve parallel performance. In doing so, we develop a new block variant that allows us to express the stability difficulties in s-step GMRES more fully. We use the algebraic structures previous established via the polynomial equivalence to support an intuitive choice for the variation in the s-step procedure, and reinforce its utility in some communication cost estimates.

6.2.4. FGMRES dynamics

Participant: David Imberti.

Grants and projects: EXA2CT 7.3.1, C2S@EXA 7.2.3

Publications: in preparation.

Abstract: The FGMRES algorithm has met with varying success and we detail theoretical relationships between FGMRES and GMRES including a geometric mean conjecture. Further, we build on the current literature regarding GMRES convergence with an analysis of the dynamical properties of FGMRES.

6.2.5. RPM Coupling Factors

Participant: David Imberti.

Grants and projects: EXA2CT 7.3.1, C2S@EXA 7.2.3

Publications: in preparation.

Abstract: We have improved the Recursive Projection Method (RPM) with a subspace version that effectively utilizes parallelism. Furthermore, we include a discussion, numerical experiments, and suggestions for the heretofor neglected coupling factor in RPM, and how they influence convergence of the algorithm.

6.2.6. Hastings-Metropolis Algorithm on Markov Chains for Small-Probability Estimation

Participant: Lionel Lenôtre.

Grants: H2MNO4 7.2.1

Publications: [13]

Abstract: Shielding studies in neutron transport, with Monte Carlo codes, yield challenging problems of small-probability estimation. The particularity of these studies is that the small probability to estimate is formulated in terms of the distribution of a Markov chain, instead of that of a random vector in more classical cases. Thus, it is not straightforward to adapt classical statistical methods, for estimating small probabilities involving random vectors, to these neutron-transport problems. A recent interacting-particle method for small-probability estimation, relying on the Hastings-Metropolis algorithm, is presented. It is shown how to adapt the Hastings-Metropolis algorithm when dealing with Markov chains. A convergence result is also shown. Then, the practical implementation of the resulting method for small-probability estimation is treated in details, for a Monte Carlo shielding study. Finally, it is shown, for this study, that the proposed interacting-particle method considerably outperforms a simple Monte Carlo method, when the probability to estimate is small.

6.2.7. A Strategy for the Parallel Implementations of Stochastic Lagrangian Methods

Participant: Lionel Lenôtre.

Grants: H2MNO4 7.2.1

Software: PALMTREE 5.3.1

Publications: [34]

Abstract: We present some investigations on the parallelization of a stochastic Lagrangian simulation. For the self sufficiency of this work, we start by recalling the stochastic methods used to solve Parabolic Partial Differential Equations with a few physical remarks. Then, we exhibit different object-oriented ideas for such methods. In order to clearly illustrate these ideas, we give an overview of the library PALMTREE that we developed. After these considerations, we discuss the importance of the management of random numbers and argue for the choice of a particular strategy. To support our point, we show some numerical experiments of this approach, and display a speedup curve of PALMTREE. Then, we discuss the problem in managing the parallelization scheme. Finally, we analyze the parallelization of hybrid simulation for a system of Partial Differential Equations. We use some works done in hydrogeology to demonstrate the power of such a concept to avoid numerical diffusion in the solution of Fokker-Planck Equations and investigate the problem of parallelizing scheme under the constraint entailed by domain decomposition. We conclude with a presentation of the latest design that was created for PALMTREE and give a sketch of the possible work to get a powerful parallelized scheme.

6.3. Numerical models and simulations applied to physics

6.3.1. Small scale modeling of porous media

Participants: Édouard Canot, Salwa Mansour.

Grants: ARPHYMAT 7.4.3, 7.4.4

Software: GLiMuH 5.4.3

Publications: [22]

Abstract: This study is devoted to the heat transfer between two spherical grains separated by a small gap; dry air is located around the grains and a liquid water meniscus is supposed to be present between them. This problem can be seen as a micro-scale cell of an assembly of solid grains, for which we are looking for the effective thermal conductivity. For a fixed contact angle and according to the volume of the liquid meniscus, two different shapes are possible for the meniscus, giving a “contacting” state (when the liquid makes a true bridge between the two spheres) and a “non-contacting” one (when the liquid is split in two different drops, separated by a thin air layer); the transition between these two states occurs at different times when increasing or decreasing the liquid volume, thus leading to a hysteresis behavior when computing the thermal flux across the domain.

6.3.2. Heat and mass transfer modeling in porous media

Participants: Édouard Canot, Salwa Mansour.

Grants: HYDRINV 7.4.5

Software: HeMaTiS (5.4.1)

Abstract: The physical model of the HeMaTiS code (5.4.1) has been recently improved by adding the diffusion process of dry air through the water steam which is created by the evaporation of the water inside the porous medium. In this fashion, not only can the heating stage of the surface of the soil be simulated but also the cooling stage. The application concerns the study of archaeological fires which were used many times a day; the possibility of alternation of heating and cooling may lead to a better interpretation of residual marks left in the ground. Work is in progress to validate the numerical results.

