# *Approches mathématiques pour la simulation multi-échelle des matériaux*

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based on a series of works by

F. Legoll, T. Lelièvre, G. Stoltz and collaborators



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# Numerical simulation of coarse-grained stochastic dynamics

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# Dissipative Particle Dynamics and the like

• Simulation of shock waves at the atomistic level requires very large systems

• Coarse-graining through stochastic dynamics which is Galilean invariant
→ friction using relative velocities (consistence with hydrodynamics)

• **Dissipative Particle Dynamics with conserved energy (DPDE)**

- can be used in nonequilibrium situations
- replace a molecule or some group of atoms by a mesoparticle
- consistent thermodynamics
- input: static properties (ab-initio), dynamical parameters

• **Collaboration** with J.-B. Maillet (CEA/DAM) and J. Brennan (Army Research Lab); 2 PhD students (A.-A. Homman and G. Faure)

# Dissipative particle dynamics with conserved energy

- Coarse-graining interpretation:
  - a (fragment of a) molecule is replaced by a mesoparticle
  - $(q_i, p_i)$ describes the center of mass of the $i$th mesoparticle
  - missing degrees of freedom described by an internal energy $\varepsilon_i$

- Evolution at constant total energy $\mathcal{H}(q, p, \varepsilon) = V(q) + \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N} \varepsilon_i$

- Microscopic state law: entropies $s_i = s_i(\varepsilon_i)$, internal temperature defined from the entropy as

$$T_i(\varepsilon_i) = \frac{1}{s_i'(\varepsilon_i)}$$

- Simplest case: harmonic internal degrees of freedom, $T(\varepsilon) = \varepsilon / C_v$

J. Bonet Avalos and A. Mackie, *Europhys. Lett.* **40**, 141-146 (1997)
P. Español, *Europhys. Lett.* **40** 631-636 (1997)

# Equations of motion

$$\begin{cases} dq_i = \dfrac{p_i}{m_i}\, dt \\ dp_i = -\nabla_{q_i} V(q)dt + \displaystyle\sum_{i\neq j} -\gamma_{ij}\chi^2(r_{ij})v_{ij}\, dt + \sigma_{ij}\chi(r_{ij})\, dW_{ij}, \\ d\varepsilon_i = \dfrac{1}{2}\displaystyle\sum_{j\neq i}\chi^2(r_{ij})\left(\gamma_{ij}v_{ij}^2 - \dfrac{\sigma_{ij}^2}{2}\left(\dfrac{1}{m_i}+\dfrac{1}{m_j}\right)\right) dt - \sigma_{ij}\,\chi(r_{ij})v_{ij}\cdot dW_{ij} \end{cases}$$

where $W_{ij} = -W_{ji}$, $\chi$ is a cut-off function and $v_{ij} = \dfrac{p_i}{m_i} - \dfrac{p_j}{m_j}$

## Invariant measures

$$\rho(dq\, dp\, d\varepsilon) = f\Big(\mathcal{H}(q,p,\varepsilon)\Big) g\left(\sum_{i=1}^N p_i\right) \exp\left(\sum_{i=1}^N s_i(\varepsilon_i)\right)\, dq\, dp\, d\varepsilon,$$

- Fluctuation-dissipation relation

$$\sigma_{ij} = \sigma, \quad \gamma_{ij} = \frac{\sigma^2\beta_{ij}(\varepsilon_i,\varepsilon_j)}{2}, \quad \beta_{ij}(\varepsilon_i,\varepsilon_j) = \frac{1}{2k_{\mathrm{B}}}\left(\frac{1}{T_i(\varepsilon_i)} + \frac{1}{T_j(\varepsilon_j)}\right)$$

# Numerical integration of DPDE: our key contribution

- "Naive" schemes lead to internal energies $\varepsilon_i < 0$: simulation stopped!
  - this happens more often for small heat capacities
  - this will necessarily happen at some point for large systems

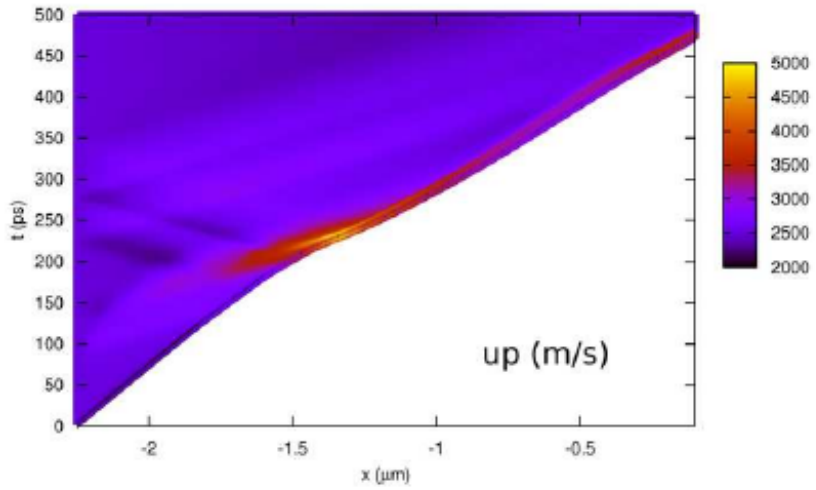
- **Stable and accurate integration schemes?**
  - Splitting strategy: Hamiltonian part vs. elementary stochastic dynamics
  - elementary stochastic dynamics reduce to a dynamics on $v_{ij}$ only
  - superimpose a Metropolis correction for discretizations of these reduced dynamics[1], even in the nonequilibrium setting considered

