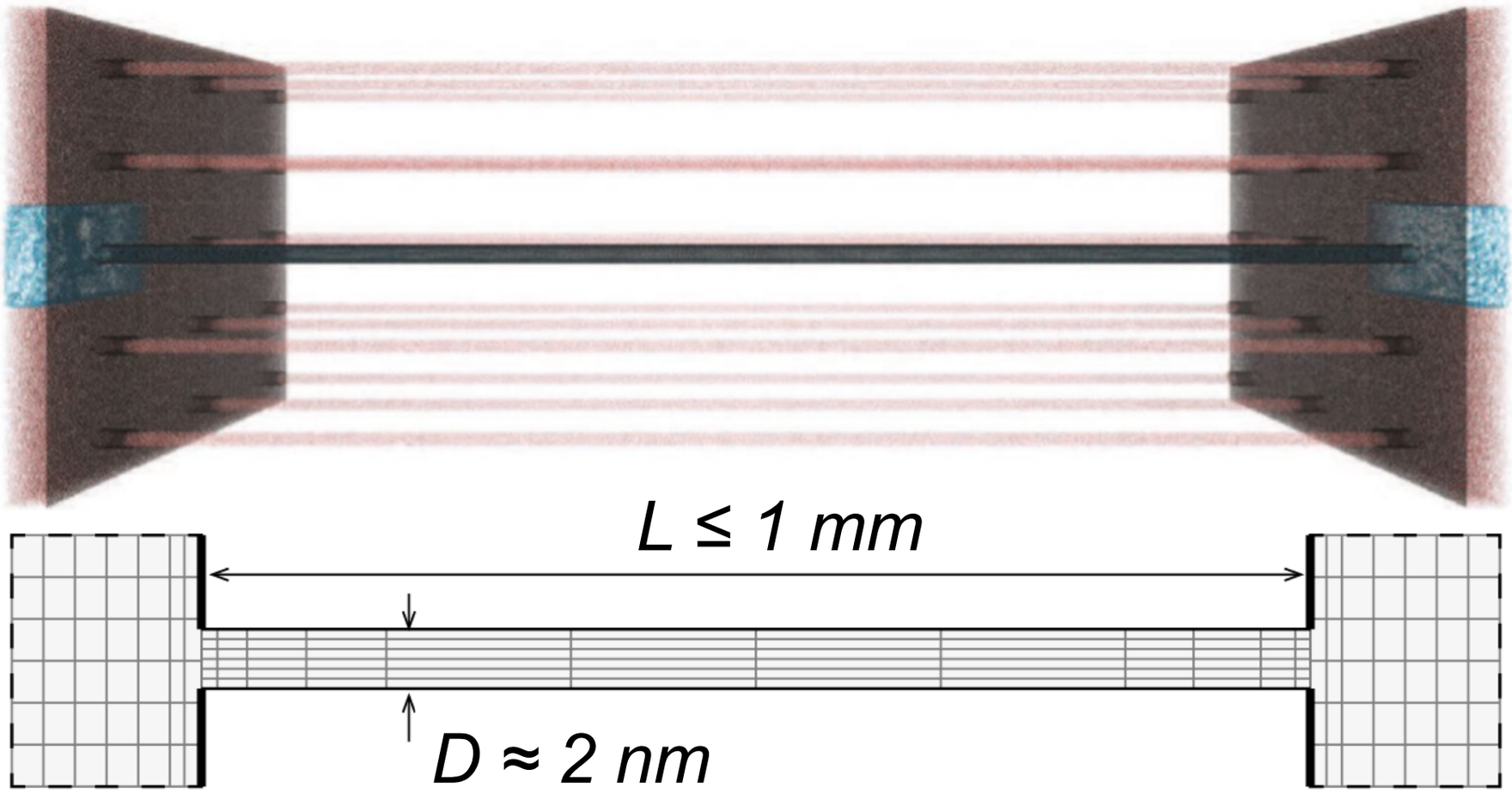
Coupling Software for Massively Parallel Molecular-Continuum Flow Simulation

Philipp Neumann

PIRE Annual Meeting

Hamburg, 19 June 2018

Motivation



K. Ritos et al. Microfluid Nanofluid 19:997-1010, 2015

- Water flow through carbon nanotube-based filtration membrane
- Navier-Stokes-Fourier description inaccurate in tubes
- Molecular dynamics simulation of complete system not affordable

