Méthodes numériques pour des modèles couplés et stochastiques d'hydrogéologie

Journée GNR MOMAS / GDR CALCUL

J. Erhel, INRIA Rennes

L'eau potable en Bretagne:

➔ 70% eaux de surface

➔ Quelques captages profonds

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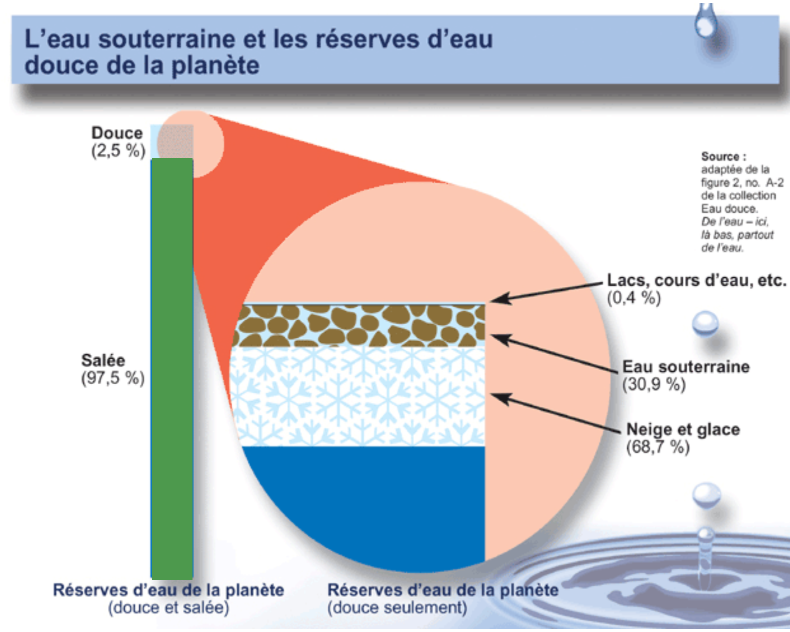

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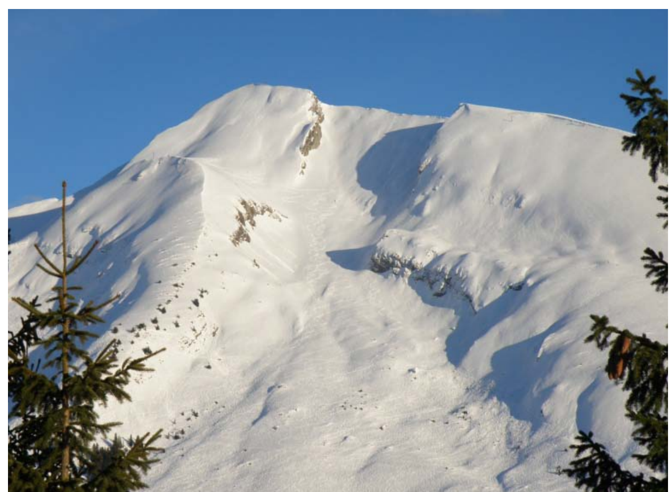


Groundwater numerical models

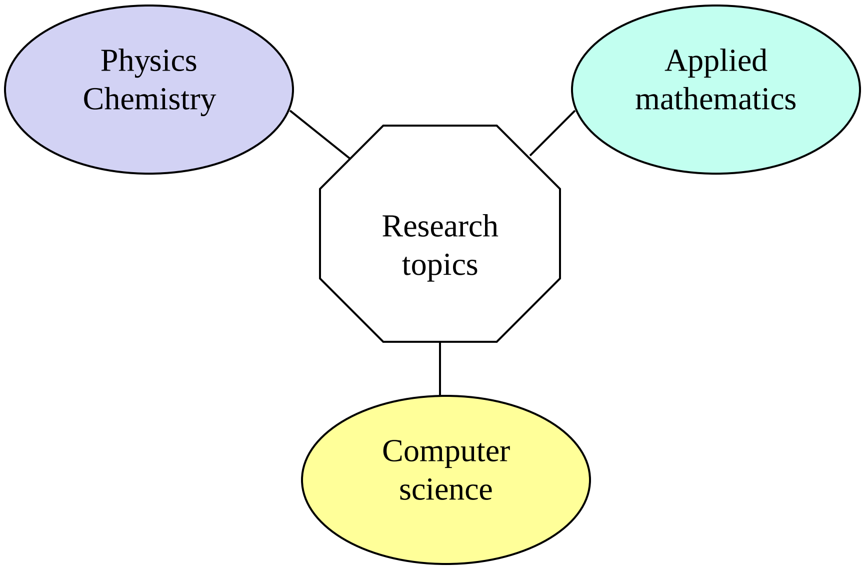
Societal impact

- Groundwater resources, pollution, remediation
- Nuclear waste storage

Scientific challenges

- Coupled nonlinear models
- Lack of data
- Heterogeneous data
- Large scale simulations

Multidisciplinary approach



Deterministic direct problems

data and process (problem statement; database)

coupled nonlinear continuous models (PDAE)
coupled nonlinear discrete model (discretization in space and time)
solving algorithm (linear and nonlinear solver, etc)

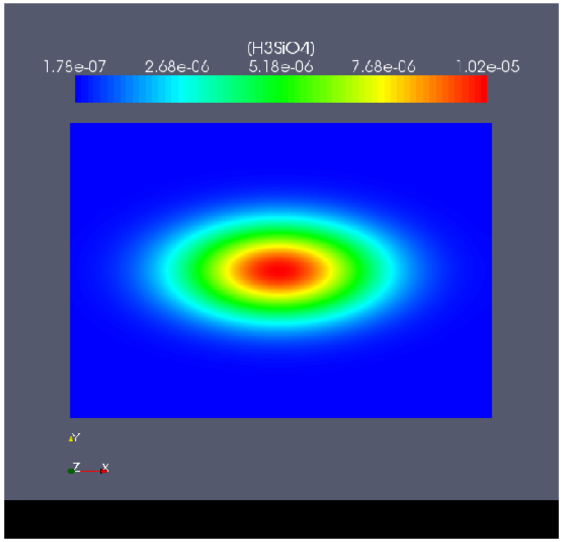
software engineering (development, debug, etc)
simulations (HPC, parallel and grid computing)

results (problem solution; database; validation)

Reactive transport models

Scientific context

• reactive transport: coupling solute transport by advection-dispersion and chemistry of aqueous and fixed species



Scientific achievements

• comparison of existing methods
• global method using a DAE solver
• simulations for Momas benchmark
• software GDAE-3D

Collaborations and technology transfer

• MOMAS: Strasbourg, Estime INRIA team, CEA
• ANDRA grant
• 3rd prize for benchmark Momas

Publications

• Ph-D thesis of C. de Dieuleveult
• JCP 2009, Comput. Geo. 2010 (2 papers)
• proceedings Parco 2006, Eccomas 2008