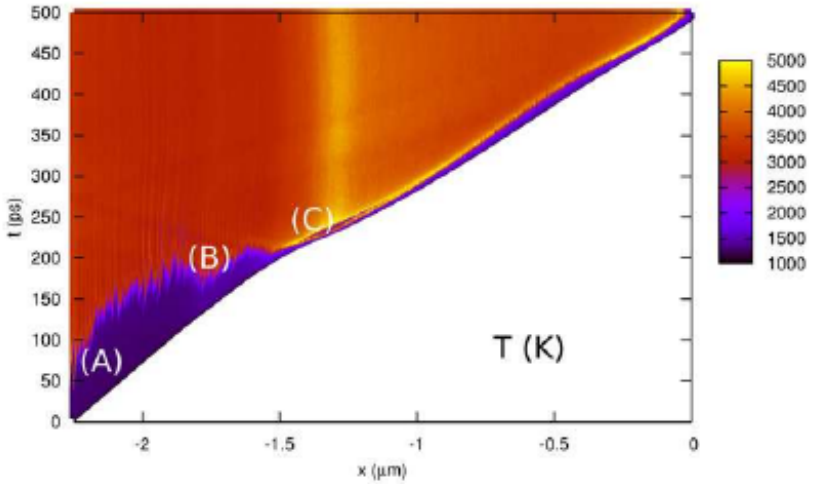
- **Pro/cons of this integrator:**
  - automatically corrects for negative internal energies (stabilization)
  - parallelization/threadability limited $\rightarrow$ dedicated schemes for that[2]

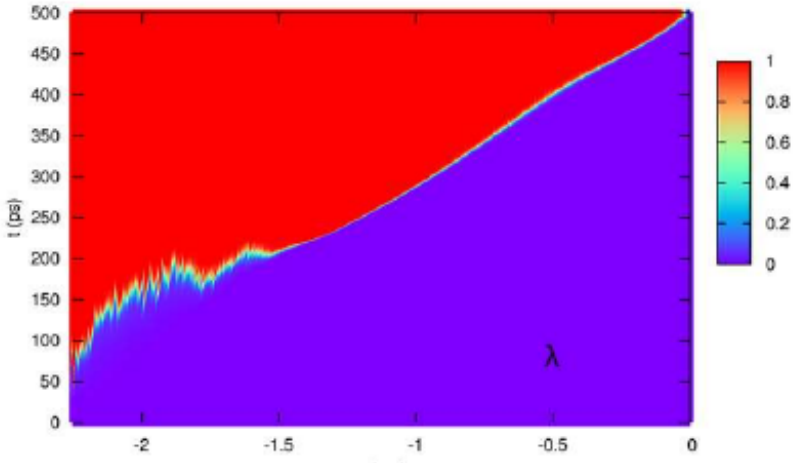
[1] G. Stoltz, *J. Comput. Phys.* (2017)

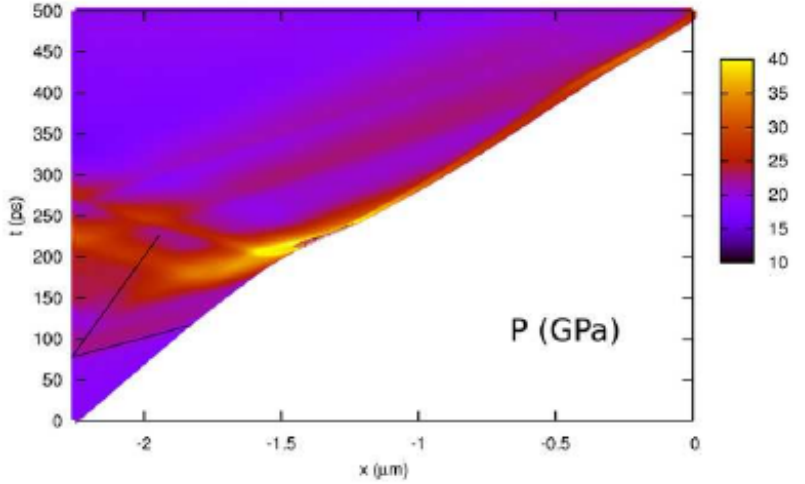
[2] A.-A. Homman, J.-B. Maillet, J. Roussel and G. Stoltz, *J. Chem. Phys* (2016)

# Detonation waves in nitromethane




Particle velocity, temperature, progress variable, pressure

J.-B. Maillet, G. Vallverdu, N. Desbiens and G. Stoltz, *Europhys. Lett.* (2011)

# Orders of magnitude of current simulations

- **At CEA/DAM**
  - number of particles $N \sim 10^6 - 10^8$
  - number of cores: several thousands, with vectorized/threadable code ExaSTAMP
  - number of steps $10^6$, timestep $\Delta t \sim 1 - 5 \times 10^{-15}$
  - CPU time: a few $\mu$s/N/ts for simple LJ potential, $\times 10 - 100$ for more complicated one

