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
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 to 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, \(T(\varepsilon) = \varepsilon/C_v\)

Equations of motion

\[
\begin{cases}
dq_i = \frac{p_i}{m_i} \ dt \\
dp_i = -\nabla q_i \ V(q) dt + \sum_{i \neq j} \gamma_{ij} \chi^2(r_{ij}) v_{ij} dt + \sigma_{ij} \chi(r_{ij}) dW_{ij},
\end{cases}
\]

\[
d\varepsilon_i = \frac{1}{2} \sum_{j \neq i} \chi^2(r_{ij}) \left( \gamma_{ij} v_{ij}^2 - \frac{\sigma_{ij}^2}{2} \left( \frac{1}{m_i} + \frac{1}{m_j} \right) \right) dt - \sigma_{ij} \chi(r_{ij}) v_{ij} \cdot dW_{ij}
\]

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

Invariant measures

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

- Fluctuation-dissipation relation

\[
\sigma_{ij} = \sigma, \quad \gamma_{ij} = \frac{\sigma^2 \beta_{ij}(\varepsilon_i, \varepsilon_j)}{2}, \quad \beta_{ij}(\varepsilon_i, \varepsilon_j) = \frac{1}{2k_B} \left( \frac{1}{T_i(\varepsilon_i)} + \frac{1}{T_j(\varepsilon_j)} \right)
\]
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\(^2\)

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Detonation waves in nitromethane

Particle velocity, temperature, progress variable, pressure

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 \( \mu s/N/\text{ts} \) 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

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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

Trypsin with various conformational states of benzamidine

Elementary time-step for the molecular dynamics $= 10^{-15} \text{s}$
Dissociation time $\approx 0.02 \text{s}$

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 \((10^{-8} \text{ to } 10^{-18})\).

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

\[
\{\tau_{z_1} < \tau_A\} \supset \{\tau_{z_2} < \tau_A\} \supset \ldots \supset \{\tau_{z_{\text{max}}} < \tau_A\} \supset \{\tau_B < \tau_A\}
\]

and simulate the successive conditional events: for \(k = 1, 2, \ldots,\)

\[
\{\tau_{z_k} < \tau_A\} \text{ knowing that } \{\tau_{z_{k-1}} < \tau_A\}
\]

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.

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

**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.


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

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Joint works with Ludovic Chamoin (LMT Cachan)

\[-\text{div} \left[ A_\varepsilon(\mu, x) \nabla u^\varepsilon(\mu, x) \right] = f(x) \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial \Omega\]

where $\mu$ is a parameter. We take

\[A_\varepsilon(\mu, x) = \lambda(\mu, x) A_\varepsilon(x), \quad \lambda(\mu, x) = \mu + (1 - \mu) \lambda_c(x)\]

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

\[-\text{div}\left[A_\varepsilon(\mu, x) \nabla u_\varepsilon(\mu, x)\right] = f(x) \text{ in } \Omega, \quad u_\varepsilon = 0 \text{ on } \partial\Omega\]

- **Direct MsFEM approach:** for each new \(\mu\),
  - compute the MsFEM basis functions:
    \[(\star) \quad -\text{div}\left[A_\varepsilon(\mu, x) \nabla \phi_i(\mu, x)\right] = 0 \text{ in } K, \quad \phi_i(\mu, \cdot) = \phi_i^0 \text{ on } \partial K\]
  - solve the global problem on \(\text{Span}\{\phi_i(\mu, \cdot), 1 \leq i \leq I\}\).
    Too expensive!

- **Our approach:** model reduction (PGD approach) on \((\star)\):
  \[
  \phi_i(\mu, x) \approx \phi_i^0(x) + \sum_{j=1}^{J} \psi_j(x) \alpha_j(\mu)
  \]
  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

\[
w_n(x, \mu) = w_{n-1}(x, \mu) + \psi_n(x) \alpha_n(\mu)
\]
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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Perform a PGD approach on $\phi^\varepsilon_i(\mu, \cdot)$, solution to

$$-\text{div}[A_\varepsilon(\mu, x) \nabla \phi^\varepsilon_i(\mu, x)] = 0 \text{ in } K, \quad \phi^\varepsilon_i(\mu, \cdot) = \phi^0_i \text{ on } \partial K$$

It amounts to writing

$$\phi^\varepsilon_i(\mu, x) \approx \phi^\varepsilon_{i,J}(\mu, x) = \phi^0_i(x) + \sum_{j=1}^{J} \psi^\varepsilon_j(x) \alpha_j(\mu)$$
PGD within MsFEM

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

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

  $$-\text{div}\left[A^\varepsilon(\mu, x)\nabla \phi^\varepsilon_i(\mu, x)\right] = 0 \text{ in } K, \quad \phi^\varepsilon_i(\mu, \cdot) = \phi^0_i \text{ on } \partial K$$

  It amounts to writing

  $$(\star) \quad \phi^\varepsilon_i(\mu, x) \approx \phi^\varepsilon_i,^J(\mu, x) = \phi^0_i(x) + \sum_{j=1}^J \psi^\varepsilon_j(x)\alpha_j(\mu)$$

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

**Alternative strategy**: PGD on global problem followed by MsFEM discretization.
Numerical results (crude discretization)

\( \mu = 1 \) (initial permeability field) \hspace{1cm} \( \mu = 0.1 \) (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 $\mu$. 

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