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MaMiCo: Two-Way Coupled Parallel-in-Time Molecular-Continuum Flow Simulation?

PinT 2022: 11th Conference on Parallel-in-Time Integration

Tuesday, July 12th, 2022

Overview: Topics of this talk

What we already have:

1) Coupled molecular-continuum flow simulations
2) Filtering system for molecular dynamics (MD) data
3) MaMiCo coupling tool

What we want to do in the future:

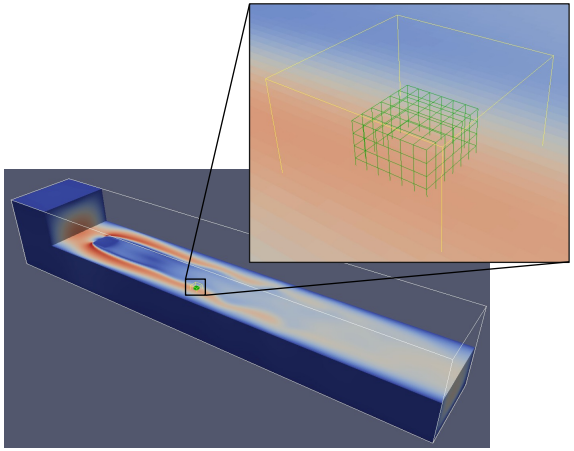
4) From Parareal to SPASD
5) Our new concept: modified SPASD variant for molecular-continuum flow in MaMiCo

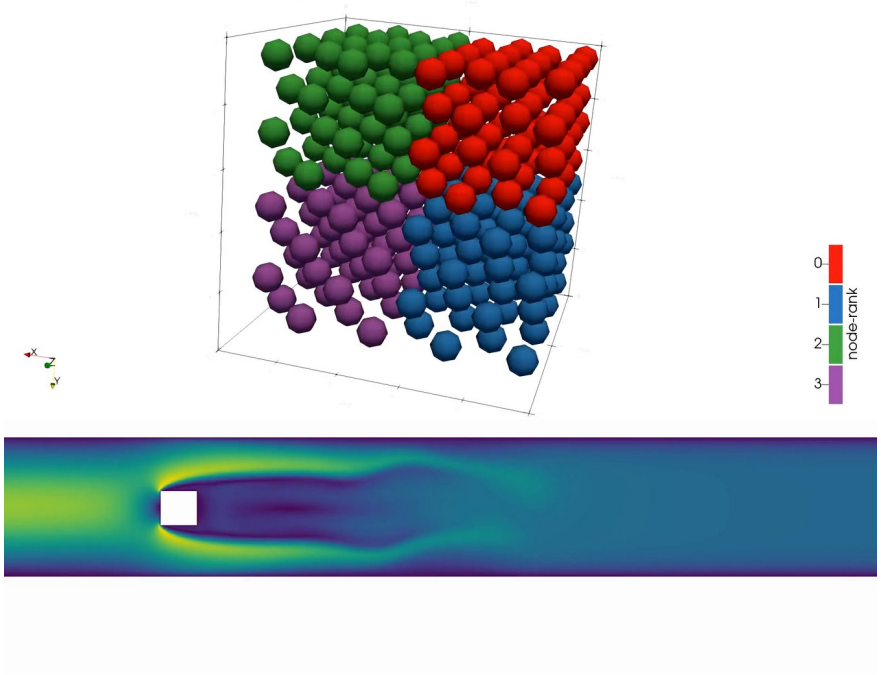
Main idea of this talk: Re-use existing continuum solver and various coupling methods for time parallelization of MD

Molecular-Continuum Coupling: Vortex Street Domain Decomposition Example

Lennard-Jones particle system (explicit time integration)