- **At Army Research Lab (Aberdeen Proving Ground)**
  - number of particles up to $N = 1,126,926,339$
  - machines: Thunder (USAF), Stampede2 (Texas Advanced Computing Center), Trinity/KNL (Los Alamos)
  - 3,000 to 8,900 nodes (Intel Xeon Phi 7250 KNL or E5-2699v3); between 4.3 and 27 PFLOPS/s (in double precision)
  - simulation time 0.5 ns

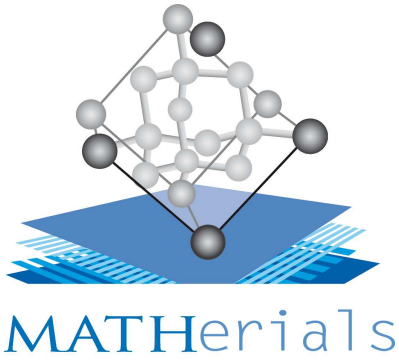
# Adaptive Multilevel Splitting algorithms for rare event simulations

Tony Lelièvre

Ecole des Ponts ParisTech and INRIA

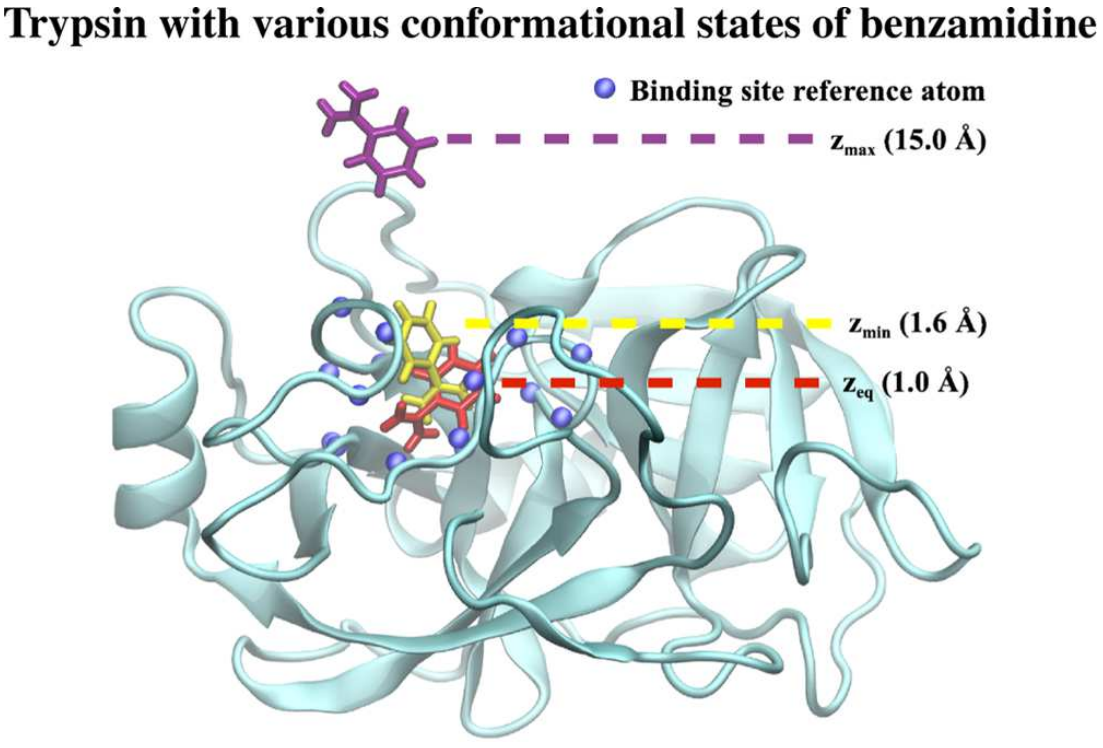
Joint work with C.-E. Bréhier, F. Cérou, M. Gazeau, L. Goudenège, A. Guyader, C. Mayne, M. Rousset and I. Teo