Global method for reactive transport using DAE

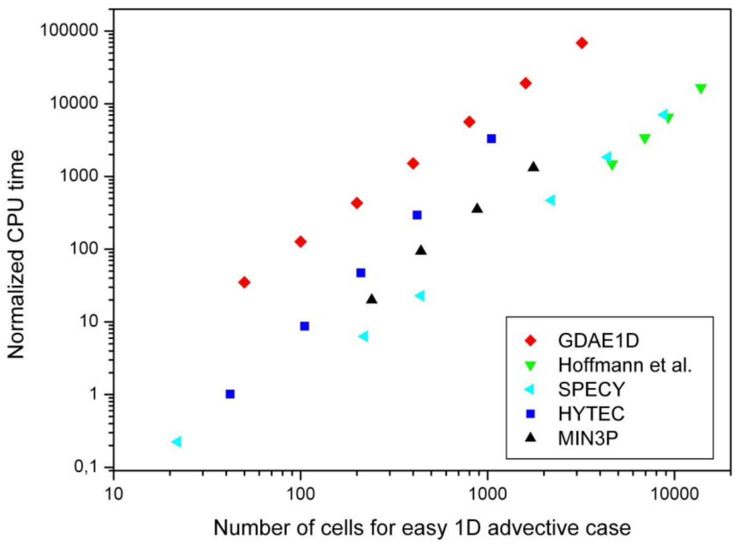
Methodology

- method of lines: spatial discretization then time discretization
- DAE system of index 1: transport and chemistry equations
- DAE solver: implicit BDF, variable order, variable timestep, control of accuracy
- embedded nonlinear solver: modified Newton, control of convergence
- currently explicit Jacobian and Newton-LU method
- libraries MT3D, SUNDIALS, UMFPACK

- Comparison with other methods
- SNIA and SIA: stability or convergence conditions
- SIA: slow convergence and nonlinear chemistry at each iteration
- DSA: adaptive timestep difficult to implement
- DSA: highly coupled nonlinear equations
- DAE: large sparse linear system and high CPU requirements

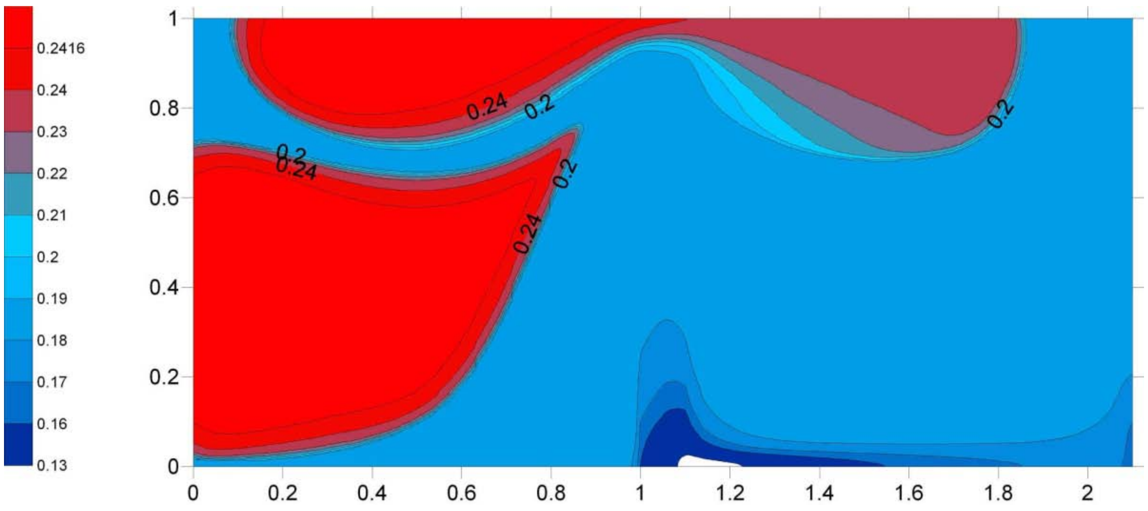
1D benchmark test case

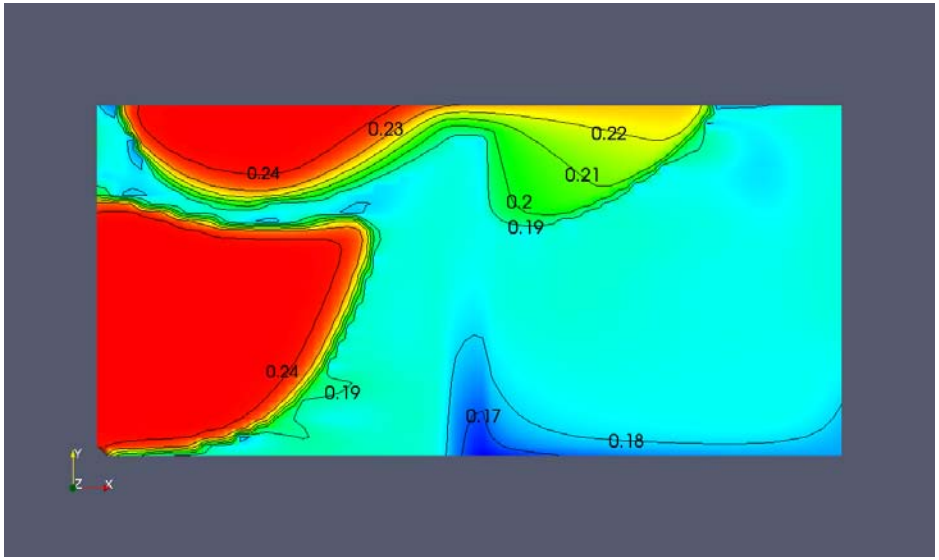
	Location of the peak	S concentration of the peak
GDAE1D	0.0175	0.966
Hoffmann et al.	0.0167	0.852
SPECY	0.0158	0.968
HYTEC	0.0170	0.286
MIN3P	0.0175	0.7248
Reference	0.01737	0.985
Mean	**0.0169**	**0.759**
Standard deviation	**$7.04\ 10^{-4}$**	**0.283**



GDAE is more accurate but slower than other methods

2D benchmark test case





One species among 13 at time t=1000
Top: Erlangen result with very fine mesh ; bottom: GDAE result with coarse mesh
Numerical dispersion due to the coarse mesh but accurate results

Perspectives for coupled models

Challenge

- reduction of CPU time in DAE methods (reduction of unknowns)
- reduction of numerical diffusion in transport and numerical dispersion
- adaptive mesh refinement
- reactive models with kinetics and precipitation-dissolution
- complex coupled models (non saturated zone, etc)

Collaboration and industrial transfer

- RISC-E network, Micas consortium, Momas group, Lille Univ
- Tunis, Barcelona, Leipzig
- Andra grant in negociation

Stochastic direct problems

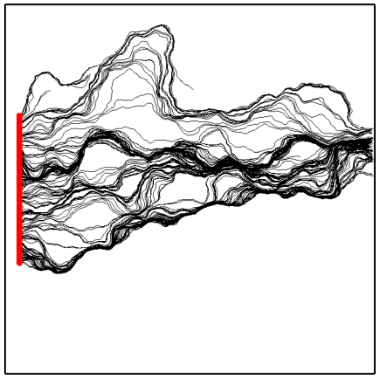
uncertain data and process (problem statement; database)

stochastic continuous models (PDAE)
stochastic discrete model (in probability, space and time)
solving algorithm (Uncertainty Quantification, solver, etc)

software engineering (development, debug, etc)
simulations (HPC, parallel and grid computing)

results (problem solution; database; statistics)