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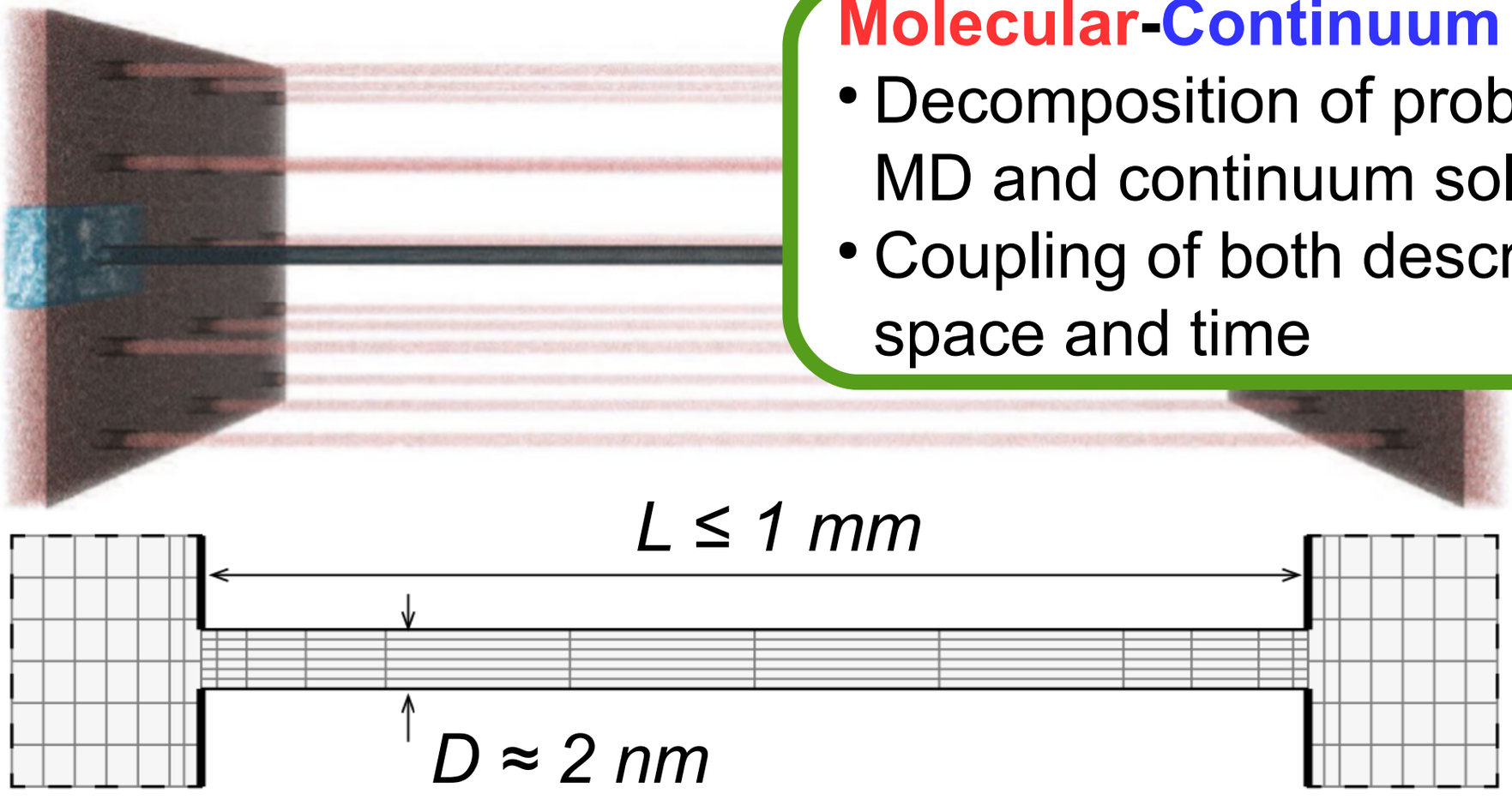

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Molecular-Continuum Methods

- Decomposition of problem into MD and continuum solver
- Coupling of both descriptions in space and time

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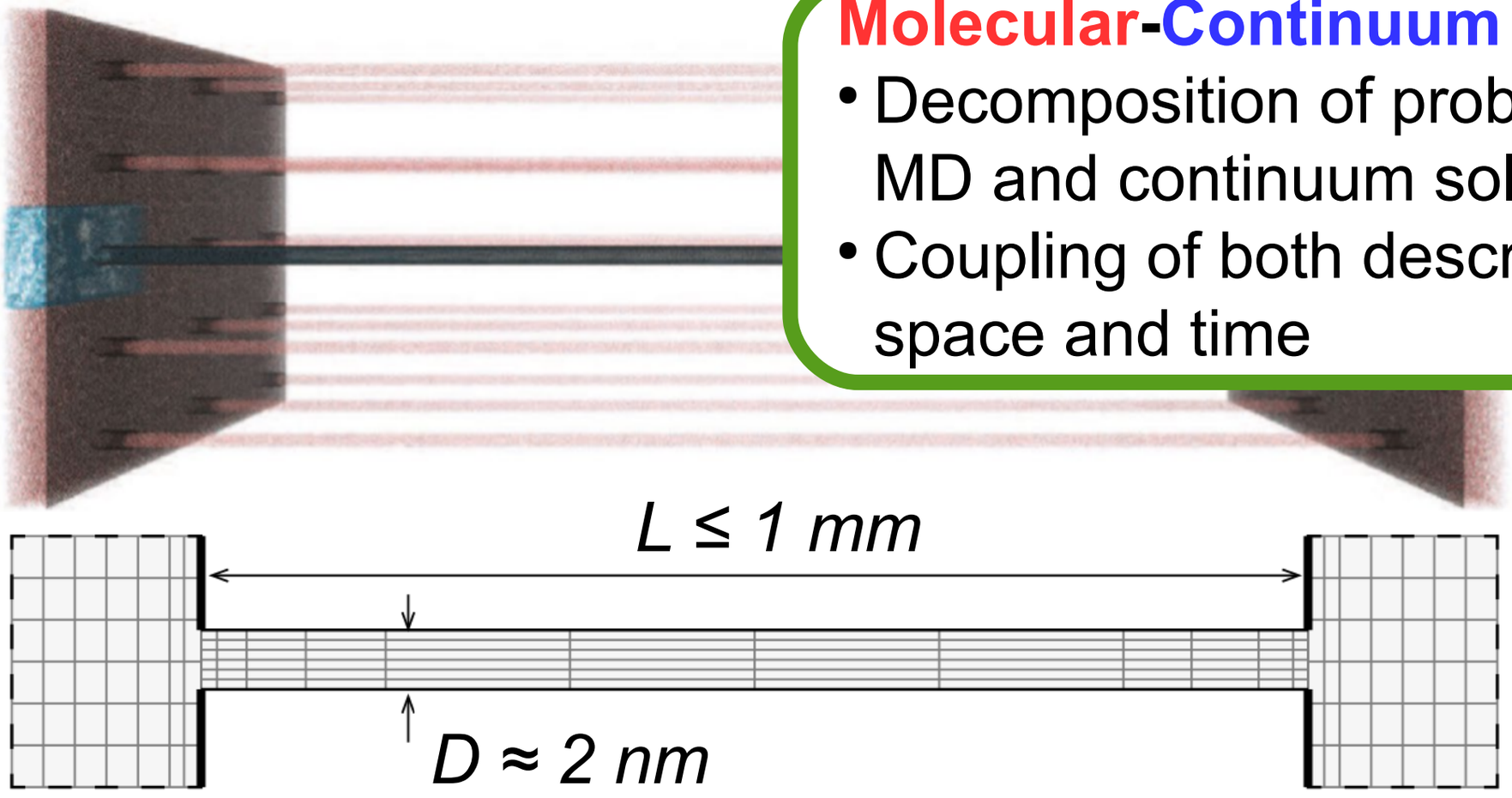

