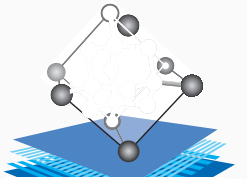


Adaptive parareal algorithms for molecular dynamics problems

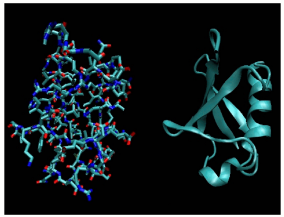
Olga Gorynina, Frédéric Legoll, Tony Lelièvre

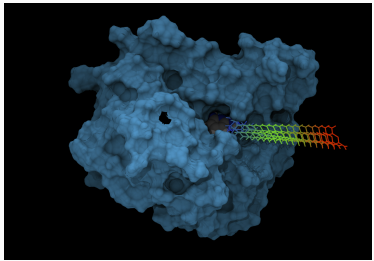
24/06/2021

SMAI 2021

Motivation

This work is motivated by molecular simulation, where we often have to simulate long trajectories of complex systems.





Typical dynamics: the Langevin equation

$$dq_t = p_t\,dt, \qquad dp_t = -\nabla V(q_t)\,dt - \gamma\,p_t\,dt + \sqrt{2\gamma\beta^{-1}}\,dW_t$$

Motivation

- Since we have to simulate long-time trajectories, it seems attractive to use the parareal algorithm, which solves initial value problems by parallel-in-time computations (domain-decomposition fashion)
- It turns out that this algorithm is not stable for MD problems when the time horizon is too large
- We therefore work with adaptive parareal algorithm, which performs simulations on shorter time slabs and paste them together, thereby allowing for a significant CPU gain (Legoll, Lelièvre and Sharma, HAL preprint 03189428, 2021)

Our goal is to apply the approach for realistic physical systems

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Parallel in time algorithm for ODEs

$$\frac{dx}{dt} = f(x), \qquad x \in \mathbb{R}^d$$

The parareal algorithm (Lions, Maday and Turinici, 2001) is based upon two integrators to propagate the system over a time ΔT:

- a fine, accurate integrator $\mathcal{F}_{\Delta T}$
- a coarse, cheap integrator $\mathcal{C}_{\Delta T}$

For instance,

$$\mathcal{F}_{\Delta T} = (\Phi_{\delta t_F})^{\Delta T/\delta t_F} \quad \text{and} \quad \mathcal{C}_{\Delta T} = (\Phi_{\delta t_C})^{\Delta T/\delta t_C} \quad \text{with} \quad \delta t_F \ll \delta t_C$$

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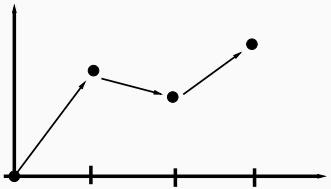
The parareal iterative procedure

- Initialization: coarse propagation that yields $\left\{x_n^{k=0}\right\}_n$:

$$\forall n, \quad x_{n+1}^{k=0} = \mathcal{C}_{\Delta T}(x_n^{k=0})$$



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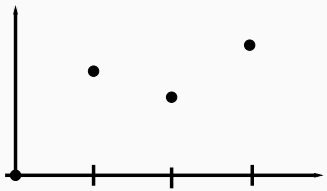

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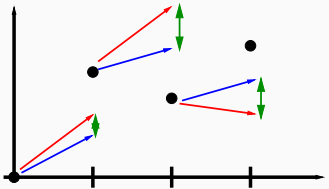

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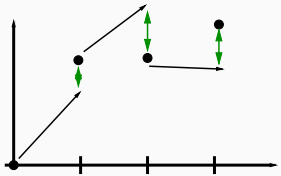

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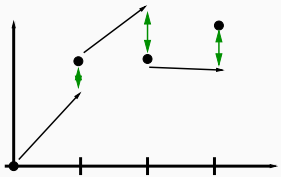

