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Université Rennes 1

Activity Report 2015

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

Creation of the Project-Team: 2004 December 06, end of the Project-Team: 2015 December 31

Keywords:

Computer Science and Digital Science:

- 6. - Modeling, simulation and control
- 6.1. - Mathematical Modeling
- 6.2. - Scientific Computing, Numerical Analysis & Optimization
- 6.3. - Computation-data interaction
- 7. - Fundamental Algorithmics
- 7.1. - Parallel and distributed algorithms
- 7.12. - Computer arithmetic

Other Research Topics and Application Domains:

- 3. - Environment and planet
- 3.3. - Geosciences
- 3.3.1. - Earth and subsoil
- 4. - Energy
- 4.1. - Fossile energy production
- 4.2. - Renewable energy production
- 4.3. - Energy delivery
- 9. - Society and Knowledge
- 9.7. - Knowledge dissemination

1. Members

Research Scientists

Jocelyne Erhel [Team leader, Inria, Senior Researcher, HdR]

Édouard Canot [CNRS, Researcher]

Géraldine Pichot [Inria, Researcher, until August 2015]

Engineer

Yvan Crenner [Inria, from October 2015]

PhD Students

Lionel Lenôtre [University of Rennes 1, October 2012-December 2015]

Benjamin Delfino [Inria, from November 2015]

Salwa Mansour [Joint PhD with Lebanese International University and AUB, Lebanon, January 2013-December 2015]

Post-Doctoral Fellow

David Imberti [Inria, until May 2015]

Visiting Scientist

Jean-Raynald de Dreuzy [CNRS, Senior Researcher, Sage member from October 2013, HdR]

Administrative Assistant

Fabienne Cuyollaa [Inria]

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 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. Highlights of the Year

5.1. Highlights of the Year

The team SAGE ended in December 2015.

N. Nassif, J. Erhel and B. Philippe published a book entitled "introduction to computational linear algebra" [23]. E. Gallopoulos, B. Philippe and A. Sameh published a book entitled "Parallelism in Matrix Computations".

6. New Software and Platforms

6.1. GENFIELD

FUNCTIONAL DESCRIPTION

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

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

6.2. GLiMuH

Grains with Liquid Meniscus under Heating

FUNCTIONAL DESCRIPTION

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

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

6.3. GRT3D

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

APP: version 2.0, April 2014, registered

Programming language: C

Current work: refactoring

FUNCTIONAL DESCRIPTION

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

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

6.4. HeMaTiS

Heat and Mass Transfer in Soils

FUNCTIONAL DESCRIPTION

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

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

6.5. PALMTREE

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

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

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

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

6.6. SBM

Skew Brownian Motion

FUNCTIONAL DESCRIPTION

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

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

6.7. TPIP

Thermal Properties by Inverse Problem

FUNCTIONAL DESCRIPTION

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

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

6.8. Zohour

FUNCTIONAL DESCRIPTION

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

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

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

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

7. New Results

7.1. Numerical algorithms

7.1.1. Introduction to computational linear algebra

Participant: Jocelyne Erhel.

Publications: [23]

Abstract: The book "Introduction to Computational Linear Algebra" presents classroom-tested material on computational linear algebra and its application to numerical solutions of partial and ordinary differential equations. The book is designed for senior undergraduate students in mathematics and engineering as well as first-year graduate students in engineering and computational science.

The text first introduces BLAS operations of types 1, 2, and 3 adapted to a scientific computer environment, specifically MATLAB. It next covers the basic mathematical tools needed in numerical linear algebra and discusses classical material on Gauss decompositions as well as LU and Cholesky's factorizations of matrices. The text then shows how to solve linear least squares problems, provides a detailed numerical treatment of the algebraic eigenvalue problem, and discusses (indirect) iterative methods to solve a system of linear equations. The final chapter illustrates how to solve discretized sparse systems of linear equations. Each chapter ends with exercises and computer projects.

7.1.2. *Hybrid algebraic sparse linear solvers*

Participants: Jocelyne Erhel, David Imberti.

Grants and projects: EXA2CT 9.2.1, EoCoE 9.2.2, C2S@EXA 9.1.2

Publications: in preparation.

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 for both fast convergence and fast computations.

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

Participant: Lionel Lenôtre.

Grants: H2MNO4 9.1.1

Publications: [12]

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.

7.1.4. *A Strategy for the Parallel Implementations of Stochastic Lagrangian Methods*

Participant: Lionel Lenôtre.