Macro dispersion models



Scientific context

• heterogeneous porous media : random field of permeability
• random velocity field given by flow model
• transport of an inert solute by advection and dispersion

Scientific achievements

• analysis of macro dispersion in 2D highly heterogeneous porous media
• reliable large scale simulations using HPC
• fast convergence of Monte-Carlo method
• software PARADIS

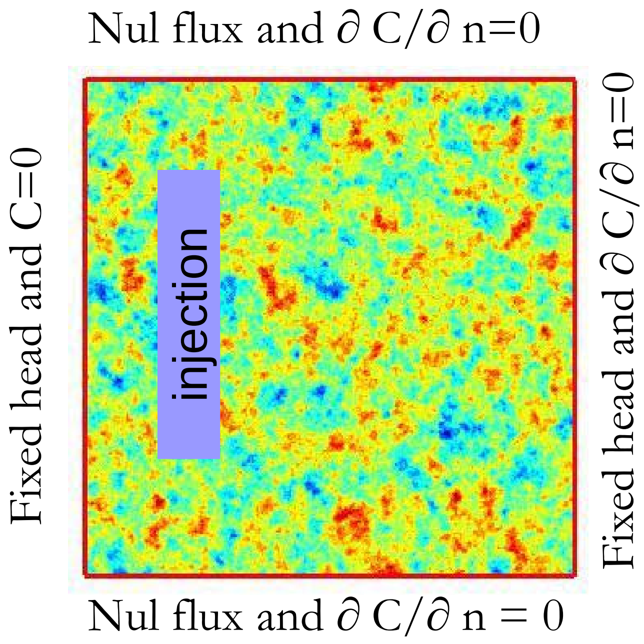
Collaborations and technology transfer

• MICAS ANR project: Univ. Le Havre, Geosciences Rennes, Univ. Lyon

Publications

• WRR 2007, WRR 2008
• proceedings Parco 2006, Eccomas 2006, EuroPar 2007, ParCFD 2007, ParCFD 2008, Mamern 2009

Macro dispersion: numerical models



- Random data

K log-normal and exponential correlation

- Flow equations

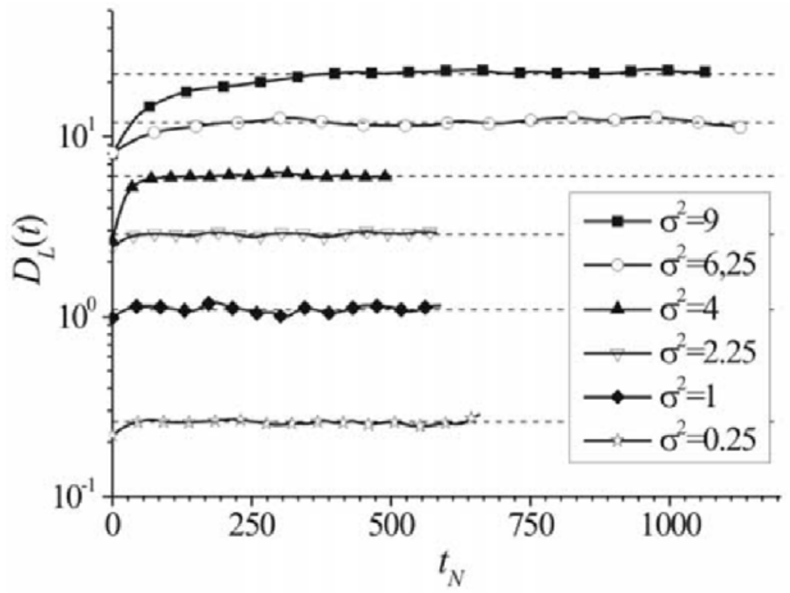
$$\epsilon V = -K \nabla h, \nabla . V = 0$$

- Advection-dispersion equations

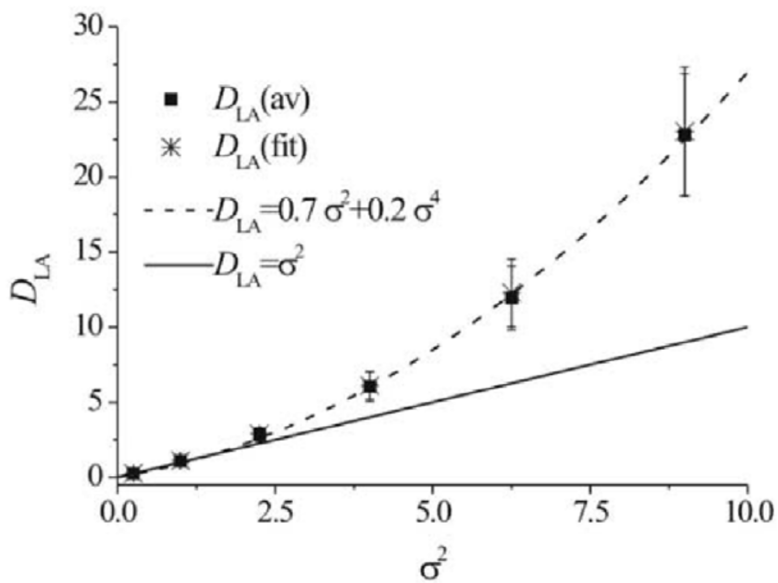
$$\frac{\partial(\epsilon c)}{\partial t} + \nabla.(\epsilon c V) - \nabla.(\epsilon d \nabla c) = 0$$

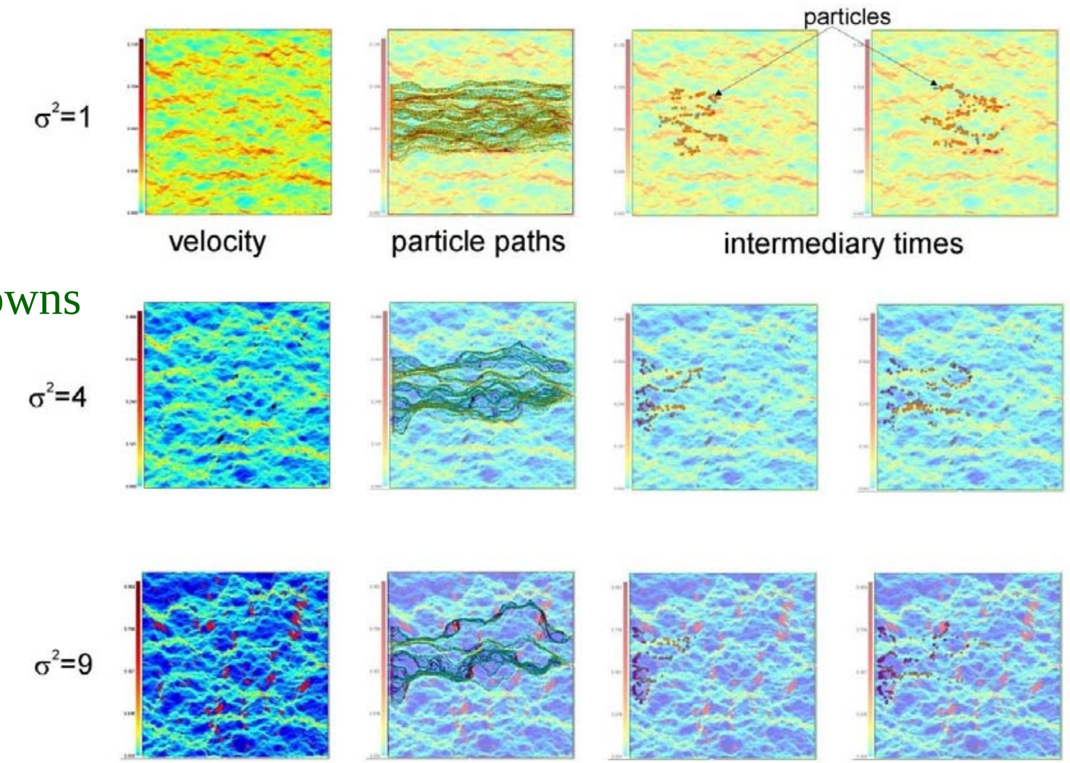
- Asymptotic behavior of dispersion coefficients ?
- Impact of heterogeneity factor σ and Peclet number Pe ?