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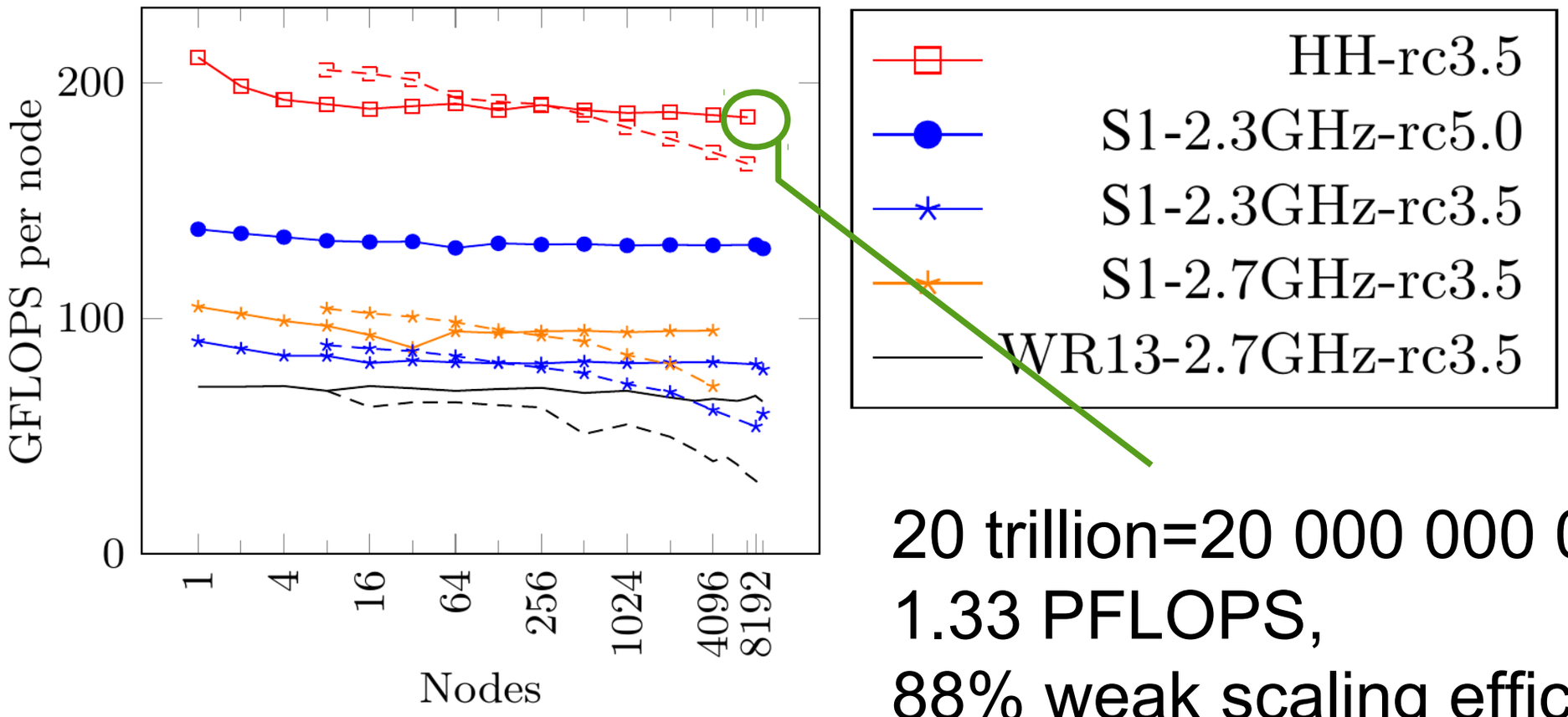
Outline

Molecular Dynamics and Its Limits

Macro-Micro-Coupling Tool (MaMiCo)
- Software Design
- Software Flexibility
- Multi-Instance Sampling

Summary and Outlook

Short-Range MD: Multi-Node



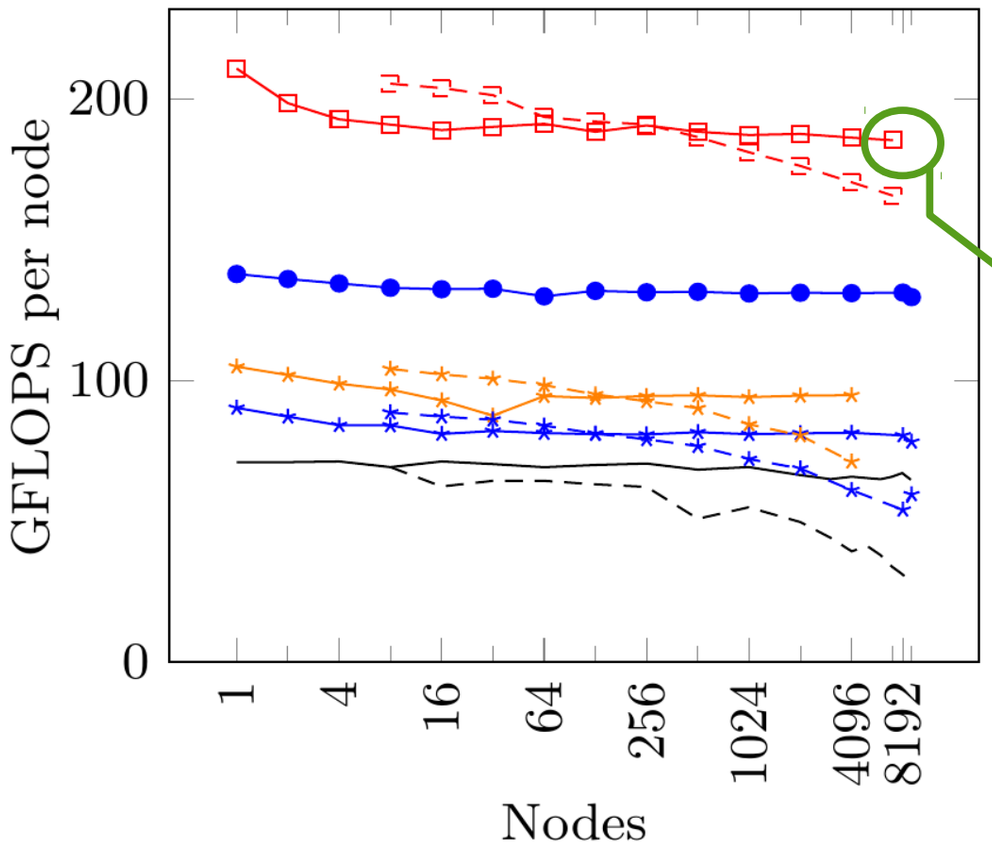
20 trillion=20 000 000 000 000 atoms,
1.33 PFLOPS,
88% weak scaling efficiency