6.3.3. Inverse problem for determining the thermo-physical properties of a porous media

Participants: Édouard Canot, Salwa Mansour.

Grants: HYDRINV 7.4.5

Software: TPIP (5.4.2)

Publications: [23]

Abstract: This study concerns the inverse problem which consists of the estimation of thermophysical properties of the soil knowing the temperature at few selected points of the domain. In order to solve this inverse problem, we used the least square criterion where we try to minimize the error function between real measures and simulated ones. The coupled system composed of the energy equation together with the three sensitivity boundary initial problems resulting from differentiating the basic energy equation with respect to the soil properties must be solved. To overcome the stiffness of our problem (due to the use of Apparent Heat Capacity method), the high nonlinearity of the coupled system and the problem of large residuals we used the Damped Gauss Newton and Levenberg-Marquardt methods. Moreover, we emphasized on the importance of the choice of ΔT (temperature range over which the phase change occurs) where for a certain initial guess the inverse problem fails to converge. We overcome this problem by chaining the inverse problems using different values of ΔT and parameters' set.

6.3.4. Geodesy

Participant: Bernard Philippe.

Grants: LIRIMA-EPIC 7.4.2.

Publications: [12].

Abstract: We solve a geodetic inverse problem for the determination of a distribution of point masses (characterized by their intensities and positions), such that the potential generated by them best approximates a given potential field.

6.4. Models and simulations for flow and transport in porous media

6.4.1. Simulating Diffusion Processes in Discontinuous Media: Benchmark Tests

Participant: Géraldine Pichot.

Grants: H2MN04 7.2.1

Software: SBM 5.2.2

Publications: [33]

Abstract: We present several benchmark tests for Monte Carlo methods for simulating diffusion in one-dimensional discontinuous media, such as the ones arising the geophysics and many other domains. These benchmarks tests are developed according to their physical, statistical, analytic and numerical relevance. We then perform a systematic study on four numerical methods.

6.4.2. Uncertainty Quantification and High Performance Computing for flow and transport in porous media

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel.

Grants: HYDRINV 7.4.5, H2MN04 7.2.1

Publications: [18]

Abstract: Stochastic models use random fields to represent heterogeneous porous media. Quantities of interest such as macro dispersion are then analyzed from a statistical point of view. In order to get asymptotic values, large scale simulations must be performed, using High Performance Computing. Non-intrusive methods are well-suited for two-level parallelism. Indeed, for each simulation, parallelism is based on domain decomposition for generating the random input and the flow matrix, parallel linear solvers and parallel particle tracker. Also, several simulations, corresponding to randomly drawn samples, can run in parallel. The balance between these two levels depends on the resources available. The software PARADIS implements flow and transport with random data and computation of macro dispersion. Simulations run on supercomputers with large 3D domains.

6.4.3. Computation of macro spreading in 3D porous media with uncertain data

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel, Mestapha Oumouni.

Grants: HYDRINV 7.4.5, H2MN04 7.2.1

Publications: [15]

Abstract: We consider an heterogeneous porous media where the conductivity is described by probability laws. Thus the velocity, which is solution of the flow equation, is also a random field, taken as input in the transport equation of a solute. The objective is to get statistics about the spreading and the macro dispersion of the solute. We use a mixed finite element method to compute the velocity and a lagrangian method to compute the spreading. Uncertainty is dealt with a classical Monte-Carlo method, which is well-suited for high heterogeneities and small correlation lengths. We give an explicit formulation of the macro dispersion and a priori error estimates. Numerical experiments with large 3D domains are done with the software PARADIS of the platform H2OLab.

6.4.4. A combined collocation and Monte-Carlo method for advection-diffusion equation of a solute in random porous media

Participants: Jocelyne Erhel, Mestapha Oumouni.

Grants: HYDRINV 7.4.5, H2MN04 7.2.1

Publications: [14]

Abstract: In this work, we present a numerical analysis of a method which combines a deterministic and a probabilistic approaches to quantify the migration of a contaminant, under the presence of uncertainty on the permeability of the porous medium. More precisely, we consider the flow equation in a random porous medium coupled with the advection-diffusion equation. Quantities of interest are the mean spread and the mean dispersion of the solute. The means are approximated by a quadrature rule, based on a sparse grid defined by a truncated Karhunen-Loève expansion and a stochastic collocation method. For each grid point, the flow model is solved with a mixed finite element method in the physical space and the advection-diffusion equation is solved with a probabilistic Lagrangian method. The spread and the dispersion are expressed as functions of a stochastic process. A priori error estimates are established on the mean of the spread and the dispersion.

6.4.5. An adaptive sparse grid method for elliptic PDEs with stochastic coefficients

Participants: Jocelyne Erhel, Mestapha Oumouni.

Grants: HYDRINV 7.4.5, H2MN04 7.2.1

Publications: [31].

Abstract: The stochastic collocation method based on the anisotropic sparse grid has become a significant tool to solve partial differential equations with stochastic inputs. The aim is to seek a vector of weights and a convenient level of interpolation for the method. The classical approach uses an a posteriori approach on the solution, which causes an additional prohibitive cost.