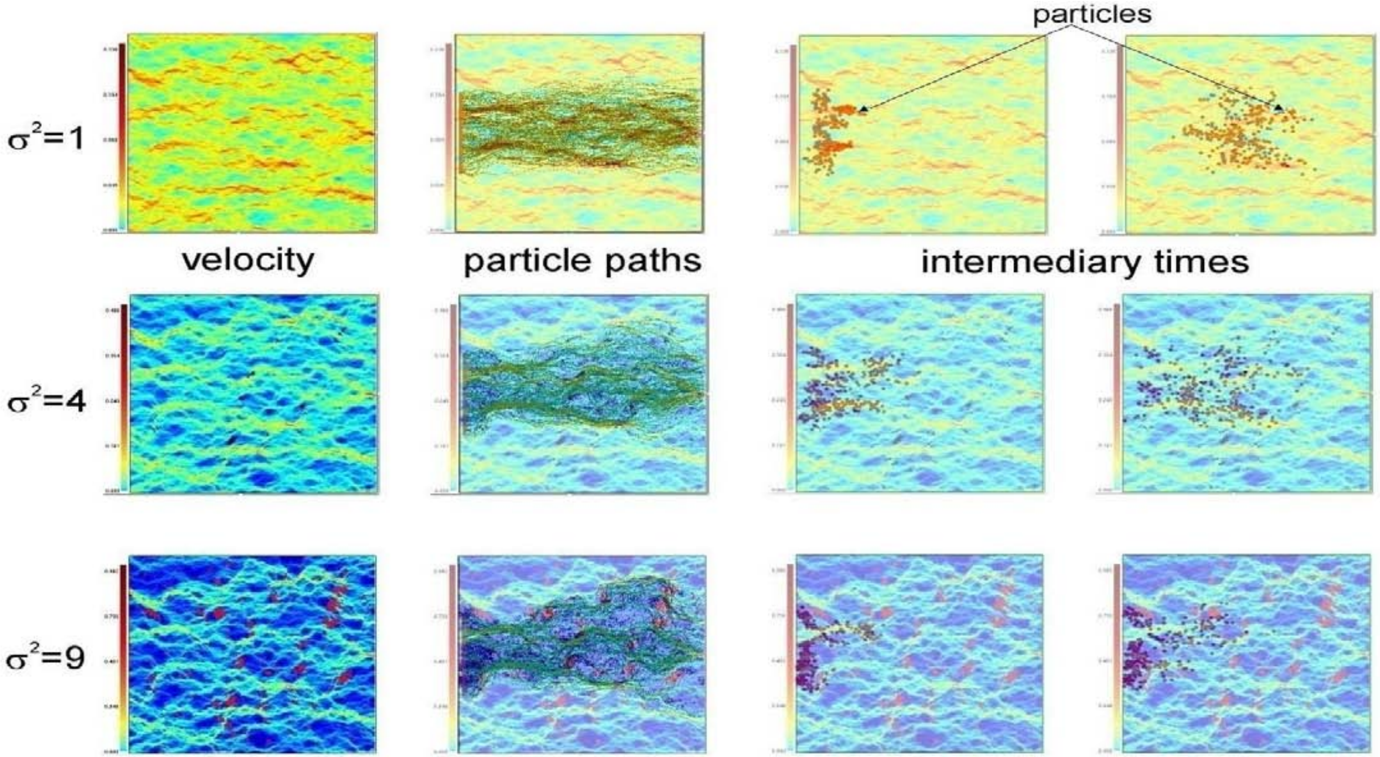
Pure advection case
Longitudinal dispersion