# Motivation 1: Simulations of biological systems

## Unbinding of a ligand from a protein



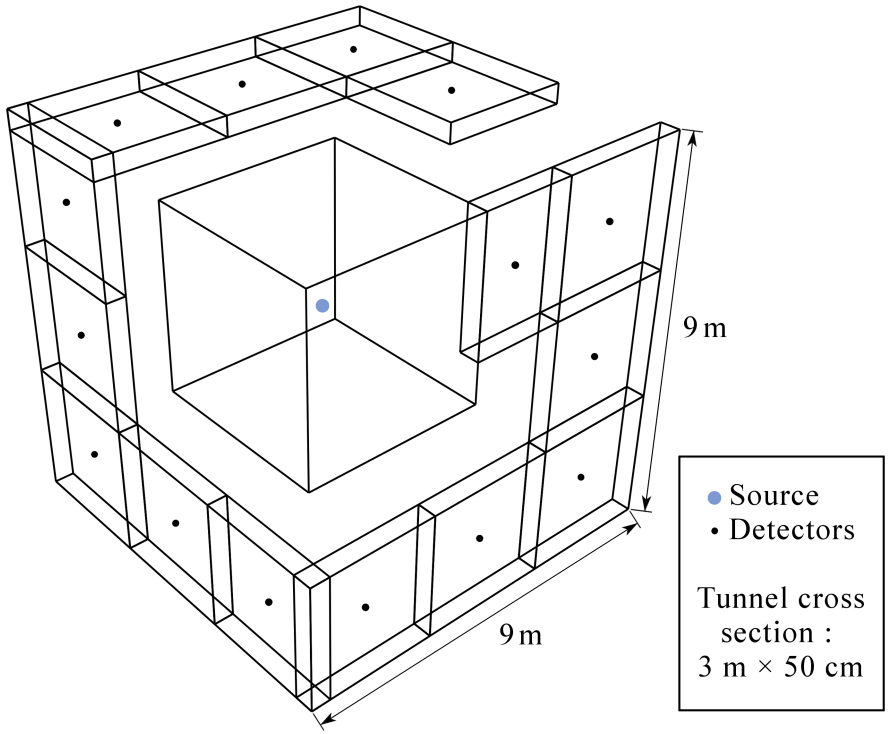

Elementary time-step for the molecular dynamics $= 10^{-15}\,\mathrm{s}$

Dissociation time $\simeq 0.02\,\mathrm{s}$

Challenge: bridge the gap between timescales

# Motivation 2: Radiation protection

## Monte Carlo particle transport




**Concrete tunnel with a neutron source**

How to compute the neutron flux at the detector ?

Challenge: the flux is very small

# Mathematical setting: rare event computation

Consider a stochastic process $(X_t)_{t\geq 0}$ and two stopping times $\tau_A$ and $\tau_B$. Objective: simulate and compute the probability of the event $\{\tau_B < \tau_A\}$ when $\mathbb{P}(\tau_B < \tau_A)$ is very small ($10^{-8}$ to $10^{-18}$).

Basic idea of splitting technique: find intermediate events which are easier to simulate:

$$\{\tau_{z_1} < \tau_A\} \supset \{\tau_{z_2} < \tau_A\} \supset \ldots \supset \{\tau_{z_{\max}} < \tau_A\} \supset \{\tau_B < \tau_A\}$$

and simulate the successive *conditional events*: for $k = 1, 2, \ldots,$

$$\{\tau_{z_q} < \tau_A\} \text{ knowing that } \{\tau_{z_{q-1}} < \tau_A\}$$

where $\tau_z = \inf\{t, \xi(X_t) > z\}$ for a well chosen real valued importance function $\xi$.

Adaptive feature: build the intermediate levels $(z_i)_{i\geq 1}$ on the fly.

$\longrightarrow$ Adaptive Multilevel Splitting algorithm [Cérou, Guyader, Stoch. Annal. Appl., (2007)]

# Numerical results

Example 1: In collaboration with the group of K. Schulten (C. Mayne and I. Teo), AMS is currently implemented in the NAMD code. We have studied the unbinding event of benzamidine from trypsin.

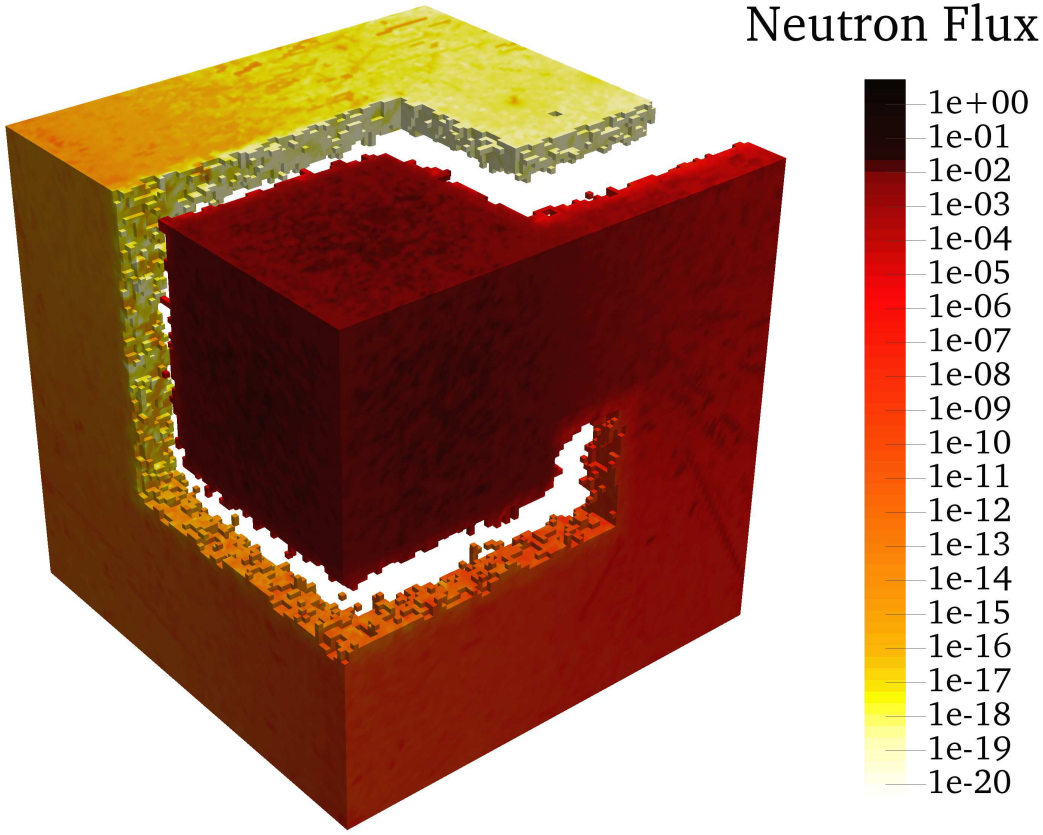
Estimated dissociation rate: $k_{off} = (260 \pm 240)s^{-1}$ which is in the same order of magnitude as the experimental rate $(600 \pm 300)s^{-1}$.