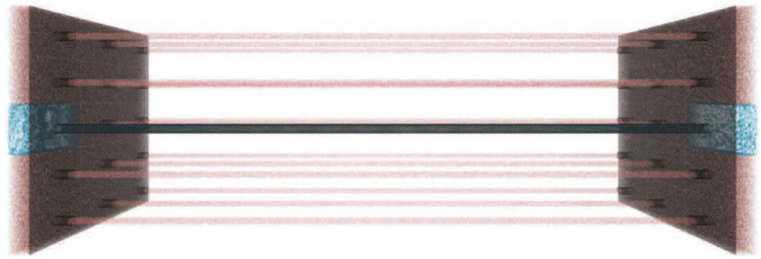
Example: ls1 mardyn

- Linked cells-based short-range MD
- Vectorized kernels via SIMD wrappers
- Different OpenMP schemes based on cell coloring and slicing
- MPI-parallel: Non-blocking collectives etc.

Tchipev, Seckler, …, Bungartz, Neumann. TweTriS: Twenty Trillion-atom Simulation. Submitted, 2018

Short-Range MD: Multi-Node





1 “SLJ-water” tube
↔ 100 000 000 atoms
but time scale O(sec)!

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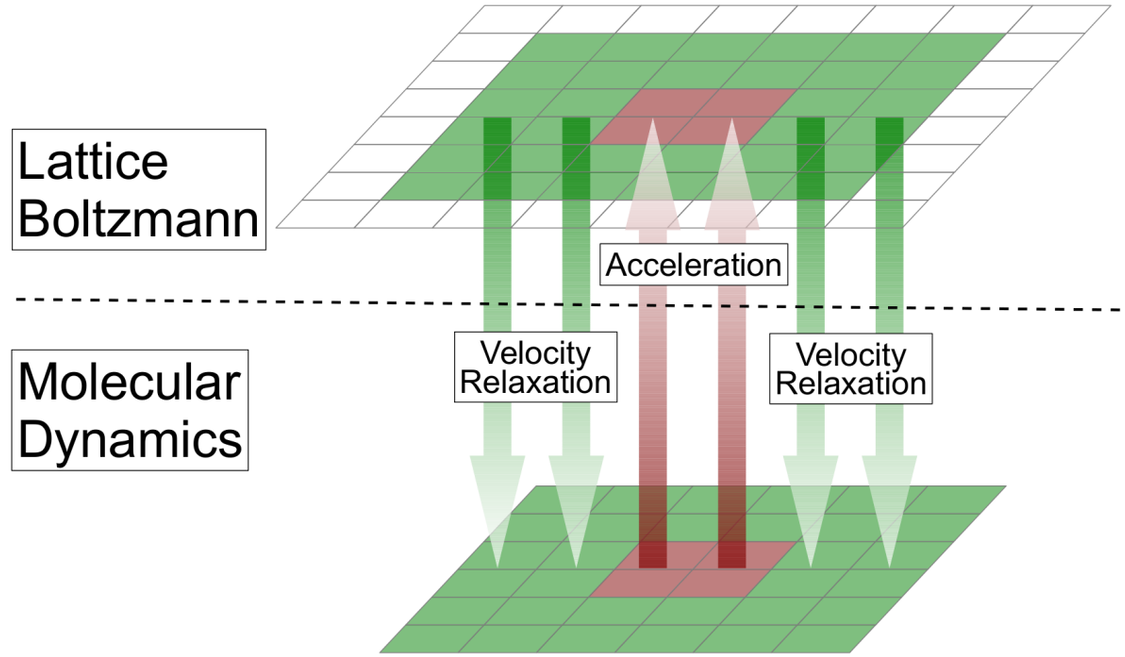
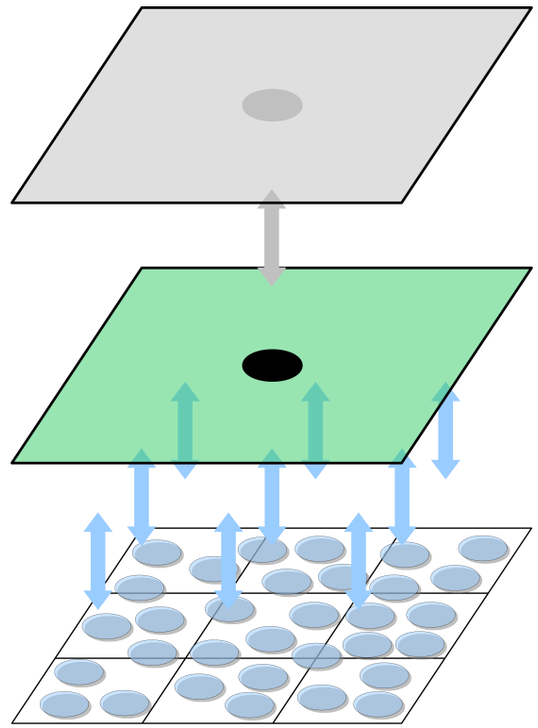
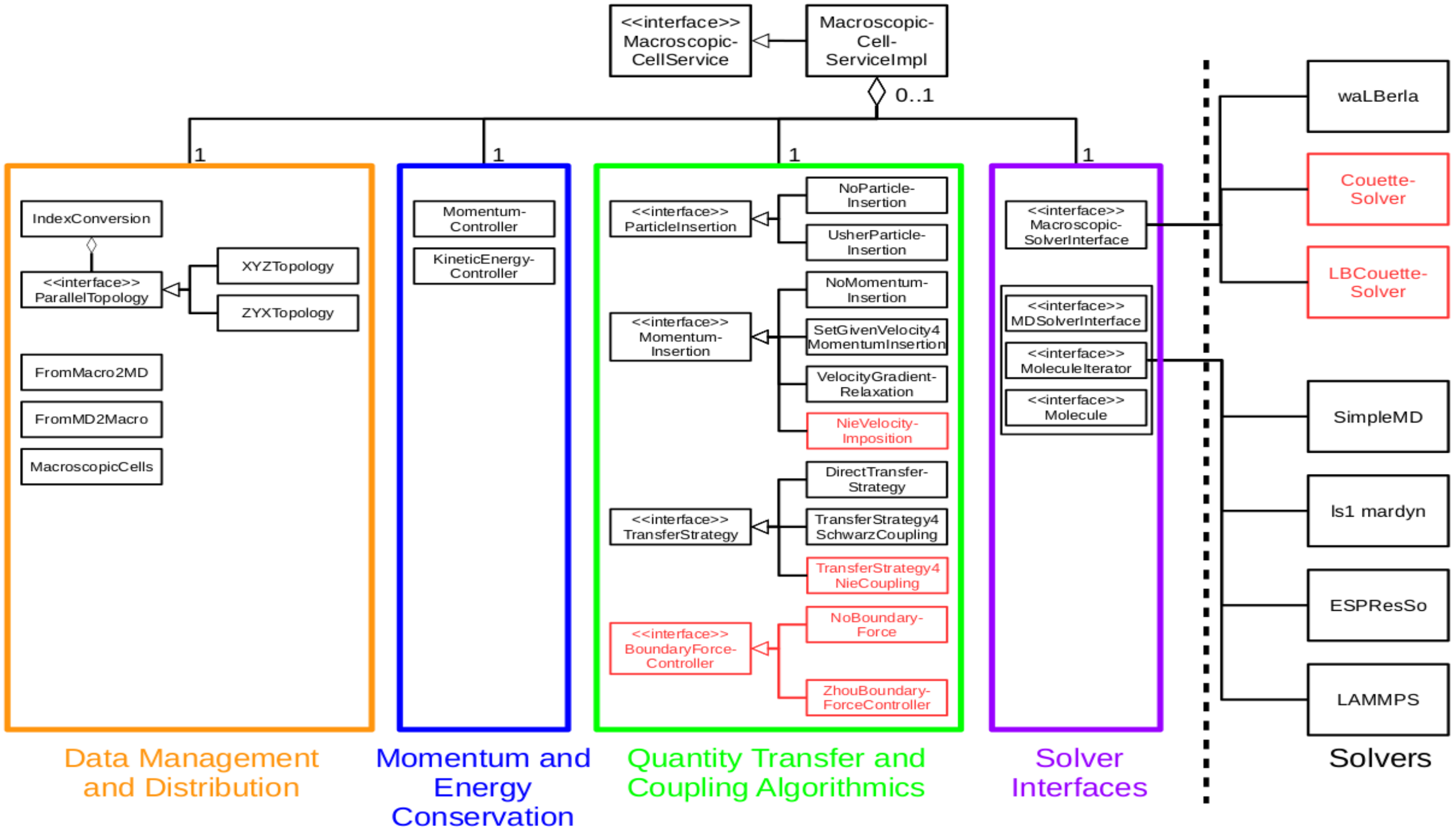
Macro-Micro-Coupling Tool (MaMiCo)