MD Domain and inner cells





3D transient flow simulation, Lattice-Boltzmann Method, on a GPU

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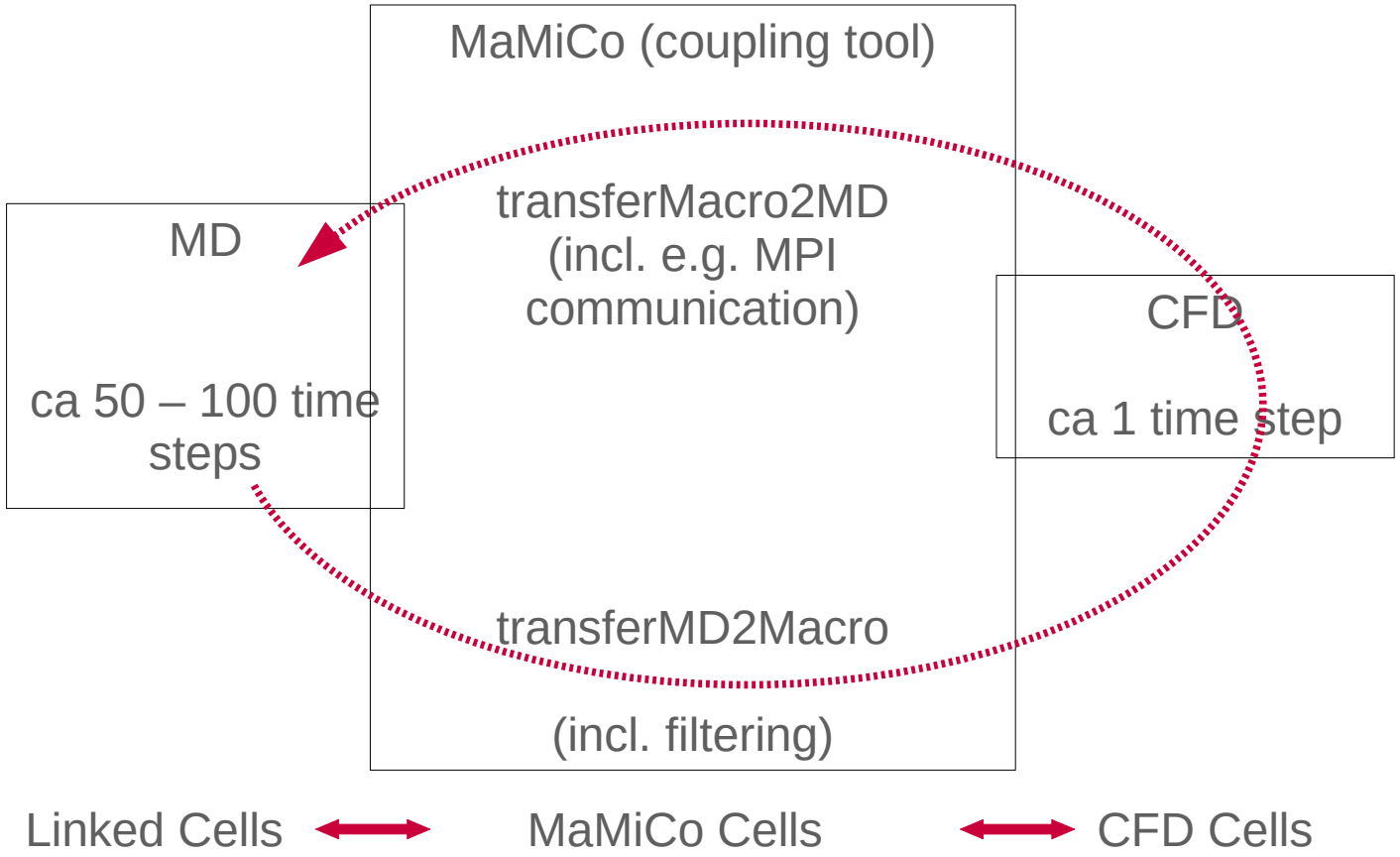
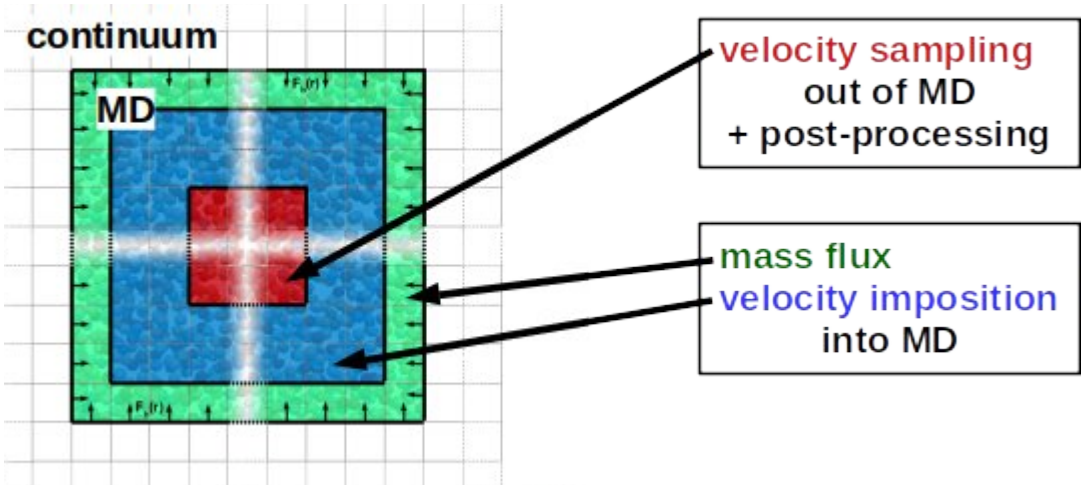
Outline