In this work, we discuss an adaptive approach of this method to calculate the statistics of the solution. It is based on an adaptive approximation of the *inverse* diffusion parameter. We construct an efficient error indicator which is an upper bound of the error on the solution. In the case of unbounded variables, we use an appropriate error estimation to compute suitable weights for the method. Numerical examples are presented to confirm the efficiency of the approach, and to show that the cost is considerably reduced without loss of accuracy.

6.4.6. Numerical analysis of stochastic advection-diffusion equation via Karhunen-Loève expansion

Participants: Jocelyne Erhel, Mestapha Oumouni.

Grants: HYDRINV 7.4.5, H2MN04 7.2.1

Publications: [32] , [25]

Abstract: In this work, we present a convergence analysis of a probabilistic approach to quantify the migration of a contaminant, under the presence of uncertainty on the permeability of the porous medium. More precisely, we consider the flow problem in a random porous medium coupled with the advection-diffusion equation and we are interested in the approximation of the mean spread and the dispersion of the solute. The conductivity field is represented by a Karhunen-Loève (K-L) decomposition of its logarithm. The flow model is solved using a mixed finite element method in the physical space. The advection-diffusion equation is computed thanks to a probabilistic Lagrangian method, where the concentration of the solute is the density function of a stochastic process. This process is solution of a stochastic differential equation (SDE), which is discretized using an Euler scheme. Then, the mean of the spread and dispersion are expressed as functions of the approximate stochastic process. A priori error estimates are established on the mean of the spread and of the dispersion. Numerical examples show the effectiveness of this approach.

6.4.7. About a generation of a log-normal correlated field

Participants: Jocelyne Erhel, Mestapha Oumouni.

Grants: HYDRINV 7.4.5, H2MN04 7.2.1

Software: GENFIELD 5.2.3

Publications: in preparation

Abstract: Uncertainty quantification often requires the generation of large realizations of stationary Gaussian random field over a regular grid.

This paper compares and analyzes the commonalities between the methods and approaches for simulating stationary Gaussian random field. The continuous spectral method is the classical approach which discretizes its spectral density to construct an approximation of the field. When the spectral density and the covariance functions decrease rapidly to zero at infinity, we prove that the spectral method is computationally attractive.

We compare also the classical methods used to simulate the field defined by its covariance function, namely the Discrete Spectral method, the Circulant Embedding approach, and the Discrete Karhunen-Loève approximation. We have found that under some assumptions on the covariance all these latter methods give the same simulations of a stationary Gaussian field on a regular grid, which are very efficient with the Fast Fourier Transform algorithm.

6.4.8. A global model for reactive transport

Participants: Édouard Canot, Jocelyne Erhel.

Grants: H2MN04 7.2.1, MOMAS 7.2.5, C2SEXA 7.2.3

Software: GRT3D 5.2.1

Thesis: [11]

Publications: [19], [16]

Abstract: In some scientific applications, such as groundwater studies, several processes are represented by coupled models. For example, numerical simulations are essential for studying the fate of contaminants in aquifers, for risk assessment and resources management. Chemical reactions must be coupled with advection and dispersion when modeling the contamination of aquifers. This coupled model combines partial differential equations with algebraic equations, in a so-called PDAE system, which is nonlinear. A classical approach is to follow a method of lines, where space is first discretized, leading to a semi-discrete differential algebraic system (DAE). Several methods have been designed for solving this system of PDAE.

In this study, we propose a global method which uses a DAE solver, where time is discretized by an implicit scheme. Then, each time step involves a nonlinear system of equations, solved by a modified Newton method. Thanks to the DAE solver, the time step is adaptively chosen in order to ensure accuracy and convergence. Moreover, the Jacobian in the nonlinear iterations is freezed as long as Newton converges fast enough, saving a lot of CPU time.

However, the size of the nonlinear system is quite large, because it involves both the differential and the algebraic variables. We show how to eliminate the differential variables, in order to reduce the size. This is equivalent to a so-called Direct Substitution Approach, but it keeps the nice features of DAE solvers.

Classicaly, the concentrations of chemical species are defined with their logarithms, assuming that they are strictly positive. This simplifies the computation of the mass action laws in the chemistry model and the computation of their derivatives. However, when a species does not exist, its concentration is replaced by a very small value and this may lead to an ill-conditioned Jacobian. We propose to use directly the concentrations, without logarithms, so that the Jacobian is then well-conditioned. Therefore, Newton method converges much faster without logarithms, allowing larger time steps and saving many computations.

We illustrate our method with two test cases, provided by the french agency for nuclear waste (ANDRA) and by the group MOMAS. We can compare our results with either analytical or other numerical solutions and show that our method is quite accurate. We also show that reducing the number of unknowns is very efficient and that dealing without logarithms reduces drastically the CPU time.

6.4.9. A chemistry model with precipitation-dissolution

Participant: Jocelyne Erhel.

Grants: H2MN04 7.2.1, MOMAS 7.2.5

Internship: Tangi Migot (Master M2, INSA and University, Rouen)

Publications: [36]

Abstract: In this study, we focus on precipitation and dissolution chemical reactions, because they induce numerical difficulties.