Grants and projects: H2MNO4 9.1.1

Software: PALMTREE 6.5

Publications: [32]

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.

7.1.5. *About a generation of a log-normal correlated field*

Participants: Jocelyne Erhel, Géraldine Pichot.

Grants: HYDRINV 9.3.3, H2MN04 9.1.1

Software: GENFIELD 6.1

Publications: [18].

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

We compare 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 design and implement a parallel algorithm related to the Discrete Spectral method.

7.2. Numerical models and simulations applied to heat transfer

7.2.1. *Small scale modeling of porous media*

Participants: Édouard Canot, Salwa Mansour.

Grants: ECOS Sud Chili (ARPHYMAT project) 9.3.2

Software: GLiMuH 6.2

Publications: [13]

Conferences: [20]

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. We consider also another process where humidity varies, for example during an evaporation or condensation process; in this situation, the shape of the menisci changes a lot, because some liquid bridges may break, and this can strongly affect the effective thermal conductivity. Then, the reorganization of the liquid menisci is predicted, especially their surface area variation; it is an important parameter for a global model of the evaporation phenomenon in wet porous media.

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

Participants: Édouard Canot, Salwa Mansour.

Grants: HYDRINV 9.3.3

Software: TPIP (6.7)

Publications: [15], [27]

Conferences: [22]

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. To take into account uncertainties of the position of the sensors, some constraints have been added to the least square problem. Results are good when the number of sensors is sufficiently large.

7.2.3. *Evaporation/Condensation in a wet granular medium: the EWGM model*

Participants: Édouard Canot, Salwa Mansour.

Grants: ECOS Sud Chili (ARPHYMAT project) 9.3.2

Software: HeMaTis (6.4)

Publications: [26], [25]

Abstract: The physical model of the HeMaTiS code (6.4) has been completed by a new variant dedicated to the unsaturated case. The pendular regime concerns the special case where a very few quantity of liquid water is contained in a granular medium. The new model involves seven variables and can be considered as a two-phase two-component one; it contains both air and water, this latter component being liquid or gas. Generally, the diffusive transport of humidity in soils is extremely slow, we numerically show that humidity is convected quickly when the medium is subjected to a strong temperature gradient. The key feature of the thermal process is the simultaneous evaporation and condensation of water near a discontinuity of the liquid layout.

7.3. Models and simulations for skew diffusion

7.3.1. *Simulating Diffusion Processes in Discontinuous Media: Benchmark Tests*

Participant: Géraldine Pichot.

Grants: H2MN04 9.1.1

Software: SBM 6.6

Publications: submitted.

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.

7.3.2. *One-dimensional skew diffusions: explicit expressions of densities and resolvent kernel*

Participants: Lionel Lenôtre, Géraldine Pichot.

Grants: H2MN04 9.1.1

Publications: [31]

Abstract: The study of skew diffusion is of primary concern for their implication in the modeling and simulation of diffusion phenomenons in media with interfaces. First, we provide results on one-dimensional processes with discontinuous coefficients and their connections with the Feller theory of generators as well as the one of stochastic differential equations involving local time. Second, in view of developing new simulation techniques, we give a method to compute the density and the resolvent kernel of skew diffusions. Explicit closed-form are given for some particular cases.

7.3.3. Algorithms for the simulation of Feller processes

Participant: Lionel Lenôtre.

Grants and projects: H2MNO4 9.1.1.

Publications: [34].

Abstract: Two new numerical schemes are created for Skew Diffusions processes. Both algorithms rely on a more generic numerical scheme that can be used for any kind of Feller processes. The proof of convergence for this generic numerical scheme is performed.

7.3.4. Theoretical results on multidimensional Skew Diffusions

Participant: Lionel Lenôtre.

Grants and projects: H2MNO4 9.1.1.

Publications: [33].

Abstract: Some significant results on the distribution of the marginal processes of multidimensional Skew Diffusions are found together with new formula. In addition, totally analytical proofs of some results and algorithms given by A. Lejay are given.

7.4. Models and simulations for flow and transport in porous fractured media

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

Participant: Jocelyne Erhel.

Grants and projects: HYDRINV 9.3.3, H2MN04 9.1.1

Publications: [14].

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.

7.4.2. A global reactive transport model applied to the MoMaS benchmark

Participant: Jocelyne Erhel.

Grants and projects: H2MN04 9.1.1

Software: GRT3D 6.3

Publications: [19].