- Mol-cont
- Filtering
- MaMiCo
- Parareal / SPASD
- Outlook: PinT in MaMiCo
- Summary

Molecular-Continuum Coupling: A Coupling Cycle



Molecular-Continuum Coupling: Cell Meshes and Overlap Regions



- MD boundary: Zhou boundary force [Zhou et al. ‘14]
- Mass flux: Particle insertion with USHER [Delgado-Buscalioni et al. ‘03]
- Velocity imposition: Nie transfer strategy [Nie et al. ‘04]

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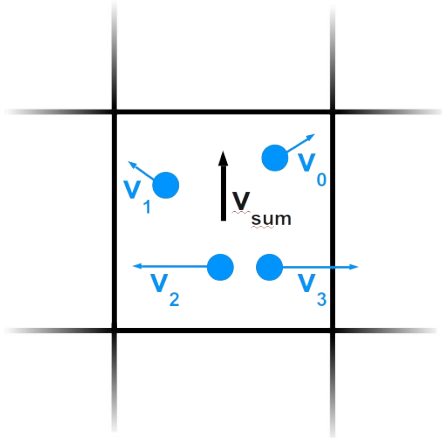
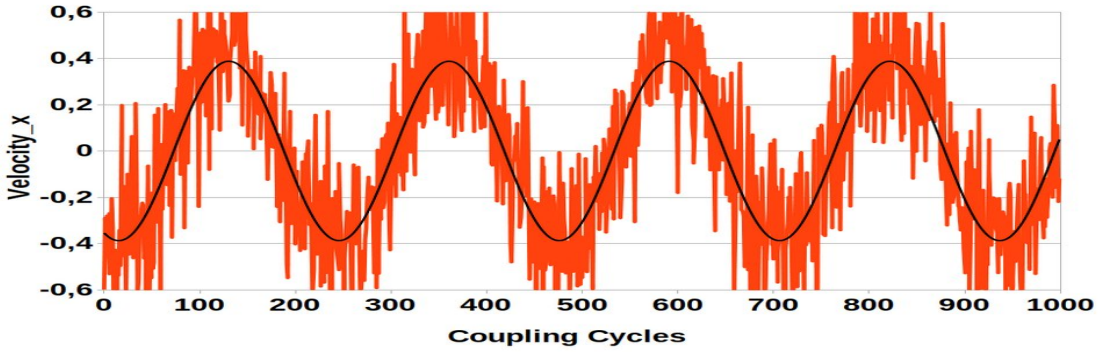
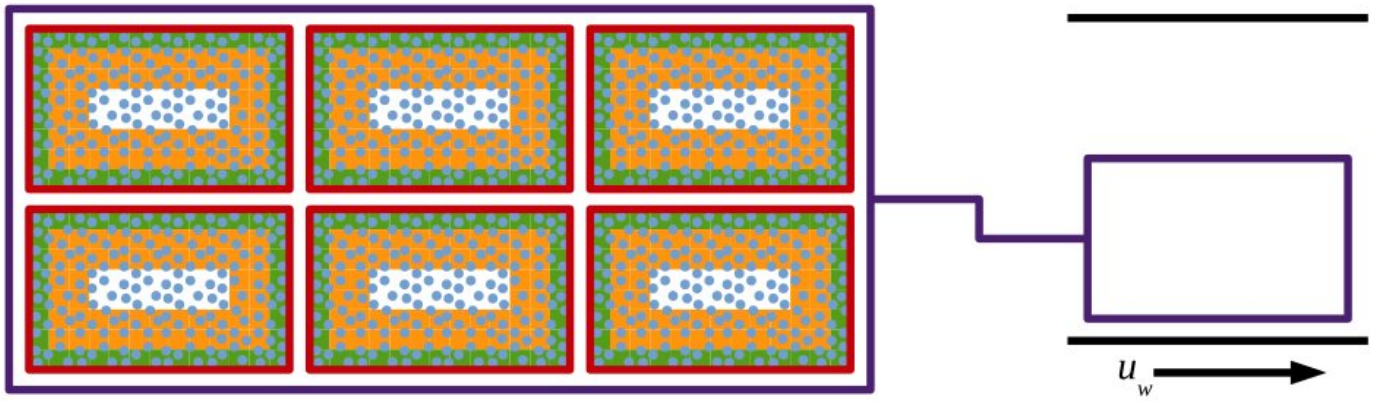
MD Quantity Sampling