We consider a set of solute species and minerals, with precipitation occuring when a saturation threshold is reached. A challenge is to detect which minerals are dissolved and which minerals are precipitated. This depends on the total quantities of chemical species. We propose an analytical approach to build a phase diagram, which provides the interfaces between the different possible cases. We illustrate our method with three examples arising from brine media and acid mine drainage.

6.4.10. Coupled models for salted aquifers

Participants: Édouard Canot, Jocelyne Erhel.

Grants: H2MN04 7.2.1, MOMAS 7.2.5, HYDRINV 7.4.5

Software: GEODENS and SELSAUM (from Tunis)

Internship: Marwen ben Refifa (Ph-D, ENIT, Tunis)

Publications: in preparation

Abstract: We study gravity driven problems in salted aquifers, when many species are present together with high concentrations. In this framework, we couple flow, transport and chemistry by using a fixed point approach. We interfaced two codes developed in Tunis: GEODENS for density driven flow and transport, and SELSAUM for geochemistry. This latter provides also the density of salted water.

6.5. Models and simulations for flow in porous fractured media

6.5.1. A Graphical User Interface for simulating flow and transport in fractured-porous media

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel, Géraldine Pichot.

Grants: H2MNO4 7.2.1

Platform: H2OLab

Publications: [21]

Abstract: The platform H2OLab can be used with a Graphical User Interface, called H2OGuilde, which is developed using a Qt framework. Launchers correspond to a main program and to a hydrogeological application. These launchers call modules or libraries, implementing discretization schemes, solving algorithms, parallel communications, etc. The interface is generic for all the launchers. It is composed of three main tabs corresponding to the three steps of a simulation: entering input data, running computations, analyzing output data. Input parameters are classified in several categories, corresponding to the physical model and the numerical algorithms chosen. Output parameters are of three types, scalar, vector and matrix. Currently, visualization is done outside of the interface.

6.5.2. Meshing Strategies and the Impact of Finite Element Quality on the Velocity Field in Fractured Media

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel, Géraldine Pichot.

Grants: FRACINI 7.1.1

Platform: H2OLab

Publications: [20]

Abstract: For solving flow within a network of fractures, Mixed Hybrid Finite Element (MHFE) method is a method of choice as it yields a symmetric positive definite linear system. However, a drawback is its sensitivity to bad aspect ratio elements. For poor-quality triangles, elementary matrices are ill-conditioned and inconsistent velocity vectors are obtained by inverting these local matrices. In our presentation, we will present different strategies for a better reconstruction of the velocity field.

7. Partnerships and Cooperations

7.1. Regional Initiatives

7.1.1. Brittany council: FRACINI project

Participants: Jean-Raynald de Dreuzy, Jocelyne Erhel, Géraldine Pichot.

Contract with Brittany council
Duration: one year from December 2013.
Title: European initiative towards models and numerical methods for simulations in fractured-porous geological media.
Coordination: Géraldine Pichot.
Partners: Geosciences Rennes.

Web page: http://www.irisa.fr/sage/
Abstract: FRACINI is an initiative funded by the Région Bretagne. It aims at gathering researchers from the European community working on models and numerical methods for simulations in fractured-porous media. Two international workshops were organized in 2014. These workshops ended up with a proposal submitted in response to the Future and Emerging Technology (FET) call of H2020 Funding.

7.2. National Initiatives

7.2.1. ANR-MN: H2MNO4 project

Participants: Édouard Canot, Jocelyne Erhel, Grégoire Lecourt, Lionel Lenôtre, Géraldine Pichot.

Contract with ANR, program Modèles Numériques
Duration: four years from November 2012.
Title: Original Optimized Object Oriented Numerical Model for Heterogeneous Hydrogeology.
Coordination: Jocelyne Erhel and Géraldine Pichot, with Fabienne Cuyollaa.
Partners: Geosciences Rennes, University of Poitiers, University of Lyon 1, Andra, Itasca.
International collaborations: University of San Diego (USA), UPC, Barcelona (Spain)
Web page: http://h2mno4.inria.fr/
Abstract: The project H2MNO4 develops numerical models for reactive transport in heterogeneous media. It defines six mathematical and computational challenges and three applications for environmental problems with societal impact (see 6.4, 5.1.1). ANR organized a review of the project in December 2014.

7.2.2. Inria Project Lab: HEMERA project

Participants: Jocelyne Erhel, Géraldine Pichot.

Title: Hemera - developing large scale parallel and distributed experiments
Duration: September 2010 - July 2014
Coordination: C. Perez, Avalon team.
Partners: 22 Inria teams.
Webpage: http://www.grid5000.fr/mediawiki/index.php/Hemera
Abstract: Hemera is an Inria Project Lab, started in 2010, that aims at demonstrating ambitious up-scaling techniques for large scale distributed computing by carrying out several dimensioning experiments on the Grid'5000 infrastructure, at animating the scientific community around Grid'5000 and at enlarging the Grid'5000 community by helping newcomers to make use of Grid'5000. The final evaluation was in December 2014.