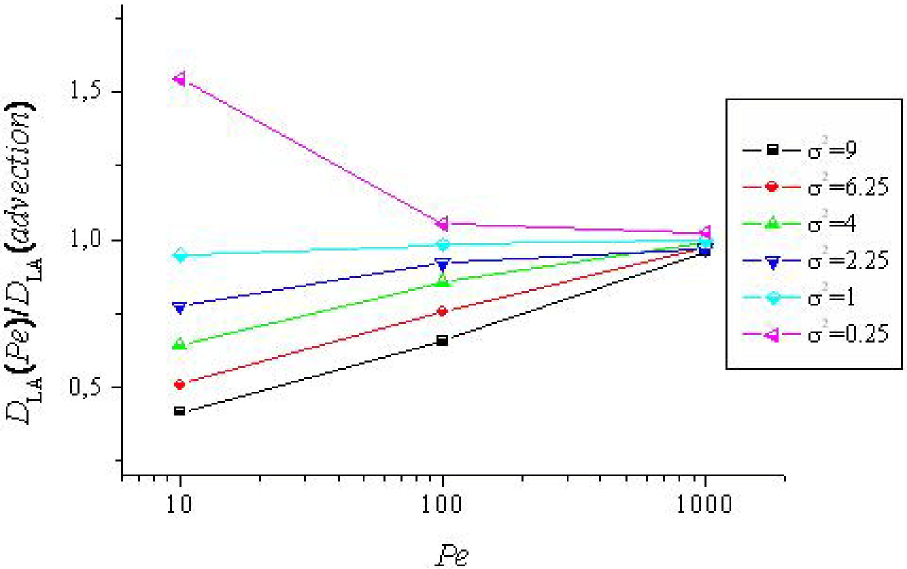


Each curve represents 100 simulations on domains with 67.1 millions of unknowns



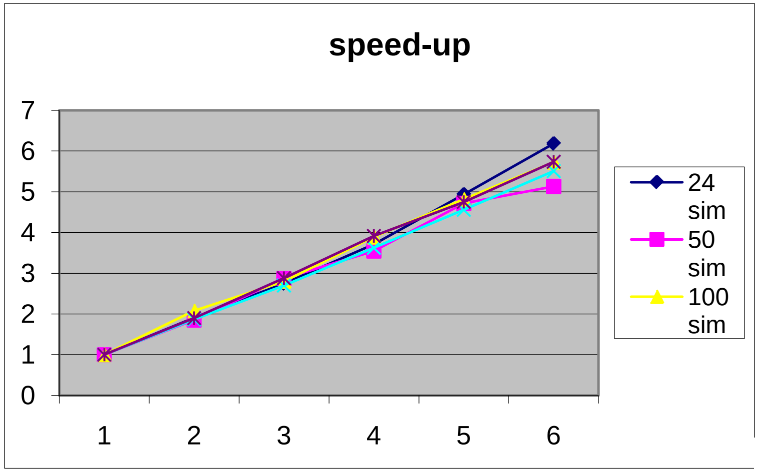


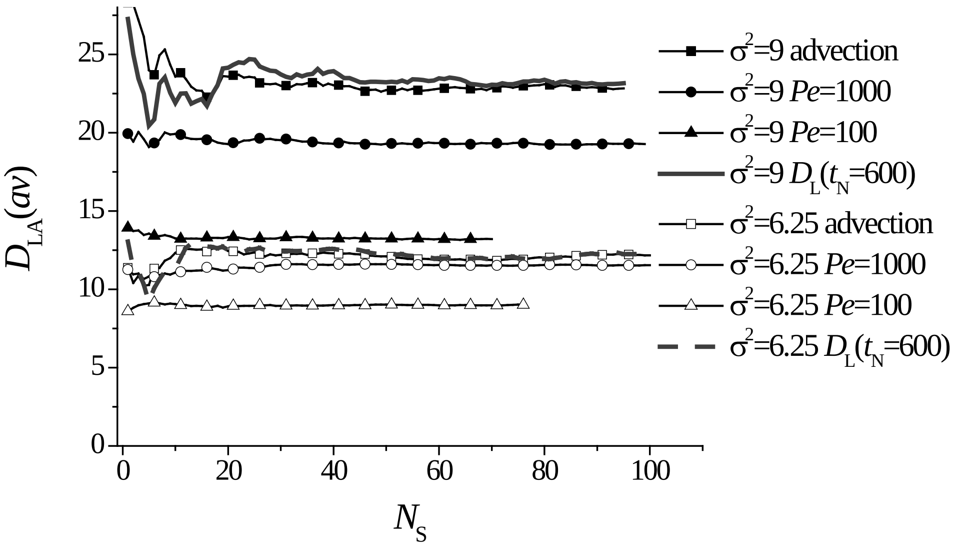


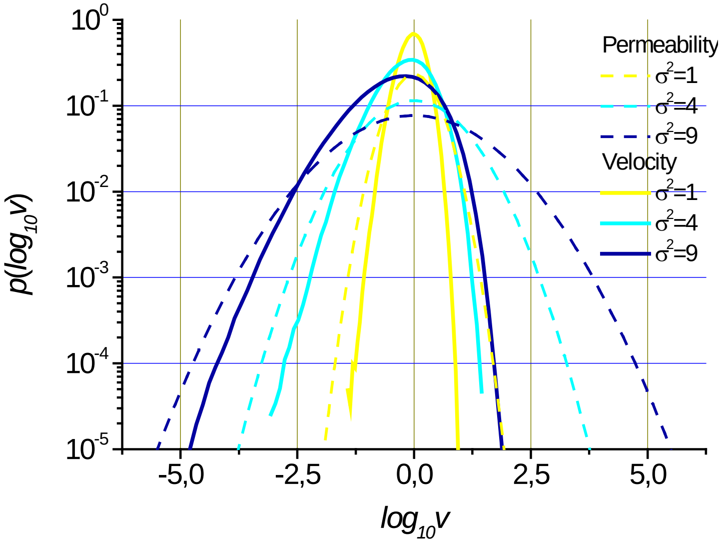


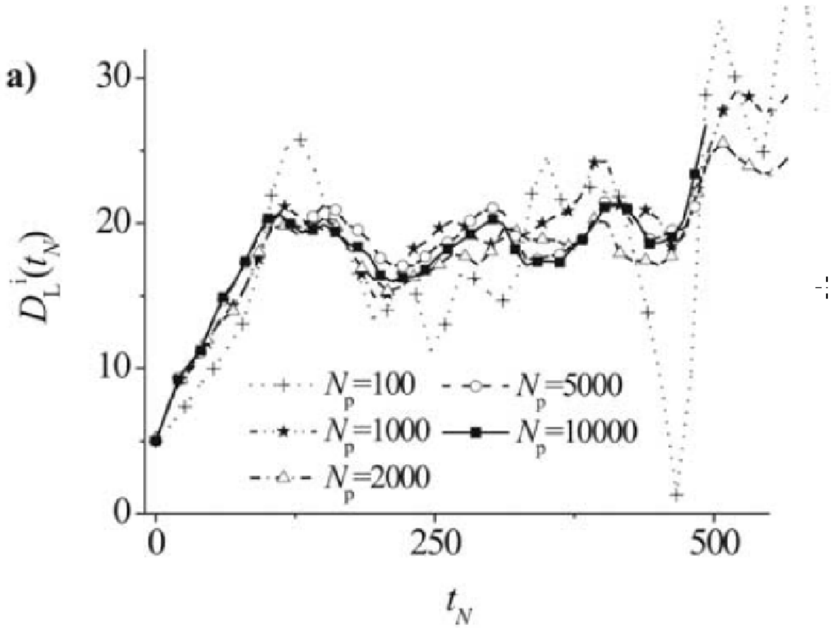
Impact of molecular diffusion

Parallel Monte Carlo simulations









Perspectives for stochastic heterogeneous media

Challenge

- Macro dispersion in 3D
- hydrodynamic dispersion
- nonlinear stochastic model (chemistry, non saturated, etc)
- non ergodic random field

Collaboration and applications

- RISC-E network, Micas consortium, ENS Cachan Bretagne, Tosca INRIA team
- Barcelona, Leipzig, San Diego

Discrete Fracture Networks models

Scientific context

- fractured media : random complex computational domain
- random velocity field given by flow model

Scientific achievements

- mesh generation for 3D networks
- conforming and non conforming methods
- reliable simulations
- software MP_FRAC