1) Velocity, density, or other values for the coupling are sampled cell-wise from the particle system and then averaged:
   1) over all particles in a cell and
   2) over all (i.e. ca 50 – 100) MD time steps corresponding to a continuum time step (= coupling cycle)
2) Resulting quantities still fluctuate with high thermal noise:



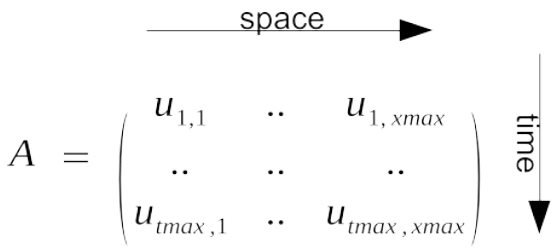
Multi-Instance Sampling



- Averaging over ensemble of MD systems
- Enables short coupling time intervals => transient simulation
- Computationally very expensive
  (N instances reduce standard deviation of noise only by a factor of $N^{1/2}$)
- We can modify N at runtime: ‘dynamic MD’

Noise Filtering with POD / PCA

- View flow quantities, e.g. a velocity component u(t, **x**), as matrix

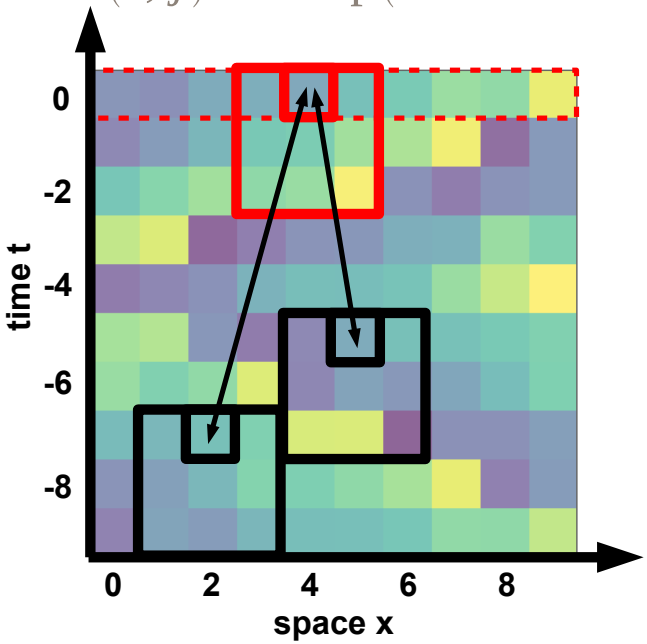


- Compute temporal auto-correlation covariance matrix $C = A\,A^T$
- Perform EVD of C
- Temporal modes $a_k(t)$ are eigenvectors of C
- Compute spatial modes $\varphi_k(x) = \sum_t A(t,x) \cdot a_k(t)$
- Obtain filtered smooth $\bar{u}(t, \mathbf{x})$ as sum over $\varphi_k(x)\, a_k(t)$ for a few k

Noise Filtering with Non-Local Means (NLM)

$$NLM[v](i) = \frac{1}{\sum_{j \in I} w(i,j)} \sum_{j \in I} w(i,j) v(j)$$

$$w(i,j) = \exp\left(-\frac{max(dist(i,j) - 2\sigma^2, 0)}{h^2}\right) * \frac{1}{1-t}$$



- We define a similarity metric dist(i,j) to compare local neighborhoods i.e. 4D space-time windows around i and j
- NLM computes weighted average of input data, weighted by similarity
- Exploits redundancy of given information to remove noise

Noise Filtering with Non-Local Means (NLM)