The team Sage was the leader of the Scientific Challenge Hydro: Multi-parametric intensive stochastic simulations for hydrogeology. The objective was to run multiparametric large scale simulations (see 6.4).

7.2.3. Inria Project Lab: C2S@EXA project

Participants: Édouard Canot, Jocelyne Erhel, Géraldine Pichot.

Title: C2S@EXA - Computer and Computational Scienecs at Exascale
Duration: from January 2012.
Coordination: S. Lanteri, Nachos team.
Partners: Inria teams working on HPC; external partners: ANDRA and CEA.
Webpage: http://www-sop.inria.fr/c2s_at_exa/
Abstract: The C2S@Exa Inria Project Lab is concerned with the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society (see 6.2, 6.4, 6.5). The team participated in several workshops.

7.2.4. GENCI: project on advanced linear solvers

Participants: Édouard Canot, Jocelyne Erhel, Grégoire Lecourt, Lionel Lenôtre, Géraldine Pichot.

Title: Scalabilité de méthodes numériques pour l'hydrogéologie
Duration: 2012
Coordination: J. Erhel and G. Pichot.
Webpage: http://www.genci.fr/
Abstract: To run large scale simulations, we defined a project, based on the platform H2OLab. We obtained and used computing time on machines located at GENCI supercomputing centers. (see 6.2, 6.4).

7.2.5. GDR MOMAS: project on reactive transport

Participant: Jocelyne Erhel.

Webpage: https://www.ljll.math.upmc.fr/cances/gdrmomas/

The working group MOMAS includes many partners from CNRS, Inria, universities, CEA, ANDRA, EDF and BRGM. It covers many subjects related to mathematical modeling and numerical simulations for nuclear waste disposal problems (see 6.4, 6.5). The team participated in workshops.

7.3. European Initiatives

7.3.1. FP7 & H2020: EXA2CT project

Type: FP7

Challenge: Special action

Instrument: Specific Targeted Research Project

Objective: Exascale computing platforms, software and applications

Duration: September 2013 - August 2016

Coordinator: S. Ashby, IMEC, Belgium

Partners: 10 partners

Inria contact: Luc Giraud

Web page: https://projects.imec.be/exa2ct/

Abstract: The goal of this project is to develop novel algorithms and programming models to tackle what will otherwise be a series of major obstacles to using a crucial component of many scientific codes at exascale, namely solvers and their constituents. The results of this work will be combined in running programs that demonstrate the application-targeted use of these algorithms and programming models in the form of proto-applications.

7.3.2. Collaborations with Major European Organizations

UPC: Universitat Politècnica de Catalunya-UPC, Institute of Environmental Assessment and Water Research (Spain)

numerical simulations in hydrogeology, reactive transport in heterogeneous media, upscaling, scientific software platform (see 5.1.1).

UFZ: Helmholtz Centre for Environmental Research-UFZ, Hydrogeology group (Germany)

numerical simulations in hydrogeology, flow in porous fractured media, scientific software platform

HPCLab: University of Patras, High Performance Information Systems Laboratory (Greece)

cooperation with B. Philippe in writing a book, and in common research on low rank approximations of matrix functions.

ERCIM: working group on numerical algorithms, high performance computing.

7.4. International Initiatives

7.4.1. LIRIMA laboratory: momappli team (Cameroon)

Participant: Bernard Philippe.

Program: Laboratoire International de Recherche en Informatique et Mathématiques Appliquées

Title: Modélisation Mathématique et Applications

Inria principal investigator: Bernard Philippe

International Partner (Institution - Laboratory - Researcher): University of Yaoundé, Cameroon - Norbert Noutchegueme

Duration: 2010-2014

See also: http://www.lirima.uninet.cm/index.php/recherche/equipes-de-recherche/momappli

Abstract: The team deals with high performance scientific computing, with a focus on reliable tools for localizing eigenvalues of large sparse matrices.

7.4.2. LIRIMA laboratory: EPIC team (Tunisia)

Participants: Édouard Canot, Jocelyne Erhel, Sinda Khalfallah, Bernard Philippe.

Program: Laboratoire International de Recherche en Informatique et Mathématiques Appliquées

Title: Problèmes Inverses et Contrôle

Inria principal investigator: Houssem Haddar, Defi team

International Partner (Institution - Laboratory - Researcher): ENIT, University of Tunis, Tunisia - LAMSIN - Amel ben Abda

Duration: 2011-2015

See also: http://www.lirima.uninet.cm/index.php/recherche/equipes-de-recherche/epic

Abstract: The team deals with nonlinear and inverse problems.

7.4.3. ECOS Sud (Argentina): ARPHYMAT project

Participant: Édouard Canot.

Program: COFECUB

Title: Processus de formation et transformation de structures de combustion archéologique

Inria principal investigator: Édouard CANOT

International Partner (Institution - Laboratory - Researcher): University of Buenos Aires (Argentina)

Duration: Jan 2012 - Dec 2014

Abstract: the project concerns numerical simulations of prehistoric fires and comparison with archaeological data in South America.