- C++-based, MPI-parallel
- 2D/3D support
- Steady-state and transient coupling
- Cell structure (re)used on particle solver side
- Macroscopic cells
  - used for data exchange with mesh-based solver
  - stored on particle solver process
- Interfaces
  - on particle side:
    - Molecule → access single particles
    - MoleculeIterator → traverse particles
    - MDSolverInterface → global properties of particle solver
  - on mesh-based solver side:
    - MacroscopicSolverInterface
      → contains cell-rank-mapping to send/recv data



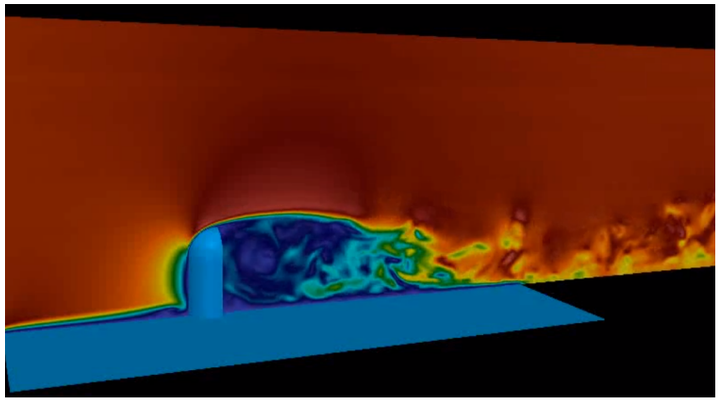


MaMiCo: Separation of Concerns

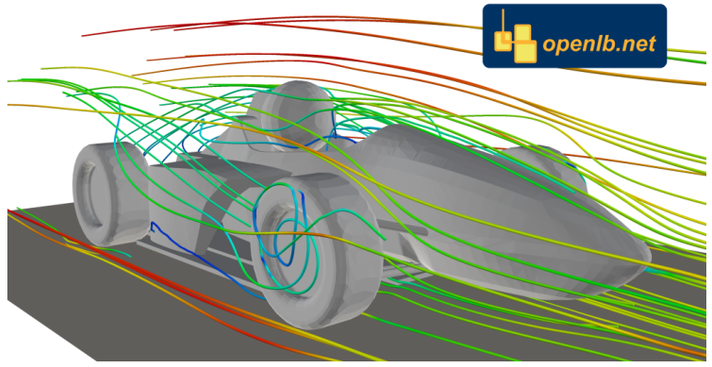


Neumann, Bian. Comput Phys Commun 220:390-402, 2017

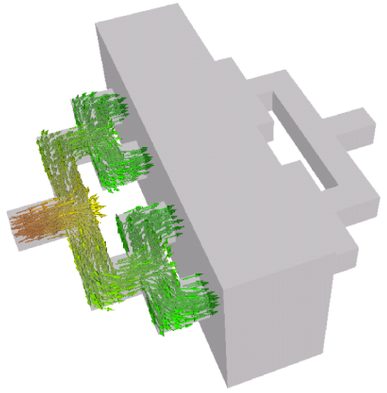
MaMiCo: Flexibility



Palabos



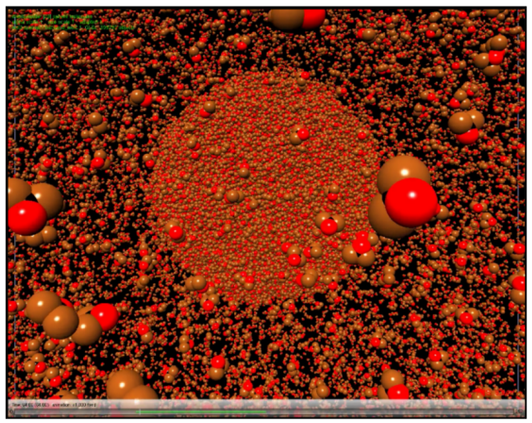
OpenLB