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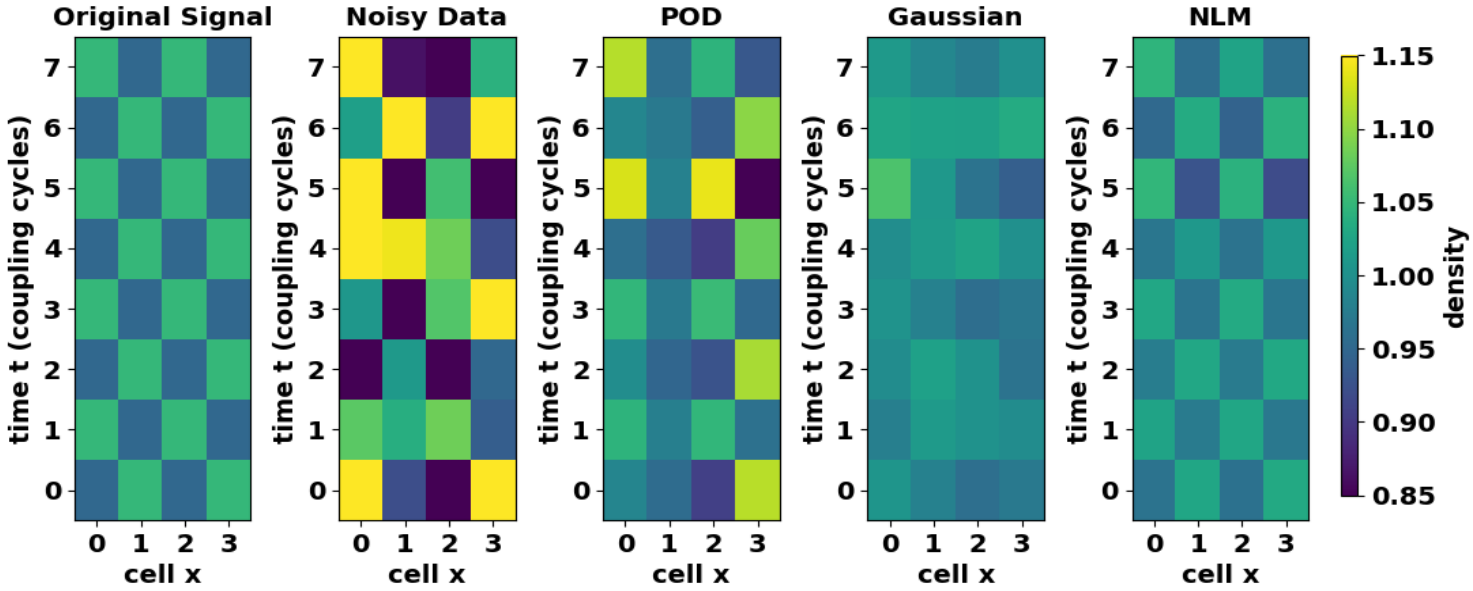

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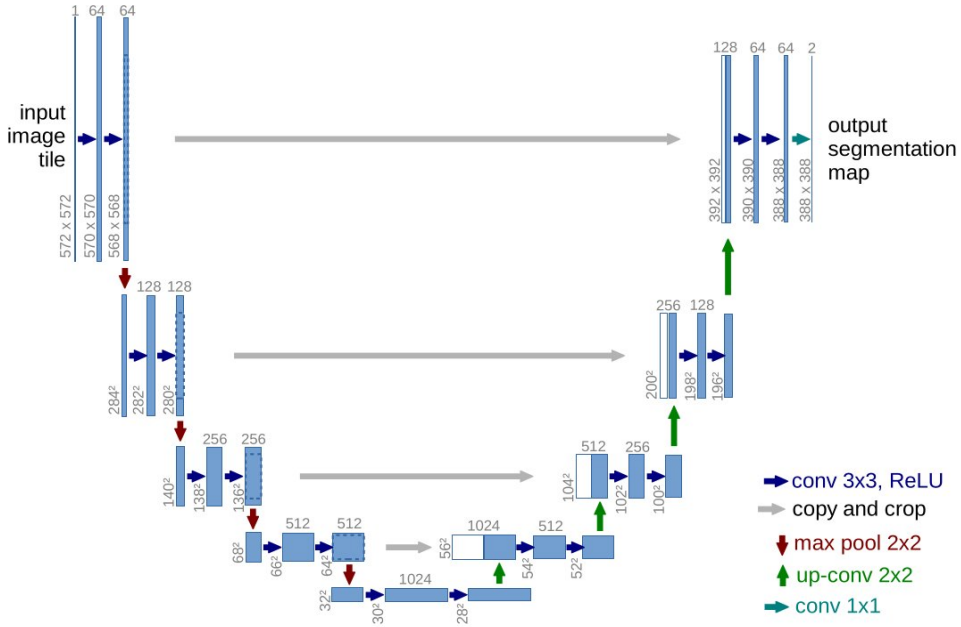
ML based Filtering, RNN + U-Net