7.4.4. ECOS Sud (Chili): ARPHYMAT project

Participant: Édouard Canot.

Program: CONICYT

Title: Processus de formation et transformation de structures de combustion archéologique : un regard interdisciplinaire

Inria principal investigator: Édouard CANOT

International Partner (Institution - Laboratory - Researcher): Universidad de Tarapaca (Chili)

Duration: Jan 2014 - Dec 2016

Abstract: Multidisciplinary study of prehistoric fire traces in South America, by means of different approaches: taphonomy of the soil, physical processes involved during the heat transfer, modeling and numerical simulations.

7.4.5. Inria Euromediterranean: HYDRINV project

Participants: Édouard Canot, Jocelyne Erhel, Sinda Khalfallah, Bernard Philippe.

Program: Euromediterranean 3+3

Title: Direct and inverse problems in subsurface flow and transport

Coordination: H. ben Ameur, ENIT, Tunisia and J. Jaffré, Inria, Paris

Inria-Rennes principal investigator: Jocelyne Erhel

International Partners (Institution - Laboratory - Researcher):

Université Ibn Tofail - Faculté des Sciences de Kénitra (Morocco) - Laboratoire Interdisciplinaire en Ressources Naturelles et en Environnement - Zoubida Mghazli

Ecole Nationale d'Ingénieurs de Tunis (Tunisia) - Laboratoire de Modélisation en Hydraulique et Environnement - Rachida Bouhlila

Universidad de Sevilla (Spain) - Department Ecuaciones Diferenciales y Anâlisis Numérico - Tomas Chacon Rebollo

Universitat Politècnica de Catalunya (Spain) - Department of Geotechnical Engineering and Geo-Sciences - Xavier Sànchez Vila

University Centre of KHEMIS MILIANA (Algeria) - Laboratoire de l'Energie et des Systèmes Intelligents - Mohammed Hachama

Ecole Mohammadia d'Ingénieurs (Morocco) - LERMA - Rajae Aboulaich

Ecole Nationale d'Ingénieurs de Tunis (Tunisia) - Laboratoire de Modélisation Mathématique et Numérique dans les Sciences de l'Ingénieur - Hend Ben Ameur

Duration: Jan 2012 - Dec 2015

The management of water resources is a problem of great importance in all countries, and is particularly acute around the Mediterranean sea. The goal is to find a reasonable balance between these resources and demand while preserving the quality of water. Towards this goal it is essential to understand and simulate flow and transport in the subsurface. The science corresponding to this topic is hydrogeology. Since models become more and more complicated and quantitative answers must be given, numerical modeling become more and more sophisticated and mathematicians must also be involved. This project brings together hydrogeologists and mathematicians from France, Spain, Algeria, Morocco and Tunisia in order to develop, analyze, and validate numerical methods for several problems arising from modeling flow and transport in the subsurface. The emphasis is put on direct nonlinear problems (air-water flow, density driven flow related to salinization, transport with chemistry) and on inverse problems.

7.4.6. Joint supervision of S. Khalfallah's PhD (Tunisia)

Participants: Jocelyne Erhel, Sinda Khalfallah.

Program: International joint supervision of PhD agreement

Title: Contribution à l'analyse mathématique et numérique de quelques problèmes issus de l'hydrogéologie

Inria principal investigator: Jocelyne Erhel

International Partner (Institution - Laboratory - Researcher): Ecole Nationale d'Ingénieurs de Tunis - LAMSIN (Tunisia) - Amel ben Abda

Duration: 2010 - 2014

Abstract: The objective is to solve data completion problems applied to hydrogeology (see 7.4.5, 7.4.2).

7.4.7. Informal International Partners

University of Purdue (USA)
High Performance Scientific Computing
University of San Diego (USA)
Hydrogeology

7.5. International Research Visitors

7.5.1. Visits of International Scientists

- Emmanuel Kamgnia, University of Yaoundé, 2 months, March-April 2014
- Nabil Nassif, American University of Beirut, 1 week, May 2014
- Stratis Gallopoulos, Uiversity of Patras, 1 week, May 2014
- Ahmed Sameh, University of Purdue, 1 week, May 2014

7.5.2. Internships (Joint supervision of Ph-D students)

- Louis-Bernard Nguenang, University of Yaoundé, 4 months, April-July 2014
- Marwen ben Refifa, University of Tunis, 5 months, April-July and Sep 2014
- Salwa Mansour, Lebanese University, 8 months, Feb-Sep 2014

7.5.3. Visits to International Teams

- Édouard Canot, ENIT Tunis, Tunisia, 1 week, November 2014 (project HYDRINV)

8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Scientific committees and review of conferences

- J. Erhel is a member of the international advisory committee of the parallel CFD conferences (Trondheim, Norway, May 2014).
- J. Erhel was reviewer for the CARI conference.