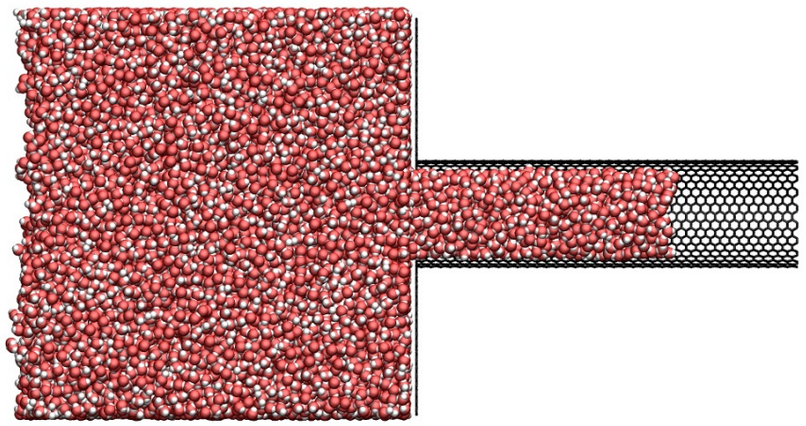
PeanoLB

waLBerla

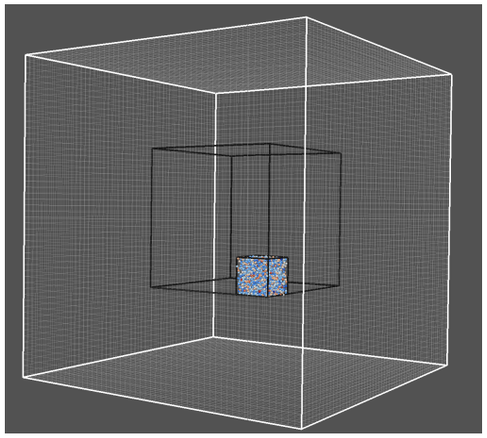
ESPResSo



ls1 mardyn



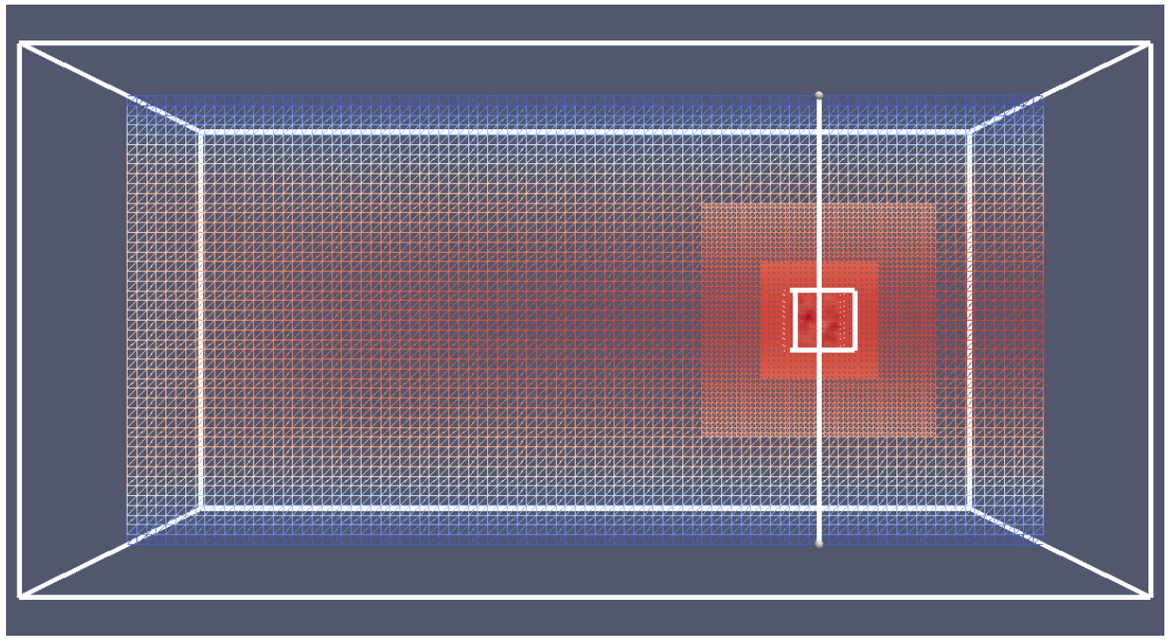
LAMMPS

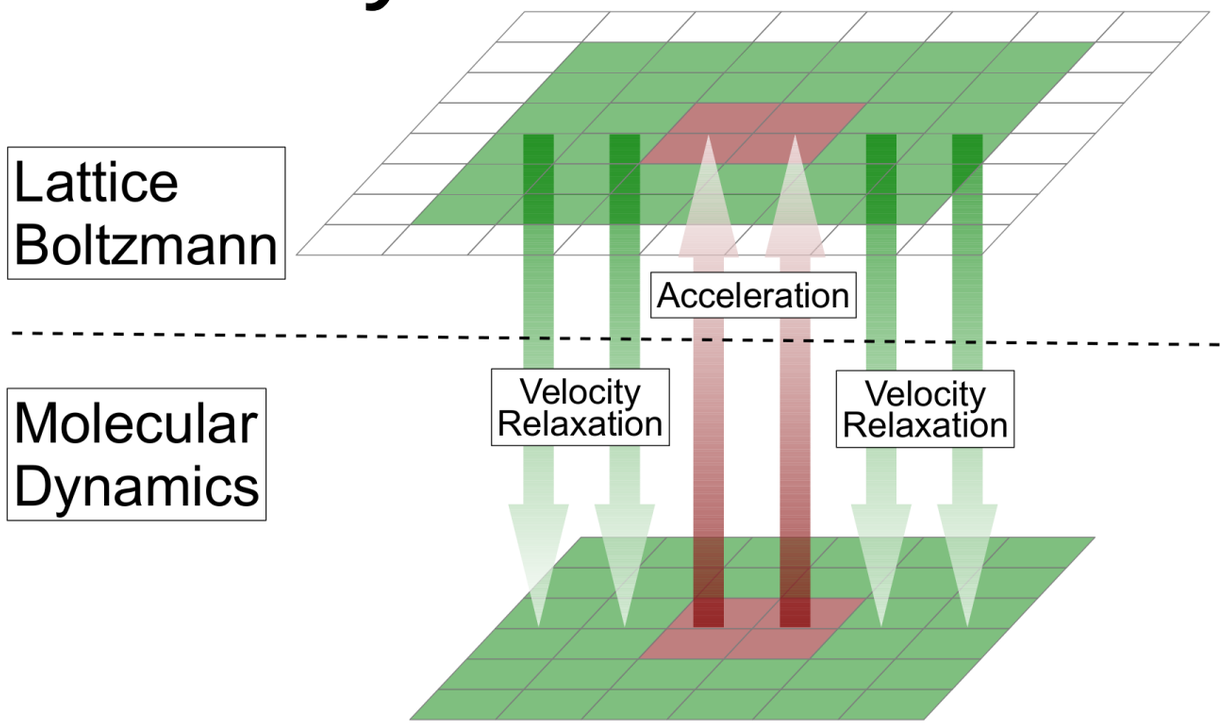


SimpleMD

P. Neumann et al. Comput Phys Commun. 200, pp. 324-335, 2016

MaMiCo: Flexibility – Case Study Channel Flow





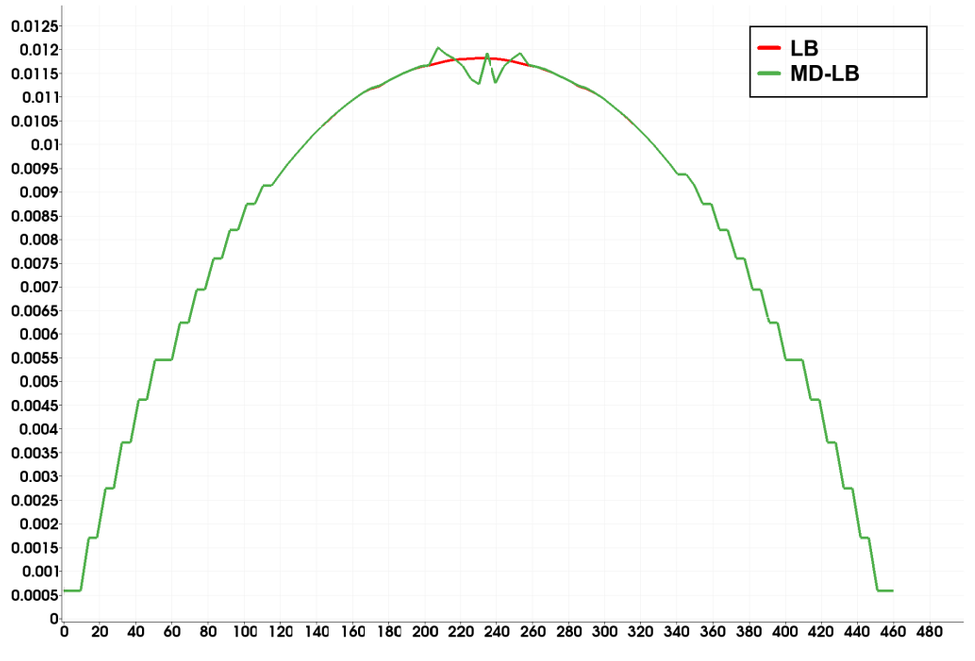
- 3D coupling based on velocity exchange
- MD → LB: Acceleration

$$f_i(\mathbf{x} + \mathbf{c}_i dt, t + dt) = f_i(\mathbf{x}, t) - \frac{1}{\tau}(f_i - f_i^{eq}) + g_i$$

$$g_i = w_i \frac{\mathbf{c}_i \mathbf{F}}{c_s^2}, \quad \mathbf{F} = \mu \cdot (\mathbf{u}^{target} - \mathbf{u}),\ \mu \in (0, 1)$$

- LB → MD: Velocity relaxation

$$\mathbf{v}_i \leftarrow \mathbf{v}_i + \lambda \cdot (\mathbf{v}_{local}^{target} - \mathbf{v}_{local}^{avg}),\ \lambda \in (0, 1)$$