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Parareal algorithm for MD simulations

- Fundamental property : $x_n^k = \mathcal{F}_{\Delta T}^n(x_0)$ for any $n \leq k$. In practice, convergence is observed in many cases over long times in a few iterations.
- In MD, we often run simulations with time steps chosen just below the stability limit (this often provides sufficient accuracy on the quantities of interest). There is hence no room for choosing $\delta t_C \gg \delta t_F$

- We thus turn to a different paradigm where $\mathcal{C}_{\Delta T}$ integrates a simpler dynamics than $\mathcal{F}_{\Delta T}$ (say with the same time step):
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- Relative error between consecutive parareal trajectories:

$$E(k,N) = \frac{\sum_{n=1}^{N} |q_n^k - q_n^{k-1}|}{\sum_{n=1}^{N} |q_n^{k-1}|}.$$

- We stop the algorithm at the first parareal iteration $\overline{k}$ for which

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Settings

- 128 tungsten atoms
- BCC lattice + periodic boundary conditions
- Langevin dynamics
- $\beta^{-1} = T = 300$ Kelvin (+ we have to revisit the time integrator)
- $V_{\mathcal{F}}$ - fine machine-learning interatomic potentials SNAP-56 (spectral neighbor analysis potentials): Wood, Cusentino, Wirth, Thompson, Physical Review B (2019)
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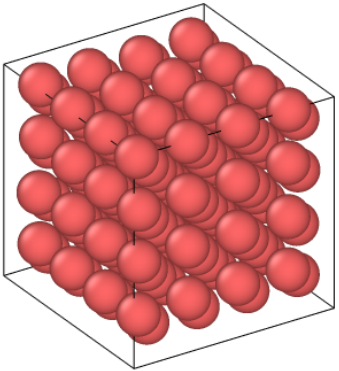

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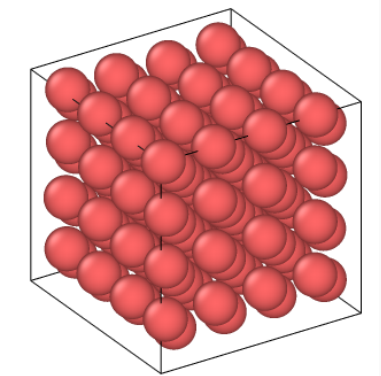

LAMMPS

We use LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) - a popular molecular dynamics software with a focus on materials modeling.

The parareal algorithm is written in Python and we use the following three LAMMPS include files

- **in.snap.WBe.simulation.box** - defines units, MD parameters, initial configuration of the atoms and simulation cell
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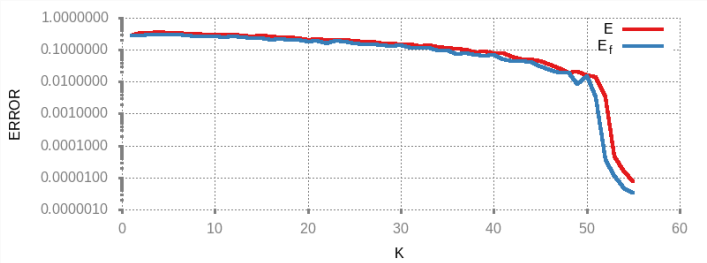
Plot of consecutive error for $N = 297$, $\Delta T = 0.005$



The gain $\Gamma = 5.4$. But for $N \geq 298$ it is not possible to work on the complete interval $[0, N]$ since, along the parareal iterations, the trajectory blows up

Remedy? Adaptive algorithm

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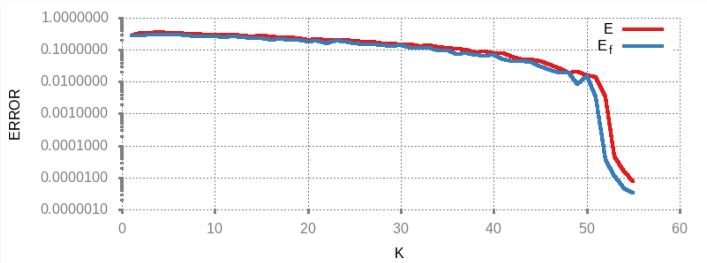