Overall simulation time: $2.3\mu s$ which is 4 orders of magnitude shorter than than the estimated dissociation time.

MD setup: about 70 000 atoms, CHARMM36 force field, NPT conditions (298 K).

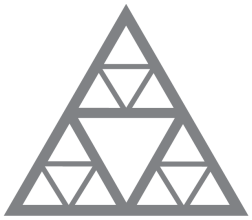
# Numerical results

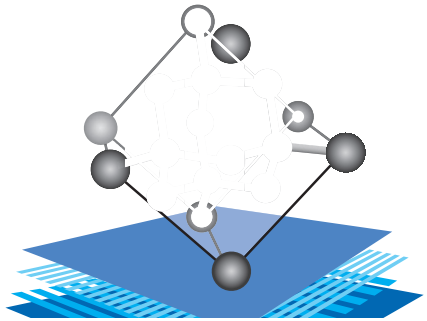
Example 2: In collaboration with CEA (Eric Dumonteil, Cheikh Diop and Henri Louvin), AMS is currently implemented in the Tripoli code.



# References


- C.-E. Bréhier, M. Gazeau, L. Goudenège , T. Lelièvre and M. Rousset, *Unbiasedness of some generalized Adaptive Multilevel Splitting algorithms*, Annals of Applied Probability 26(6), 2016.
- F. Cérou, A. Guyader, T. Lelièvre and D. Pommier, *A multiple replica approach to simulate reactive trajectories*, Journal of Chemical Physics 134, 2011.
- I. Teo, C. Mayne, K. Schulten and T. Lelièvre, *Adaptive multilevel splitting method for molecular dynamics calculation of benzamidine-trypsin dissociation time*, Journal of Chemical Theory and Computation 12(6), 2016.





# Multiscale computations based on MsFEM: model reduction and goal-oriented a posteriori error estimation

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Ecole des Ponts & project-team MATHERIALS, INRIA Paris

*Joint works with Ludovic Chamoin (LMT Cachan)*

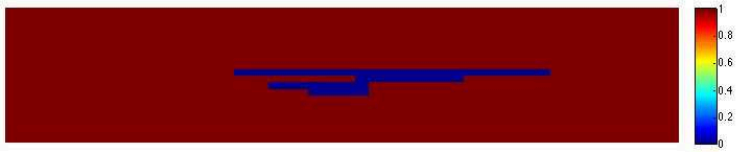
# Problem of interest (SPE 10, http://www.spe.org/web/csp/index.html)

$$-\mathrm{div}\big[A_\varepsilon(\mu,x)\nabla u^\varepsilon(\mu,x)\big] = f(x) \ \text{ in } \Omega, \qquad u^\varepsilon = 0 \ \text{ on } \partial\Omega$$

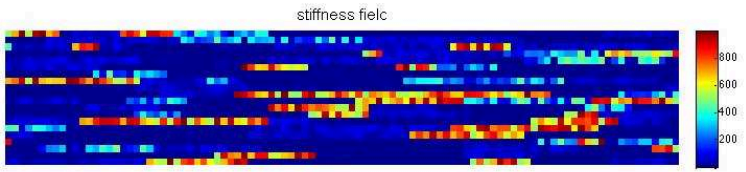
where $\mu$ is a parameter. We take

$$A_\varepsilon(\mu,x) = \lambda(\mu,x)A_\varepsilon(x), \qquad \lambda(\mu,x) = \mu + (1-\mu)\lambda_c(x)$$

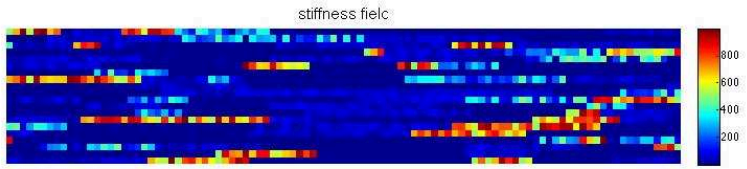
Depending on the value of $\mu$, the central channel is present or not.
Very large contrast in $A_\varepsilon$: $10^6$



Representation of $\lambda_c(x)$




$A_\varepsilon(\mu,x)$ for $\mu = 1$




$A_\varepsilon(\mu,x)$ for $\mu = 0.1$

# Model reduction approaches

$$-\mathrm{div}\Big[A_\varepsilon(\mu,x)\nabla u^\varepsilon(\mu,x)\Big] = f(x) \ \text{ in } \Omega, \qquad u^\varepsilon = 0 \ \text{ on } \partial\Omega$$

- Direct MsFEM approach: for each new $\mu$,
  - compute the MsFEM basis functions:

$$(\star) \quad -\mathrm{div}\Big[A_\varepsilon(\mu,x)\nabla \phi_i^\varepsilon(\mu,x)\Big] = 0 \text{ in } K, \qquad \phi_i^\varepsilon(\mu,\cdot) = \phi_i^0 \text{ on } \partial K$$

  - solve the global problem on Span $\{\phi_i^\varepsilon(\mu,\cdot), \quad 1 \le i \le I\}$.

  Too expensive!