Abstract: Reactive transport models are very useful for groundwater studies such as water quality, safety analysis of waste disposal, remediation, and so on. The MoMaS group defined a benchmark with several test cases. We present results obtained with a global method and show through these results the efficiency of our numerical model.

7.4.3. About some numerical models for geochemistry

Participant: Jocelyne Erhel.

Grants and projects: H2MN04 9.1.1

Publications: [16], [17].

Abstract: Reactive transport models are very useful to study the fate of contaminants in groundwater. These models couple transport equations with geochemistry equations. In this talk, we focus on precipitation and dissolution chemical reactions, because they induce numerical difficulties.

We consider a set of solute species and minerals, with precipitation occurring 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.

7.4.4. Power-averaging method to characterize and upscale permeability in DFNs

Participants: Jean-Raynald de Dreuzy, Géraldine Pichot.

Publications: [21].

Abstract: In a lot of geological environments, permeability is dominated by the existence of fractures and by their degree of interconnections. Flow properties depend mainly on the statistical properties of the fracture population (length, apertures, orientation), on the network topology, as well as on some detailed properties within fracture planes. Based on an extensive analysis of 2D and 3D DFNs as well as on reference connectivity structures, we investigate the relation between the local fracture structures and the effective permeability. Defined as the relative weight between the two extreme harmonic and arithmetic means, the power-law averaging exponent gives a compact way to compare fracture network hydraulics. It may further lead to some comprehensive upscaling rules.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. ANDRA project

Participants: Yvan Crenner, Benjamin Delfino, Jean-Raynald de Dreuzy, Jocelyne Erhel.

Contract with ANDRA (National Agency for Nuclear Waste)

Duration: three years from November 2015.

Title: reactive transport in fractured porous media

Coordination: Jocelyne Erhel.

Partners: Geosciences Rennes.

Web page: <http://www.irisa.fr/sage/>

Abstract: Even in small numbers, fractures must be carefully considered for the geological disposal of radioactive wastes. They critically enhance diffusivity, speed up solute transport, extend mixing fronts and, in turn, modify the physicochemical conditions of reactivity around possible storage sites. Numerous studies in various fields have shown that fractures cannot be simply integrated within an equivalent porous medium with a simple enhancement of its petro-physical properties (porosity and permeability). We propose a combined numerical and experimental approach to determine the influence on reactivity of typical fracture patterns found in some radioactive waste applications.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR-MN: H2MNO4 project

Participants: Yvan Crenner, Benjamin Delfino, Jean-Raynald de Dreuzy, Jocelyne Erhel, 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 Cuyolla.

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. We organized a project meeting in February.

9.1.2. *Inria Project Lab: C2S@EXA project*

Participants: Édouard Canot, Yvan Crenner, Jocelyne Erhel, Géraldine Pichot.

Title: C2S@EXA - Computer and Computational Sciences 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. The team participated in several workshops.

9.1.3. *GENCI: project on advanced linear solvers*

Participants: Yvan Crenner, Jocelyne Erhel, David Imberti, Lionel Lenôtre, Géraldine Pichot.

Title: Numerical models for hydrogeology

Duration: 2015

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 and on a new GMRES solver. We obtained and used computing time on machines located at GENCI supercomputing centers.

9.1.4. *GDR MOMAS: projects on multiphase flow and reactive transport*

Participants: Benjamin Delfino, Jocelyne Erhel.

Title: Workshops on multiphase flow and reactive transport

Duration: 2015

Coordination: J. Erhel

Partner: IFPEN

Webpage: <http://www.irisa.fr/sage/RTworkshop> and <https://www.ljll.math.upmc.fr/cances/gdrmomas/>

Abstract: 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. The team participated in a workshop on multiphase flow and organized an international workshop on reactive transport, in Paris, with IFPEN.

9.2. European Initiatives

9.2.1. FP7 & H2020 Projects: EXA2CT project

Participants: Jocelyne Erhel, David Imberti.