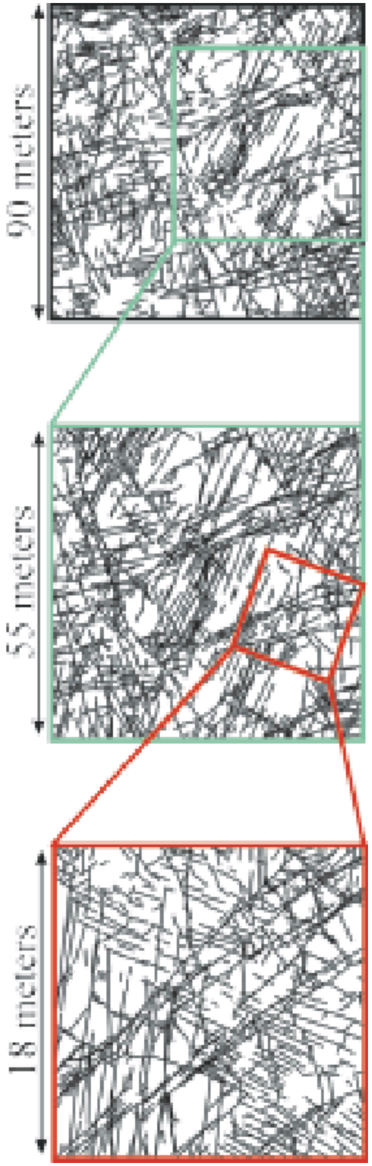
Collaborations and technology transfer

- MICAS ANR project: Univ. Le Havre, Geosciences Rennes, Univ. Lyon

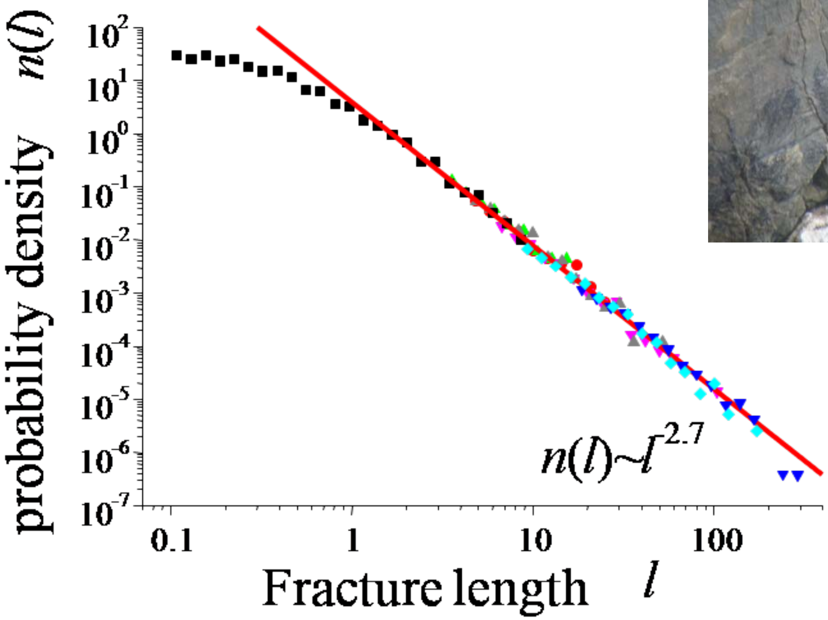
Publications

- SISC 2009, Applicable Analysis 2010 (accepted), WRR 2010 (accepted)
- proceedings PDPTA 2005, PARCO 2006, Mamern 2009

Discrete Fracture Networks : natural media



Site of Hornelen, Norwegen

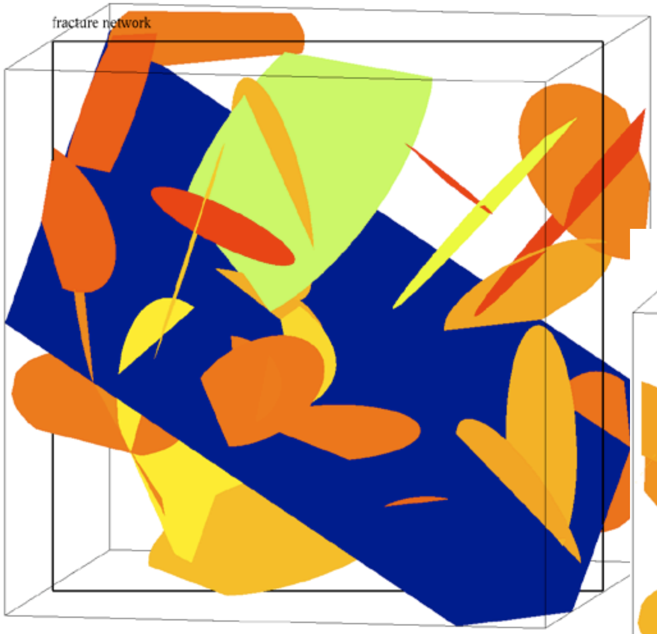


Fractures exist at any scale with no correlation

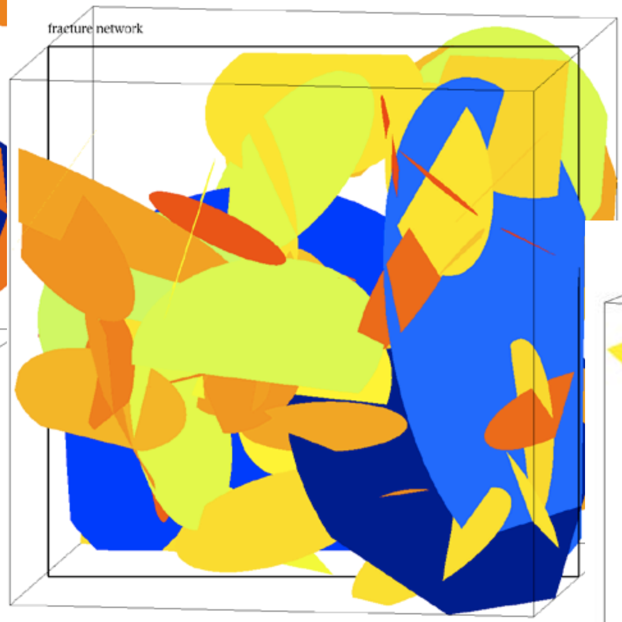
Fracture length is a parameter of heterogeneity

Power law distribution

Discrete Fracture Networks : stochastic generation



a=2.5



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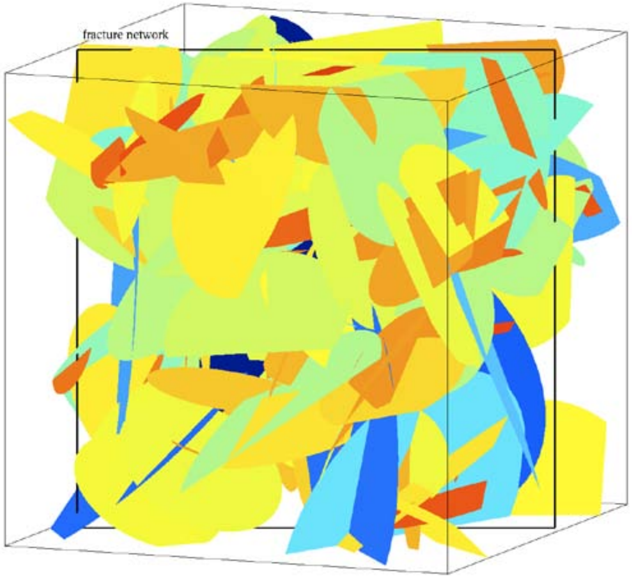