- Current WIP: Hybrid ML model based on RNN + U-Net
- Can learn and predict MD data, so that computationally expensive MD computations can be skipped



[Ronneberger et al. '15]

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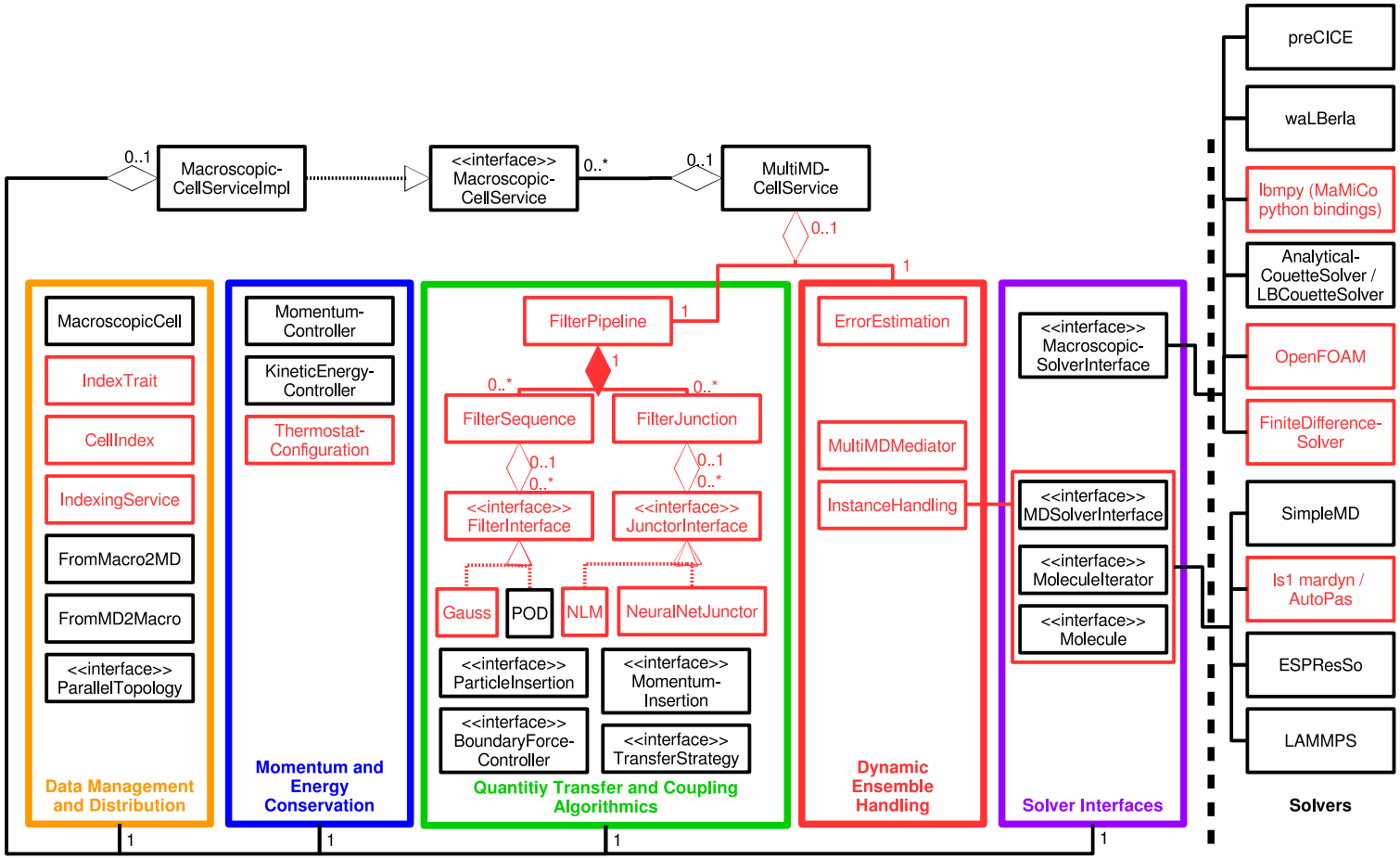
MaMiCo Coupling Tool / C++ Framework