Title: EXascale Algorithms and Advanced Computational Techniques

Programm: FP7

Duration: September 2013 - August 2016

Coordinator: S. Ashby, IMEC, Belgium

Partners:

Fraunhofer-Gesellschaft Zur Foerderung Der Angewandten Forschung E.V (Germany)

Interuniversitair Micro-Electronica Centrum Vzw (Belgium)

Intel Corporations (France)

Numerical Algorithms Group Ltd (United Kingdom)

Systems Solutions for Research (Germany)

Universiteit Antwerpen (Belgium)

Universita della Svizzera italiana (Switzerland)

Universite de Versailles Saint-Quentin-En-Yvelines. (France)

Vysoka Skola Banska - Technicka Univerzita Ostrava (Czech Republic)

Inria contact: Luc Giraud

Abstract: Numerical simulation is a crucial part of science and industry in Europe. The advancement of simulation as a discipline relies on increasingly compute intensive models that require more computational resources to run. This is the driver for the evolution to exascale. Due to limits in the increase in single processor performance, exascale machines will rely on massive parallelism on and off chip, with a complex hierarchy of resources. The large number of components and the machine complexity introduce severe problems for reliability and programmability. The former of these will require novel fault-aware algorithms and support software. In addition, the scale of the numerical models exacerbates the difficulties by making the use of more complex simulation algorithms necessary, for numerical stability reasons. A key example of this is increased reliance on solvers. Such solvers require global communication, which impacts scalability, and are often used with preconditioners, increasing complexity again. Unless there is a major rethink of the design of solver algorithms, their components and software structure, a large class of important numerical simulations will not scale beyond petascale. This in turn will hold back the development of European science and industry which will fail to reap the benefits from exascale. The EXA2CT project brings together experts at the cutting edge of the development of solvers, related algorithmic techniques, and HPC software architects for programming models and communication. It will take a revolutionary approach to exascale solvers and programming models, rather than the incremental approach of other projects. We will produce modular open source proto-applications that demonstrate the algorithms and programming techniques developed in the project, to help boot-strap the creation of genuine exascale codes.

9.2.2. FP7 & H2020 Projects: EOCOE project

Participant: Jocelyne Erhel.

Program: EINFRA-5-2015

Project acronym: EoCoE

Project title: Energy oriented Center of Excellence for computer applications

Duration: 36 months

Coordinator: CEA

Other partners: organisme, labo (pays) : 12 other partners

Abstract: the EoCoE objectives aims at firstly, to design, test and spread new methodological and organisational paradigms (Objectives 1, 3, and 4) driven by the users communities and, secondly, to contribute to mathematical and computer sciences challenges on the whole HPC tool chain (Objective 2).

9.3. International Initiatives

9.3.1. Inria International Labs: *LIRIMA Afrique, EPIC team (Tunisia)*

Participants: Édouard Canot, Jocelyne Erhel.

Program: Laboratoire International de Recherche en Informatique et Mathématiques Appliquées

Title: Problèmes Inverses et Contrôle

Inria principal investigator: Housseem 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.

9.3.2. International Program *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.

9.3.3. Inria *Euromediterranean: HYDRINV project*

Participants: Édouard Canot, Jocelyne Erhel.

Program: **Euromediterranean 3+3**

Title: Direct and inverse problems in subsurface flow and transport

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

Inria-Rennes principal investigator: Jocelyne Erhel

Duration: Jan 2012 - Dec 2015

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 Análisis Numérico - Tomas Chacon Rebollo

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

University Centre of KHEMIS MILIANA (Algeria) - Laboratoire de l'Énergie 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 Ameer

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.

9.4. International Research Visitors

9.4.1. Visits of International Scientists

- Nabil Nassif, American University of Beirut, Lebanon, April, 1 week
- Lamia Guellouz, ENIT, Tunisia, May, 1 week

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

- Marwen ben Refifa, University of Tunis, 5 months, April-July 2015
- Salwa Mansour, Lebanese University, 8 months, Feb-Sep 2015

9.4.3. Visits to International Teams

- Lionel Lenôtre visited Pr. Dr. Sylvie Roelly and her students at Potsdam University, Potsdam, Germany, one week, December 2015.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific events organization

- J. Erhel organized with T. Faney and A. Michel, from IFPEN, an international MoMaS workshop on reactive transport (Paris, France, November 2015).

10.1.2. Scientific events selection

- J. Erhel is a member of the international advisory committee of the parallel CFD conferences (Trondheim, Norway, May 2014).
- J. Erhel was a member of the scientific committee of the international conference MAMERN 2015 (Pau, France, June 2015).
- J. Erhel was a member of the program committee of the workshop Visualization in Environmental Sciences 2015 (co-event of EuroVis 2015, Cagliari, Italy, May 2015)

10.1.3. journals: editorial Boards

- J. Erhel is member of the editorial board of ETNA.
- J. Erhel is member of the editorial board of ESAIM:Proceedings and Surveys.
- J. Erhel is the scientific coordinator of the website Interstices (since June 2012).
See <https://www.interstices.info>.