8.1.2. Organization of workshops

- J. Erhel organized with Klaus Johannsen, from University of Bergen, the session "'High-performance computing, visualization and scientific workflow"', at the international conference "'Computational Methods in Water Resources (CMWR, Stuttgard, Germany, May 2014).
- G. Pichot organized two workshops in Rennes (April, 28-30, 2014 and June, 24-26, 2014) funded by the Brittany council (see 7.1.1) and Inria to prepare the Future and Emerging Technology (FET) Open proposal, called GEOPRISM, submitted in september 2014.
- G. Pichot organized with A. Fumagalli (Politecnico di Milano, Italy) a mini-symposium session (6 countries, 7 speakers) at the SIAM Annual Meeting AN14, within the SIAM Geosciences track, on *Modeling and Numerical Issues for fractured porous media.*.

8.1.3. Editorial Boards

- B. Philippe is one of the four chief-editors of the electronic journal ARIMA (revue Africaine de la Recherche en Informatique et Mathématiques Appliquées).
- B. Philippe is managing editor of the electronic journal ETNA (Electronic Transactions on Numerical Analysis).

- J. Erhel and G. Pichot are editors of the proceedings of Domain Decomposition XXI (LNCSE, Springer) [29]
- J. Erhel is member of the editorial board of ETNA.
- J. Erhel is member of the editorial board of ESAIM:Proceedings.

8.1.4. Steering committees

- J. Erhel is a member of the steering committee of the Réseau National des Systèmes Complexes.
- J. Erhel is the scientific coordinator of the website Interstices (since June 2012).
  See http://www.interstices.info.

8.1.5. Review of papers

- É. Canot was reviewer for the journals EABE, ASME-JHT.
- J. Erhel was reviewer for the journals ADWR, ETNA, SISC.
- M. Oumouni was reviewer for the journal JOMP.
- G. Pichot was reviewer for the journal ADWR.

8.1.6. Review of proposals

- J. Erhel was reviewer for proposals submitted to ACSPRF, ANR (ASTRID call), Shell-NWO-FOM.

8.1.7. Inria, IRISA and University committees

- É. Canot is member of the CLHSCT (Commité Local Hygiène Sécurité Conditions de Travail), of Inria-Rennes, from September 2010.
- J. Erhel was member of the Comité Technique d'Etablissement Public of Inria, until December 2014.
- J. Erhel was member of Conseil d'Administration of Inria, until December 2014.
- G. Pichot is responsible for the domain "environment" at IRISA.
- G. Pichot is member of the Conseil de département MAM of Polytech Lyon.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

- S. Khalfallah is teaching assistant (permanent position since September 2012) in mathematics at the University of Kairouan, Tunisia.
- L. Lenôtre is teaching assistant (contrat doctoral avec mission d'enseignement) in mathematics at the University of Rennes 1.
- É. Canot and J. Erhel: Master M2; title: Cours de modélisation et calcul scientifique; 12 hours; INSA, Rennes, France.
- É. Canot and G. Lecourt: Master M2; title: TP de modélisation et calcul scientifique; 12 hours; INSA, Rennes, France.
- É. Canot: Master M2; one week; ENIT, Tunis, Tunisia.

8.2.2. Supervision

PhD: S. Sabit, University of Rennes 1, May 2014, advisors J. Erhel with É. Canot.

PhD in progress: S. Khalfallah, University of Rennes 1 and University of Tunis, October 2009, co-advisors J. Erhel and A. ben Abda.

PhD in progress: L. Lenôtre, University of Rennes 1, October 2012, co-advisors A. Lejay (Inria Nancy) and G. Pichot, with J. Erhel.

PhD in progress: S. Mansour, University of Rennes 1 with LIU and AUB (Beiruth, Lebanon), January 2013, co-advisors É. Canot, M. Muhieddine and N. Nassif.

PhD in progress: L.-B. Nguenang, University of Yaoundé 1, October 2011, advisors E. Kamgnia with B. Philippe.

PhD in progress: M. ben Refifa, University of Tunis, October 2013, advisors Rachida Bouhlila with J. Erhel and É. Canot.

8.2.3. Juries

- PhD: S. Moufawad, University of Paris 6, Mathematics, December 2014. Reviewer J. Erhel.
- PhD: V. Vostrikov, University of Pau, Mathematics, December 2014. Reviewer and chair J. Erhel.
- PhD: S. Scialò, Politecnico di Torino, 2014. Reviewer G. Pichot.

8.3. Popularization

- J-R. de Dreuzy, J. Erhel and G. Pichot presented a poster entitled "Une eau souterraine très sollicitée", at Rencontres de la Transition Ecologique en Bretagne, January 2014 [39].
- J. Erhel gave a talk entitled "la terre se met aux maths", at lycée Descartes, Rennes, in March 2014 [38].
- J. Erhel participated in the panel on "Parle-t-on d'informatique comme on parle des autres sciences?", congrès SIF, Poitiers, France, Feb 2014
- The text "Henry Darcy et sa loi" from J. Erhel was published in the book brèves de maths [37]
- É. Canot, J. Erhel and L. Lenôtre, with M-O. Cordier, N. Lacaux, C. Lafon and J. Stainer, were in charge of the two stands Inria and Interstices at Village des sciences, Chartres de Bretagne, Sep 2014.
- J. Erhel and M-O. Cordier, with Espace des Sciences de Rennes, invited J.-P. Delahaye to celebrate the ten years of Interstices and to give a conference about the bitcoin, Rennes, October 2014.
- L. Lenôtre gave a talk at Conf'Lunch, Inria Rennes, December 2014.