a=4.5

Discrete Fracture Networks : conforming mesh

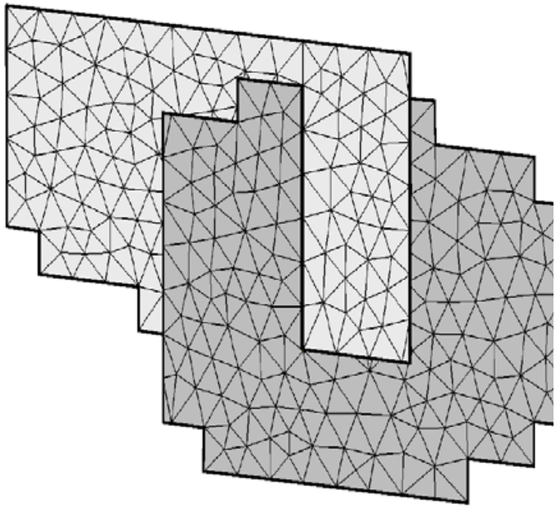
flow equations

impervious matrix

Poiseuille law and mass continuity in each fracture

Continuity of hydraulic head h

and flux V.n at each intersection



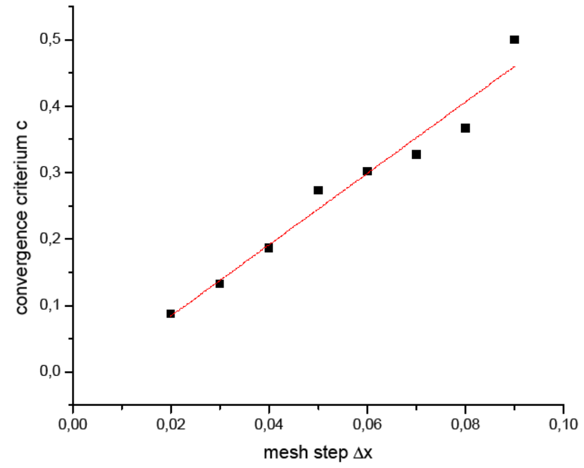
Spatial discretization

conforming mesh

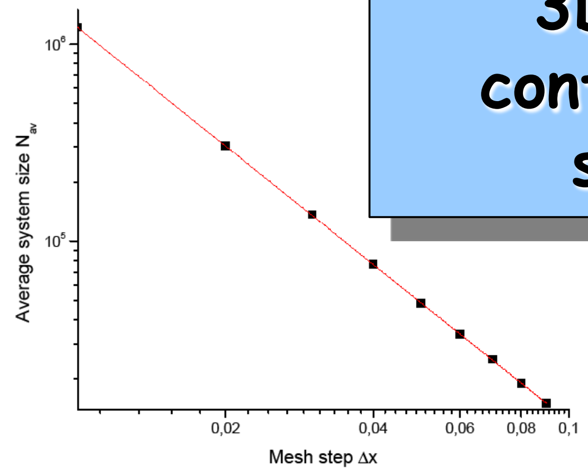
mixed hybrid finite element method

easy to apply interface conditions

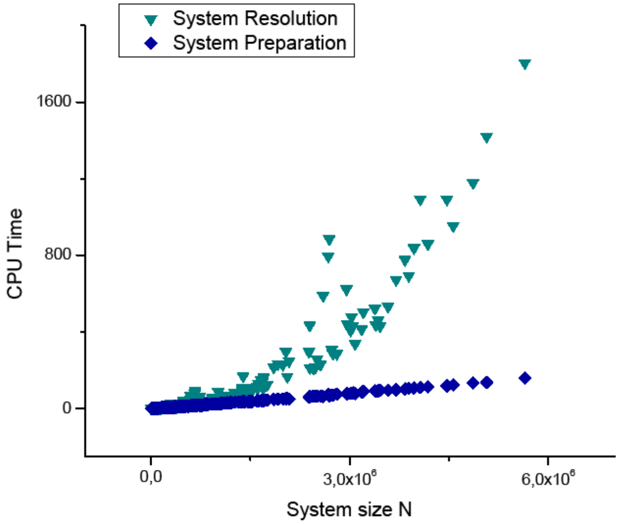
3D DFN with conforming mesh simulations



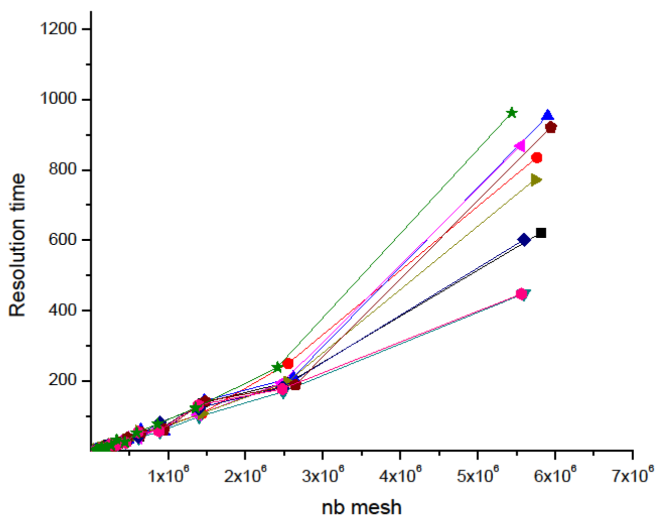
Convergence of spatial discretization



System size



CPU time with sparse direct solver



CPU time with PCG + AMG

Discrete Fracture Networks : non conforming mesh

Interface conditions written using mortar spaces

Geometrically conforming intersections

slave side and master side for each intersection

no edge common to more than 2 fractures

mass continuity through all edges of intersections

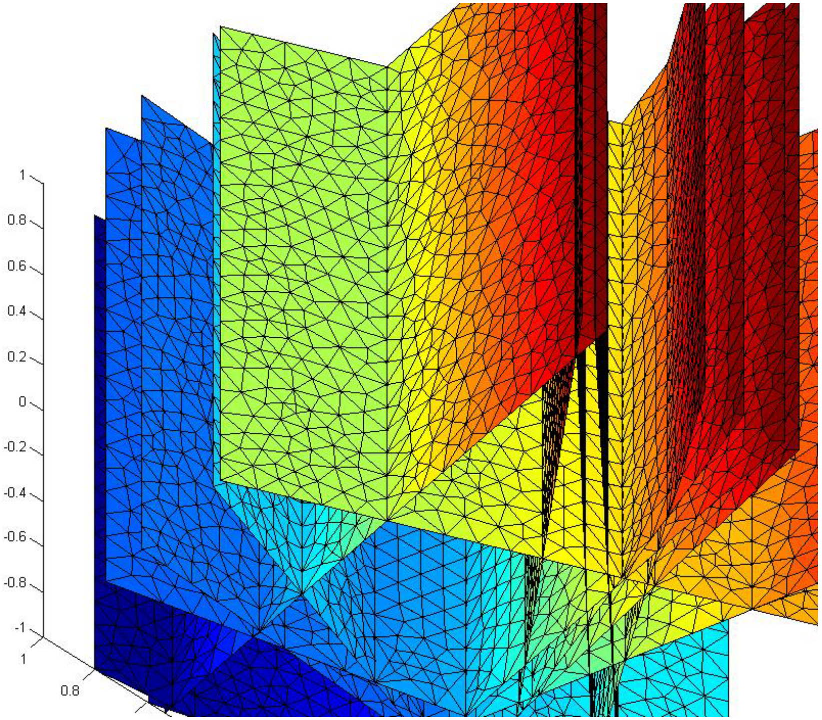
Geometrically non conforming intersections