10.1.4. Journals: Reviewing

- J. Erhel was reviewer for the journals ADWR, CONHYD, GMDD, LAA.
- L. Lenôtre was reviewer for the journal ETNA.
- M. Oumouni was reviewer for the journal JOMP.
- G. Pichot was reviewer for the journal Computers & Geosciences.

10.1.5. Review of proposals

- J. Erhel was reviewer for a proposal submitted to ICT15, Vienna Science and Technology fund.

10.1.6. Research administration

- É. Canot is member of the CLHSCT (Comité Local Hygiène Sécurité Conditions de Travail), of Inria-Rennes, from September 2010.
- J. Erhel is the correspondent of Maison de la Simulation for Inria Rennes.
- J. Erhel is the AMIES correspondent for Inria Rennes, from September 2015.
- J. Erhel was a member of the Inria local committee Post-Doc 2015.
- G. Pichot is responsible for the domain "environment" at IRISA, from June 2013 until August 2015.
- G. Pichot is member of the Conseil de département MAM of Polytech Lyon.
- G. Pichot was a member of the Inria local committee CORDI-S 2015.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

J. Erhel: Master M2; title: Cours de modélisation et calcul scientifique; 12 hours; INSA, Rennes, France.

É. Canot: Master M2; title: TP de modélisation et calcul scientifique; 12 hours; INSA, Rennes, France.

10.2.2. Supervision

PhD: L. Lenôtre, University of Rennes 1, November 2015, co-advisors A. Lejay (Inria Nancy) and G. Pichot, with J. Erhel.

PhD: S. Mansour, University of Rennes 1 with LIU and AUB (Beiruth, Lebanon), December 2015, co-advisors É. Canot, M. Muhieddine and N. Nassif.

PhD in progress: B. Delfino, University of Rennes 1, November 2015, co-advisors J.-R. de Dreuzy and J. Erhel.

PhD in progress: P.-M. Gibert, University of Lyon, October 2015, co-advisors D. Tromeur-Dervout and J. Erhel.

PhD in progress: M. ben Refifa, University of Tunis, October 2013, advisors R. Bouhlila and É. Canot.

10.2.3. Juries

- PhD: A. Abeduwia, University of Littoral Côte d'Opale (Calais), Mathematics, December 2015. Reviewer J. Erhel.
- PhD: C. Robinson, University of Rennes 1, Mathematics, December 2015. Committee member J. Erhel.
- HdR: A. Beaudoin, University of Poitiers, Geosciences, December 2015. Committee member J. Erhel.

10.3. Popularization

- J. Erhel is co-author of two documents published in Interstices, about modelling ice sheet evolution and estimating the contribution of Antarctica and Greenland to sea-level rise. [30], [29]
- J. Erhel was one of the coordinators of the Interstices publications devoted to climate change and COP21. She is co-author of the quiz on this subject. [28]
- J. Erhel gave a talk at the show "solutions COP21", held in Grand Palais, Paris, December 2015.
- J. Erhel contributed to the new version of the spelling book for computer science (l'informatique de A à Z), published in November 2015. She was one of the coordinators of the project and she wrote several cards.
- J. Erhel gave a talk in 180 seconds entitled "Enjeux pour les Eaux souterraines: Energie et Environnement", during the Inria scientific days, Nancy, June 2015.
- J. Erhel presented the challenges for groundwater at the meeting between Inria and Sénat, January 2015.
- L. Lenôtre gave a talk at "Lycée René Descartes de Rennes" on the diffusion phenomena and their underlying stochastic processes, February 2015.
- L. Lenôtre participated in the "Fête de la science de Rennes" at Inria stand.