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- On the time-slab $[0, N]$, we run the parareal algorithm until E is
  - either smaller than the convergence threshold δ_{conv}
  - or larger than an explosion threshold δ_{expl} (attained at parareal iteration # k_{cur})
- In the blow-up case, for the iteration k_{cur}, we find the first time iteration $1 + \widetilde{m}_1 \leq N$ for which E exceeds δ_{expl}, and we shorten the slab to $[0, \widetilde{m}_1]$.
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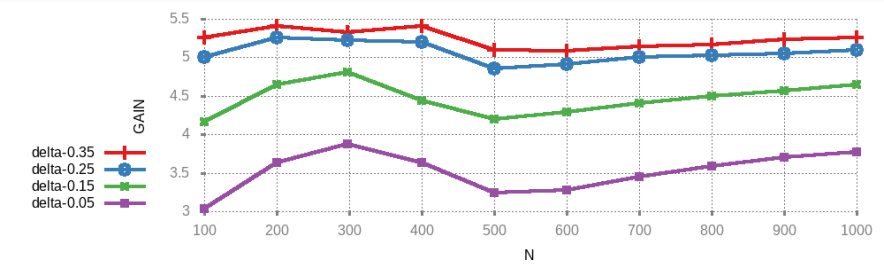

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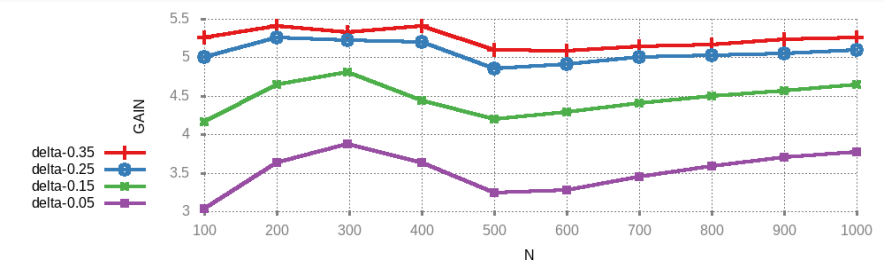

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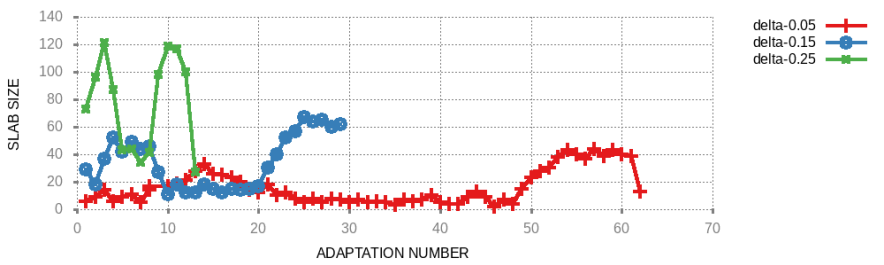
Explosion threshold

The slab sizes are such that $E \leq \delta_{\text{expl}}$:

- if δ_{expl} is chosen large, there is no adaptation: classical parareal
- if δ_{expl} is chosen small, the slabs are short: no parallelism anymore
- the optimal choice of δ_{expl} is somewhere in-between

List of the sizes of the time-slabs found by the algorithm for $N = 1000$:



Perspectives (all in progress)

Investigate the feasibility of the adaptive algorithm for realistic problems in the high performance computing context:

- Efficiency of the algorithm for computation of material properties:
  - elastic constants
  - dynamical quantities (diffusion coefficients of vacancies)
- Further comparison of the adaptive algorithm and the classical parareal
- Computational gain using different couples of SNAP potentials