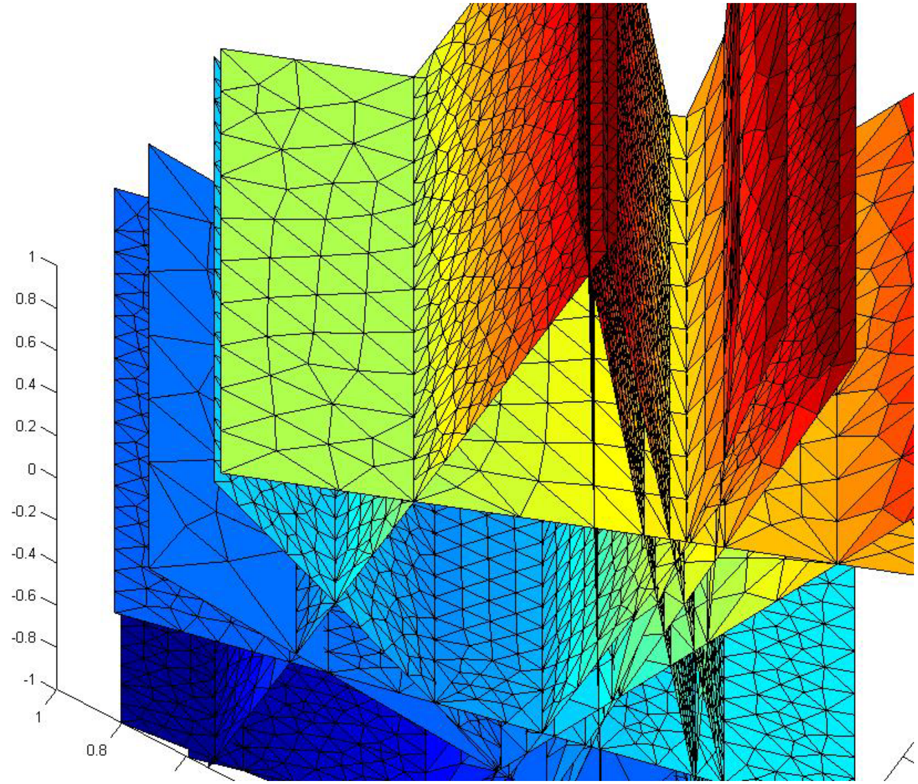
intersections partly common to more than 2 fractures

several unknowns : fracture, master and slave

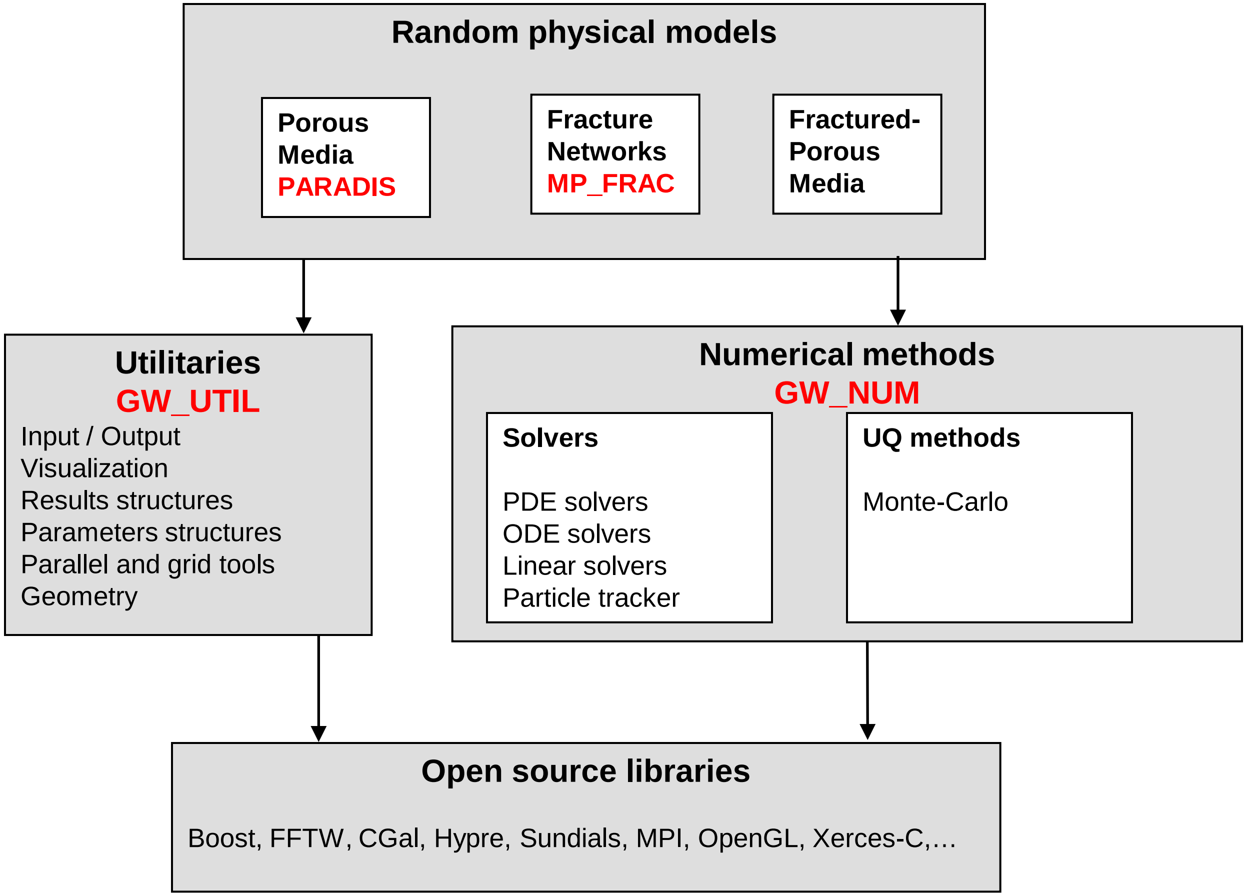
similar to a second level of mortar method

3D DFN with non conforming mesh simulations





H2OLab software platform



H2OLab methodology

- **Optimization and Efficiency**
  - Use of free numerical libraries and own libraries
  - Test and comparison of numerical methods
  - Parallel computation (distributed and grid computing)
- **Genericity and modularity**
  - Object-oriented programming (C++)
  - Encapsulated objects and interface definitions
- **Maintenance and use**
  - Intensive testing and collection of benchmark tests
  - Documentation : user's guide, developer's guide
  - Database of results and web portal
- **Collaborative development**
  - Advanced Server (Gforge) with control of version (SVN),...
  - Integrated development environments (Visual, Eclipse)
  - Cross-platform software (Cmake, Ctest)
  - Software registration and future free distribution

Numerical models in hydrogeology
Current and future work

Coupled nonlinear problems

- Chemistry with kinetic and precipitation-dissolution reactions
- Bioremediation, non saturated zone, saltwater intrusion
- ANDRA and MOMAS project

Porous and fractured media

- Coupling heterogeneous matrix and Discrete Fracture Network
- Subdomain decomposition for solving the linear system
- MICAS (ANR) project

Uncertainty Quantification methods

- Convergence results for macro-dispersion and for stochastic DFN
- Preliminary experiments with stochastic collocation methods
- MICAS and CO-ADVISE (People) projects

Inverse problems

- Data completion and parameter estimation
- HYDROMED (INRIA-MED) and CO-ADVISE projects