- Our approach: model reduction (PGD approach) on $(\star)$:

$$\phi_i^\varepsilon(\mu,x) \approx \phi_i^0(x) + \sum_{j=1}^{J} \psi_j^\varepsilon(x)\alpha_j(\mu)$$

for (hopefully) a small number $J$ of terms. The decomposition is built iteratively (greedy algorithm).

# Proper Generalized Decomposition (Ladevèze, Chinesta, Nouy, . . . )

Idea to compute $w(x, \mu)$:

- represent the solution as a linear combination of tensor products of small-dimensional functions:

$$w(x, \mu) = \sum_{j \geq 1} \psi_j(x) \alpha_j(\mu)$$

- look iteratively for the best tensor product: once some approximation

$$w_{n-1}(x, \mu) = \sum_{j=1}^{n-1} \psi_j(x) \alpha_j(\mu)$$

has been computed, improve it by considering

$$w_n(x, \mu) = w_{n-1}(x, \mu) + \psi_n(x) \alpha_n(\mu)$$

# PGD within MsFEM

- For a given parameter $\mu_0$, perform a MsFEM computation and adapt the discretization parameters ($H$, $h$ and oversampling).

  This discretization will be kept unchanged.

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  This discretization will be kept unchanged.

- Perform a PGD approach on $\phi_i^\varepsilon(\mu, \cdot)$, solution to

$$-\mathrm{div}\big[A_\varepsilon(\mu, x)\nabla\phi_i^\varepsilon(\mu, x)\big] = 0 \text{ in } K, \qquad \phi_i^\varepsilon(\mu, \cdot) = \phi_i^0 \text{ on } \partial K$$

  It amounts to writing

$$(\star) \qquad \phi_i^\varepsilon(\mu, x) \approx \phi_i^{\varepsilon, J}(\mu, x) = \phi_i^0(x) + \sum_{j=1}^{J} \psi_j^\varepsilon(x)\alpha_j(\mu)$$

# PGD within MsFEM

- For a given parameter $\mu_0$, perform a MsFEM computation and adapt the discretization parameters ($H$, $h$ and oversampling).

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$$-\mathrm{div}\big[A_\varepsilon(\mu,x)\nabla\phi_i^\varepsilon(\mu,x)\big]=0 \text{ in } K, \qquad \phi_i^\varepsilon(\mu,\cdot)=\phi_i^0 \text{ on } \partial K$$

  It amounts to writing

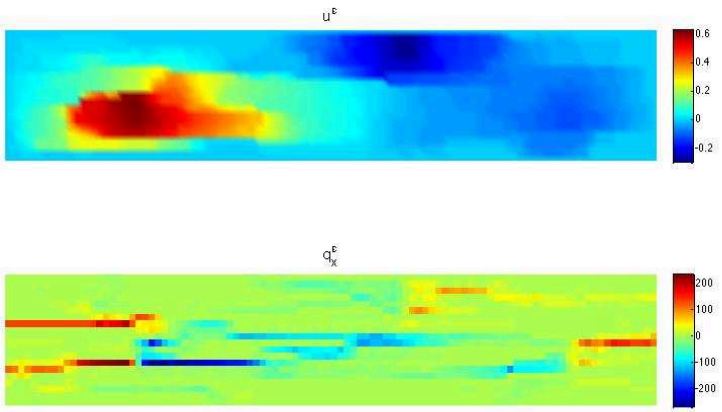
$$(\star) \qquad \phi_i^\varepsilon(\mu,x)\approx\phi_i^{\varepsilon,J}(\mu,x)=\phi_i^0(x)+\sum_{j=1}^{J}\psi_j^\varepsilon(x)\alpha_j(\mu)$$

- For each new $\mu$:
  - evaluate the basis functions $\phi_i^{\varepsilon,J}(\mu,x)$ using $(\star)$
  - solve the global problem on Span $\left\{\phi_i^{\varepsilon,J}(\mu,\cdot),\ 1\le i\le I\right\}$.
  - estimate the error

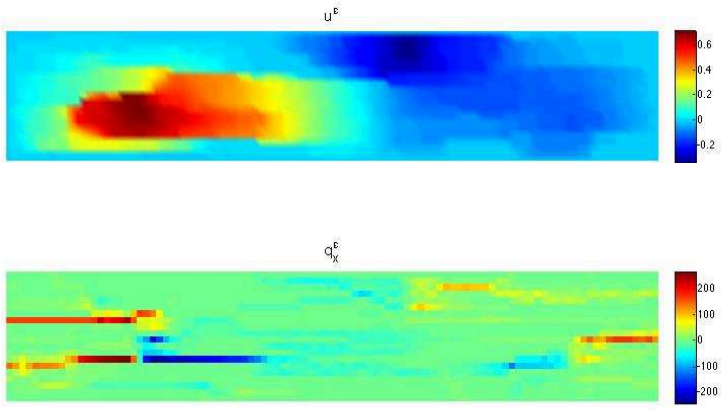
Alternative strategy: PGD on global problem followed by MsFEM discretization