11. Bibliography

Major publications by the team in recent years

- [1] K. BURRAGE, J. ERHEL. *On the performance of various adaptive preconditioned GMRES*, in "Numerical Linear Algebra with Applications", 1998, vol. 5, pp. 101-121
- [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

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Doctoral Dissertations and Habilitation Theses

- [11] L. LENÔTRE. *Study and Simulation of Skew Diffusion Processes*, Université Rennes 1, November 2015, <https://hal.inria.fr/tel-01247310>

Articles in International Peer-Reviewed Journals

- [12] F. BACHOC, A. BACHOUCH, L. LENÔTRE. *Hastings-Metropolis algorithm on Markov chains for small-probability estimation*, in "ESAIM: Proceedings", January 2015, vol. 48, 33 p. [DOI : 10.1051/PROC/201448013], <https://hal.inria.fr/hal-01058939>
- [13] E. CANOT, R. DELANNAY, S. MANSOUR, M. MUHIEDDINE, R. MARCH. *Effective thermal conductivity of a wet porous medium – Presence of hysteresis when modeling the spatial water distribution for the pendular régime*, in "ASME, Journal of Heat Transfert,", 2015, <https://hal.inria.fr/hal-01245690>
- [14] J. ERHEL, Z. MGHAZLI, M. OUMOUNI. *An adaptive sparse grid method for elliptic PDE with stochastic coefficients*, in "Computer Methods in Applied Mechanics and Engineering", 2015, 27 p. , <https://hal.inria.fr/hal-01199183>
- [15] S. MANSOUR, É. CANOT, M. MUHIEDDINE. *Identification of the Thermophysical Properties of the Soil by Inverse Problem*, in "ASME, Journal of Heat Transfert,", 2015, 9 p. , <https://hal.inria.fr/hal-01096787>

Invited Conferences

- [16] J. ERHEL, T. MIGOT. *About some numerical models for geochemistry*, in "6th International Conference on High Performance Scientific Computing", Hanoi, Vietnam, 2015, <https://hal.inria.fr/hal-01197268>
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Conferences without Proceedings

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- [21] J.-R. D. DREUZY, J. MAILLOT, C. DARCEL, P. DAVY, Y. MÉHEUST, G. PICHOT. *Power-averaging method to characterize and upscale permeability in DFNs*, in "AGU Fall Meeting 2015", San Francisco, United States, American Geophysical Union, December 2015, pp. H53I-03, <https://hal-insu.archives-ouvertes.fr/insu-01241866>
- [22] S. MANSOUR, É. CANOT, M. MUHIEDDINE, R. MARCH, J. A. CORDERO. *Estimation of the Thermophysical Properties of the Soil by Inverse Problem, using Experimental Data during Liquid/Vapour Phase Change*, in "InterPore 7th Conference on Porous Media", Padua, Italy, May 2015, <https://hal.inria.fr/hal-01245719>

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- [23] N. NASSIF, J. ERHEL, B. PHILIPPE. *introduction to computational linear algebra*, taylor and francis group, 2015, <https://hal.inria.fr/hal-01196689>
- [24] B. PHILIPPE, A. SAMEH, E. GALLOPOULOS. *Parallelism in Matrix Computations*, springer, 2016 [DOI : 10.1007/978-94-017-7188-7], <https://hal.inria.fr/hal-01257695>

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- [25] É. CANOT. *Le modèle EWGM : Implémentation numérique 1-D des variantes A et B*, IRISA, Équipe SAGE, 2015, 11 p. , <https://hal.inria.fr/hal-01245769>
- [26] É. CANOT, S. MANSOUR, R. DELANNAY. *Evaporation/Condensation of water in a granular medium, restricted to the pendular regime: the EWGM model*, IRISA, équipe SAGE, 2015, 18 p. , <https://hal.inria.fr/hal-01245758>
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Scientific Popularization

- [28] J. ERHEL, C. LEININGER, A. ROUSSEAU. *10 questions à propos de la COP21*, in "Interstices", 2015, <https://hal.inria.fr/hal-01247312>
- [29] M. NODET, J. ERHEL. *Des outils mathématiques pour prévoir la fonte des calottes polaires*, in "Interstices", 2015, <https://hal.inria.fr/hal-01247302>
- [30] M. NODET, J. ERHEL. *Modéliser et simuler la fonte des calottes polaires*, in "Interstices", 2015, <https://hal.inria.fr/hal-01247299>

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- [32] L. LENÔTRE. *A Strategy for Parallel Implementations of Stochastic Lagrangian Simulation*, November 2015, working paper or preprint, <https://hal.inria.fr/hal-01066410>
- [33] L. LENÔTRE. *Some functionals of n-dimensional skew diffusions*, October 2015, working paper or preprint, <https://hal.inria.fr/hal-01212628>
- [34] L. LENÔTRE. *Two numerical schemes for the simulation of skew diffusions using their resolvent kernel*, October 2015, working paper or preprint, <https://hal.inria.fr/hal-01206968>