From Parareal to SPASD

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Algorithm 1 Traditional Parareal algorithm

1: Initialization:
   Compute initial iteration with Coarse propagator: $U_0^{n+1} = \mathcal{G}(U_0^n)$ for all $0 \leq n \leq N$.
2: Assume sequence $\{U_k^n\}$ is known for some $0 \leq n \leq N$ and $k \geq 0$:
   Correction:
      (a) Advance with Coarse propagator in serial: $\mathcal{G}(U_k^n)$ for all $0 \leq n \leq N-1$.
      (b) Advance with Fine propagator in parallel: $\mathcal{F}(U_k^n)$ for all $0 \leq n \leq N-1$.
      (c) Compute correction: $\delta_k^n = \mathcal{F}(U_k^n) - \mathcal{G}(U_k^n)$ for all $0 \leq n \leq N-1$.
   Prediction:
      Advance with Coarse propagator in serial: $\mathcal{G}(U_{k+1}^n)$ for all $0 \leq n \leq N-1$.
   Refinement:
      Combine the correction and prediction terms: $U_{k+1}^{n+1} = \mathcal{G}(U_{k+1}^n) + \mathcal{F}(U_k^n) - \mathcal{G}(U_k^n)$
3: Repeat *Step 2* to compute U_{k+2}^n for all $1 \leq n \leq N$ until a termination-condition is satisfied.

[Blumers et al. ‘19]

From Parareal to SPASD

1) ‘SPASD’ = ‘Supervised PinT algorithm for long-time Lagrangian simulations of stochastic dynamics’ [Blumers et al. ‘19]
2) Basic idea: Use a low-dimensional macroscopic system as a coarse predictor to supervise state of particle simulator
3) Results of particle system correct the mean-field flow prediction and provide microscopic details
4) Unlike traditional Parareal: Macro-model can be inconsistent with microscale description, but the deviation is corrected by SPASD algorithm

From Parareal to SPASD

Algorithm 2 SPASD

1: Initialization:

Compute initial iteration with Coarse propagator: $U_0^{n+1} = \mathcal{G}(U_0^0)$ for all $0 \leq n \leq N$.

2: Assume sequence $\{U_k^n\}$ is known for some $0 \leq n \leq N$ and $k \geq 0$:

Correction:

(a) Filter solution to remove noise: $\mathcal{F}\{U_k^n\}$

(b) Advance with Coarse propagator in serial: $\mathcal{G}(\mathcal{F}\{U_k^n\})$ for all $0 \leq n \leq N-1$.

(c) Map the macroscopic state to microscopic space: $\mathcal{R}\{U_k^n\}$

(d) Advance with Fine propagator in parallel: $\mathcal{F}(\mathcal{R}\{U_k^n\})$ for all $0 \leq n \leq N-1$.

(e) Project the microscopic state to macroscopic state: $\mathcal{P}\{\mathcal{F}(\mathcal{R}\{U_k^n\})\}$

(f) Compute the correction: $\delta_k^n \equiv \mathcal{P}\{\mathcal{F}(\mathcal{R}\{U_k^n\})\} - \mathcal{G}(\mathcal{F}\{U_k^n\})$ for all $0 \leq n \leq N-1$.

Prediction:

Advance with Coarse propagator in serial: $\mathcal{G}(\mathcal{F}\{U_{k+1}^n\})$ for all $0 \leq n \leq N-1$

Refinement:

Combine the correction and the prediction terms:

$U_{k+1}^{n+1} = \mathcal{G}(\mathcal{F}\{U_{k+1}^n\}) + \mathcal{P}\{\mathcal{F}(\mathcal{R}\{U_k^n\})\} - \mathcal{G}(\mathcal{F}\{U_k^n\})$ for all $0 \leq n \leq N-1$.

3: Repeat *Step 2* to compute U_{k+2}^n for all $1 \leq n \leq N$ until a termination-condition is satisfied.