# Numerical results (crude discretization)

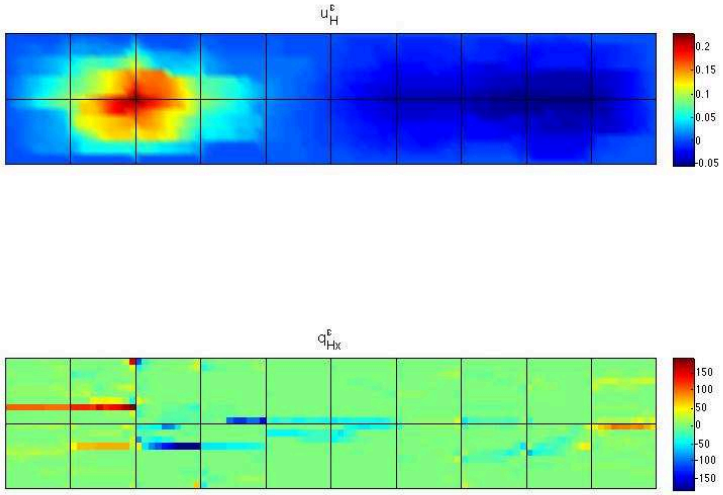
$\mu = 1$ (initial permeability field)

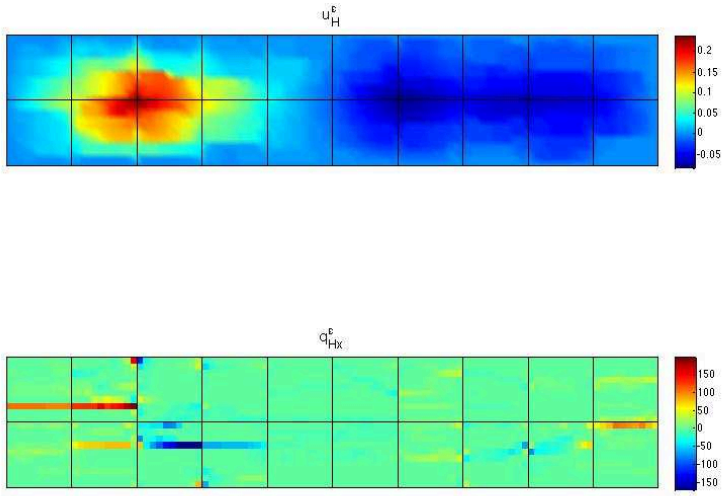



$\mu = 0.1$ (central channel removed)

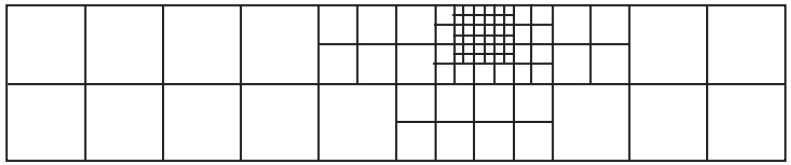



MsFEM solution (no oversampling):

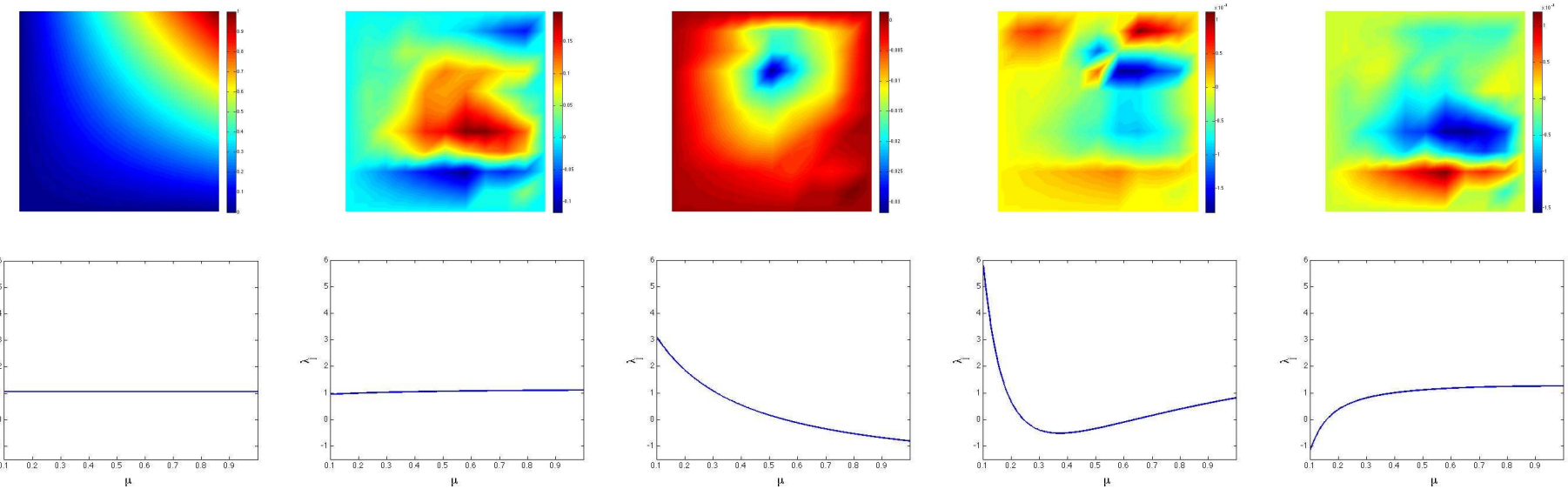


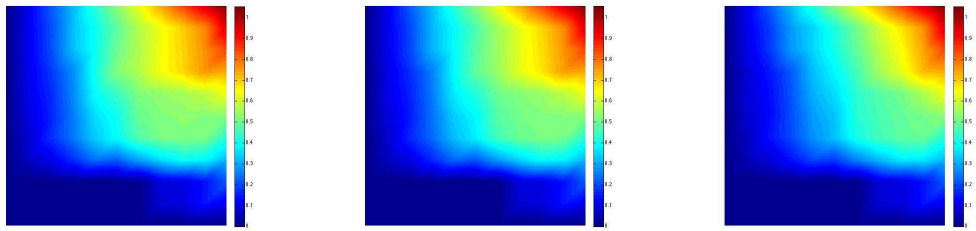
# PGD approach for the computation of $\phi_i^\varepsilon(\mu, \cdot)$