9. Bibliography

Major publications by the team in recent years

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[2] J. CARRAYROU, J. HOFFMANN, P. KNABNER, S. KRÄUTLE, C. DE DIEULEVEULT, J. ERHEL, J. VAN DER LEE, V. LAGNEAU, K. MAYER, K. MACQUARRIE. *Comparison of numerical methods for simulating strongly non-linear and heterogeneous reactive transport problems. The MoMaS benchmark case*, in "Computational Geosciences", 2010, vol. 14, n^{o} 3, pp. 483-502

[3] P. CHARTIER, B. PHILIPPE. *A Parallel Shooting Technique for Solving Dissipative ODE's, Part 1: Theoretical Analysis; Part 2: Numerical Implementation*, in "Computing", 1993, vol. 51, n^{o} 3-4, pp. 209-236

[4] R. CHOQUET, J. ERHEL. *Newton-GMRES algorithm applied to compressible flows*, in "International Journal for Numerical Methods in Fluids", 1996, vol. 23, pp. 177-190

[5] M. CROUZEIX, B. PHILIPPE, M. SADKANE. *The Davidson Method*, in "SIAM, Journal on Scientific and Statistical Computing", 1994, vol. 15:1, pp. 62-76

[6] J.-R. DE DREUZY, A. BEAUDOIN, J. ERHEL. *Asymptotic dispersion in 2D heterogeneous porous media determined by parallel numerical simulations*, in "Water Resource Research", 2007, vol. 43, n^o W10439, doi:10.1029/2006WR005394

[7] J. ERHEL, S. RAULT. *Algorithme parallèle pour le calcul d'orbites : Parallélisation à travers le temps*, in "Technique et science informatiques", 2000, vol. 19, n^o 5

[8] H. HOTEIT, J. ERHEL, R. MOSÉ, B. PHILIPPE, P. ACKERER. *Numerical Reliability for Mixed Methods Applied to Flow Problems in Porous Media*, in "Computational Geosciences", 2002, vol. 6, pp. 161-194

[9] M. MUHIEDDINE, É. CANOT, R. MARCH, R. DELANNAY. *Coupling heat conduction and water-steam flow in a saturated porous medium*, in "International Journal for Numerical Methods in Engineering", 2011, vol. 85, n^o 11, pp. 1390-1414 [*DOI :* 10.1002/NME.3022]

[10] Y. SAAD, M. YEUNG, J. ERHEL, F. GUYOMARC'H. *A deflated version of the Conjugate Gradient Algorithm*, in "SIAM Journal on Scientific Computing", 2000, vol. 21, n^o 5, pp. 1909-1926

Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] S. SABIT. *Numerical methods for reactive transport*, Université Rennes 1, May 2014, https://tel.archives-ouvertes.fr/tel-01057870

Articles in International Peer-Reviewed Journals

[12] A. ABDELMOULA, M. MOAKHER, B. PHILIPPE. *A Slepian framework for the inverse problem of equivalent gravitational potential generated by discrete point masses*, in "Inverse Problems in Science and Engineering", 2014, 19 p. , https://hal.inria.fr/hal-00919094

[13] F. BACHOC, A. BACHOUCH, L. LENÔTRE. *Hastings-Metropolis Algorithm on Markov Chains for Small-Probability Estimation*, in "ESAIM: Proceedings", 2014, 33 p. , https://hal.inria.fr/hal-01058939

[14] J. ERHEL, Z. MGHAZLI, M. OUMOUNI. *A combined collocation and Monte Carlo method for advection-diffusion equation of a solute in random porous media* , in "ESAIM: Proceedings", 2014, vol. 45, pp. 328 - 337, https://hal.inria.fr/hal-01088570

Invited Conferences

[15] A. BEAUDOIN, J.-R. DE DREUZY, J. ERHEL, M. OUMOUNI. *Computation of macro spreading in 3D porous media with uncertain data*, in "SIAM Conference on Uncertainty Quantification", Savannah, United States, April 2014, https://hal.inria.fr/hal-01093101

[16] J. ERHEL. *A global reactive transport model*, in "Momas workshop", Marseille, France, November 2014, https://hal.inria.fr/hal-01093115

[17] J. ERHEL. *Parallel sparse linear solvers and applications in CFD*, in "Journée Calcul Intensif Distribué dans l'Industrie", Paris, France, January 2014, https://hal.inria.fr/hal-01093122

[18] J. ERHEL. *Uncertainty Quantification and High Performance Computing for flow and transport in porous media*, in "Workshop on Spatial Statistics and Uncertainty Quantification on Supercomputers", Bath, United Kingdom, May 2014, https://hal.inria.fr/hal-01093104

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