[Blumers et al. ‘19]

From Parareal to SPASD

1) Unlike traditional Parareal: fine and coarse propagator encompass other operations now:
   1) Mapping operator $\mathscr{R}$ (Macro → MD)
   2) Projection operator $\mathscr{P}$ (MD → Macro)
   3) Filtering operator $\mathscr{F}$ (to remove stochastic noise)
2) These operators link the two scales, i.e. translate between microscopic and macroscopic model

From Parareal to SPASD

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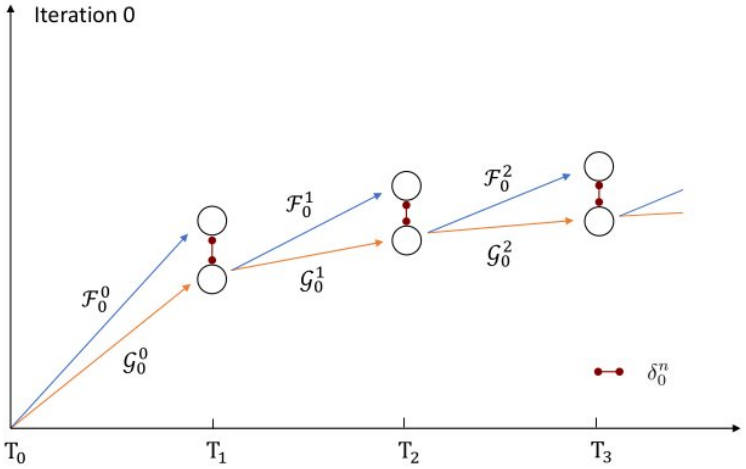

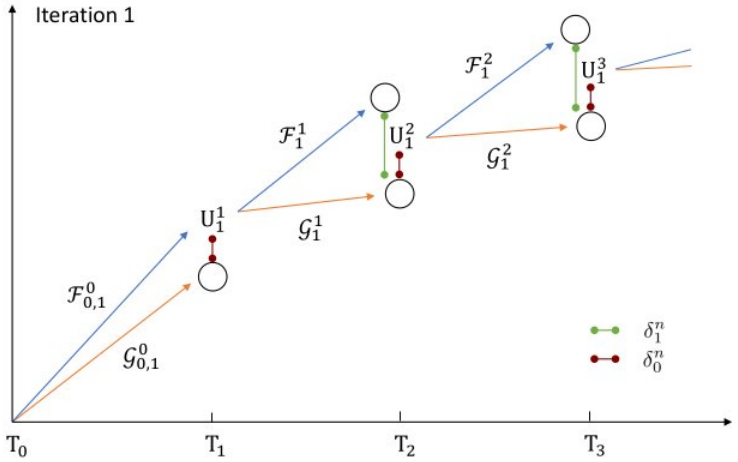

[Blumers et al. '19]

Our new concept: modified SPASD variant for molecular-continuum flow

1) In original SPASD, the continuum solver is introduced only as a coarse predictor to enable time parallelization of the particle system
2) For coupled molecular-continuum flow, we already have a continuum solver, but for a different purpose: To span larger spatial scales / extend the simulation domain
3) Idea: Use continuum solver for **both** now
4) Mapping operation to DPD is cheap (use flow quantity directly), mapping operation to MD requires interpolation, velocity-relaxation, equilibration of particle system etc

New concept: SPASD in MaMiCo

Idea: Re-use the existing feature implementation, which were made for molecular-continuum coupling, to enable parallel-in-time computations, examples:

1) Mapping operation $\mathscr{R}$ to MD requires to initialize a new particle simulation instance (at a 'future' state), but we have this already: Multi-instance MD handling, dynamic MD + checkpoints, etc ...

2) Projection $\mathscr{P}$ (MD $\rightarrow$ Macro) can be complex (quantity sampling, shift-timestep etc.) but we also have this already :-)

New concept: SPASD in MaMiCo

Idea: Re-use the existing feature implementation, which were made for molecular-continuum coupling, to enable parallel-in-time computations, examples:

3) Mapping operation $\mathscr{R}$ to MD requires interpolation, velocity-relaxation, equilibration of particle system etc,
but we have this already: USHER, Nie coupling, momentum-insertion, transfer strategy …

4) Filtering $\mathscr{F}$ between propagators can be complex (transient 3D data), but we have this already:
MaMiCo filtering subsystem, POD, NLM, ML module :-)

Summary

1) Molecular-Continuum simulations extend the applicability of MD to larger simulation domains and time scales
2) MaMiCo: open-source C++ mol-cont coupling framework

   https://github.com/HSU-HPC/MaMiCo
3) SPASD: Extended Parareal with additional mapping, projection, filtering operations, for supervised PinT particle method
4) Future idea: Re-use the existing feature implementations, which were made for molecular-continuum coupling, to enable parallel-in-time computations in MaMiCo