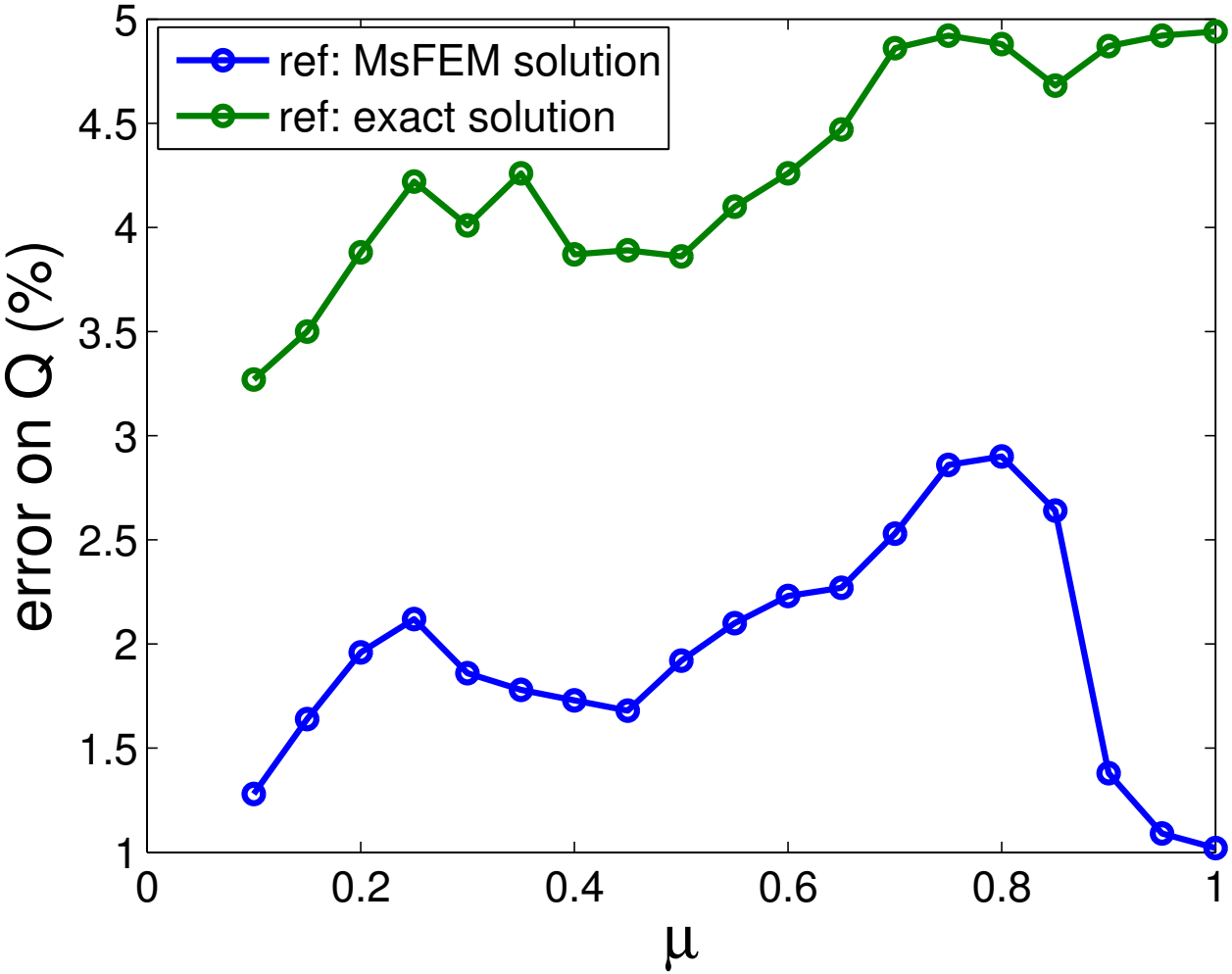
PGD modes $\psi_j^\varepsilon(x)$ (top) and $\alpha_j(\mu)$ (bottom), $j = 1, \ldots, 5$:



MsFEM basis functions $\phi_i^0(x) + \sum_{j=1}^{J} \psi_j^\varepsilon(x)\alpha_j(\mu)$ ($\mu$ =1, 0.5 and 0.1):

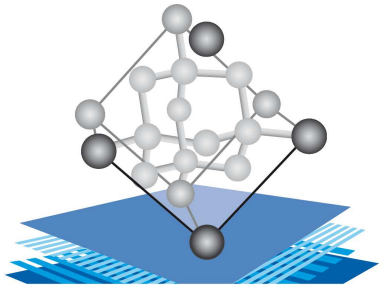


# Error estimation (identical MsFEM discretization for any $\mu$)




The error remains under 5% for all $\mu$.

https://www.rocq.inria.fr/matherials/

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