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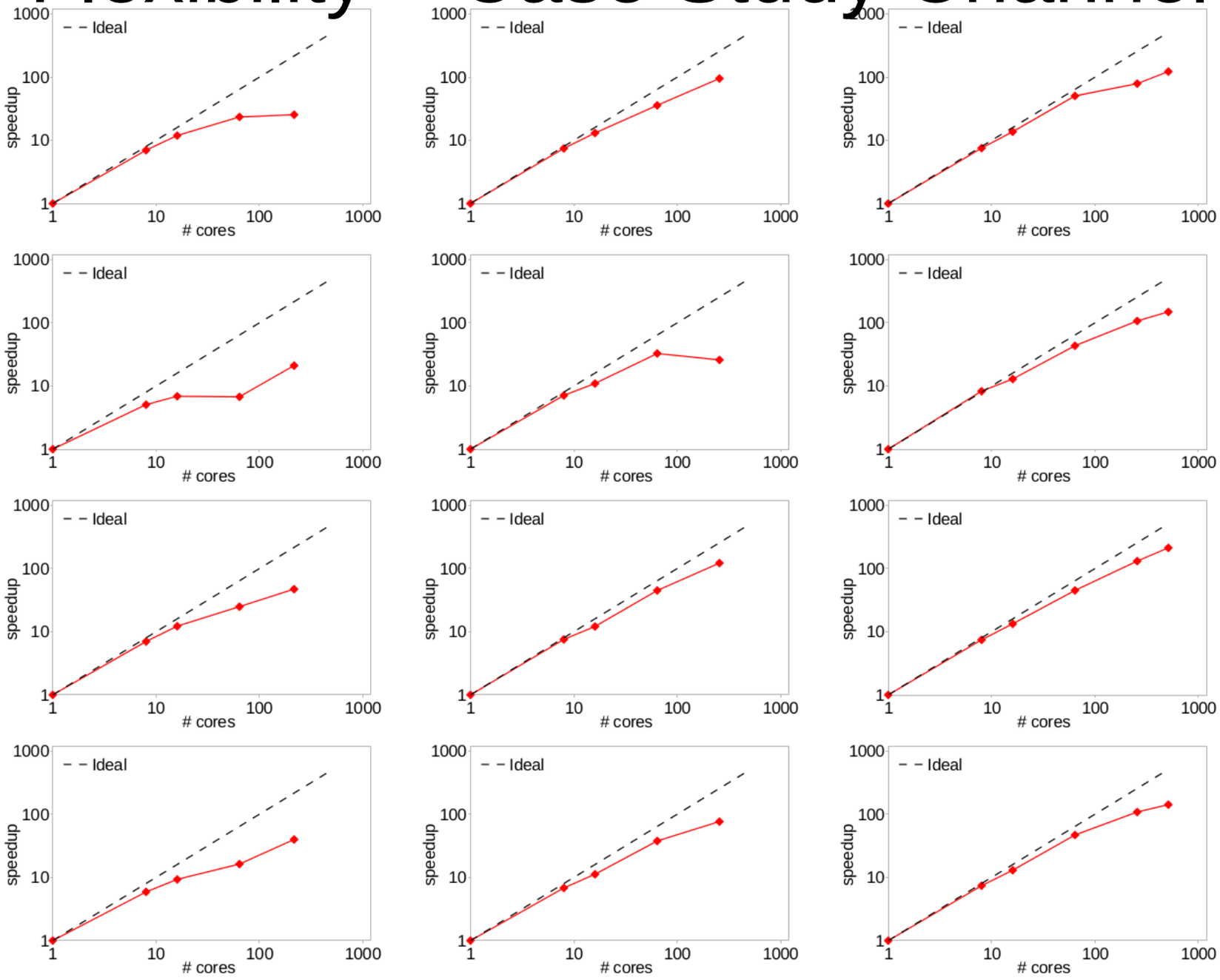

MD-30 MD-60 MD-120

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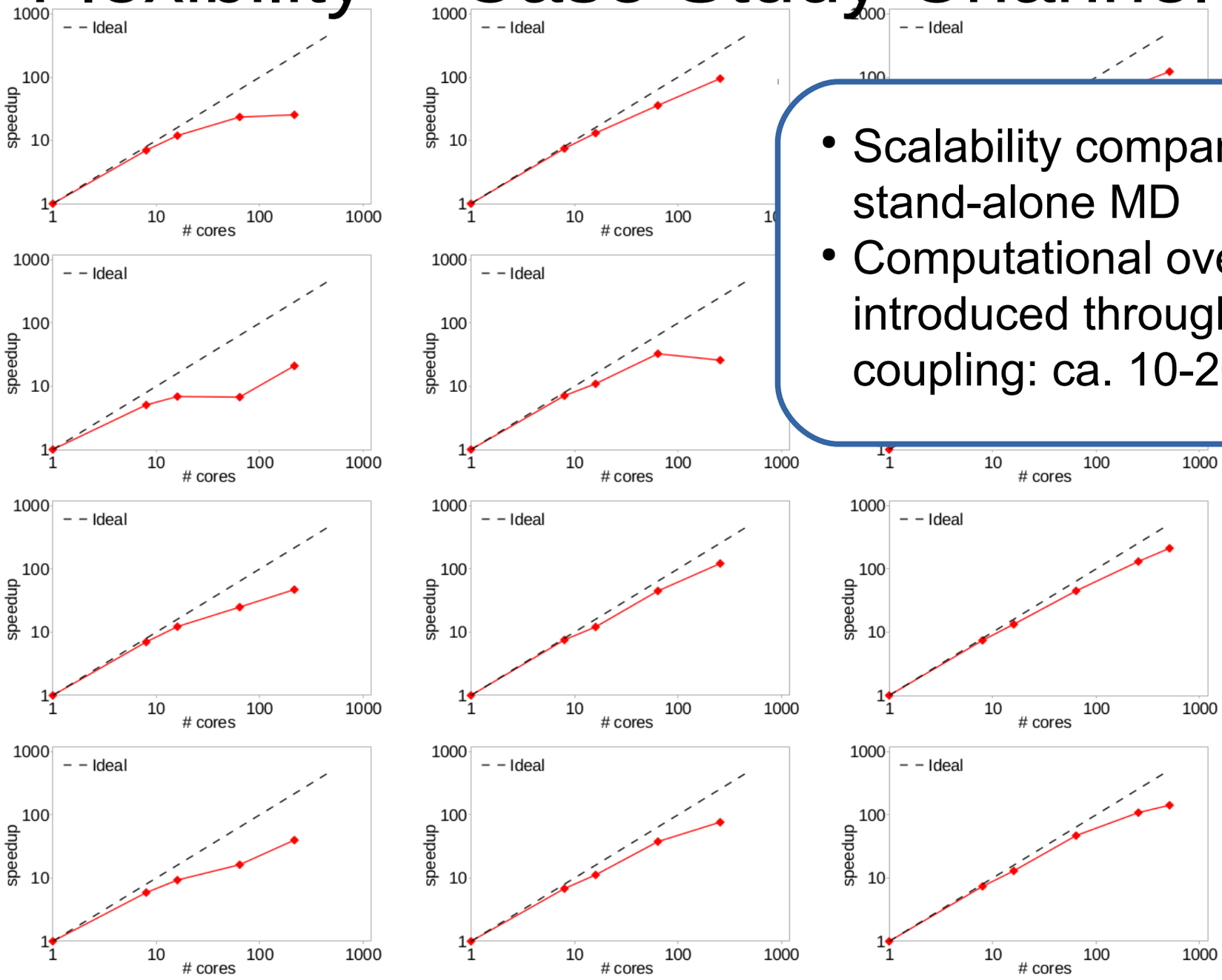


MD-30 MD-60 MD-120

- Scalability comparable to stand-alone MD
- Computational overhead introduced through coupling: ca. 10-20%

P. Neumann et al. Comput Phys Commun. 200, pp. 324-335, 2016

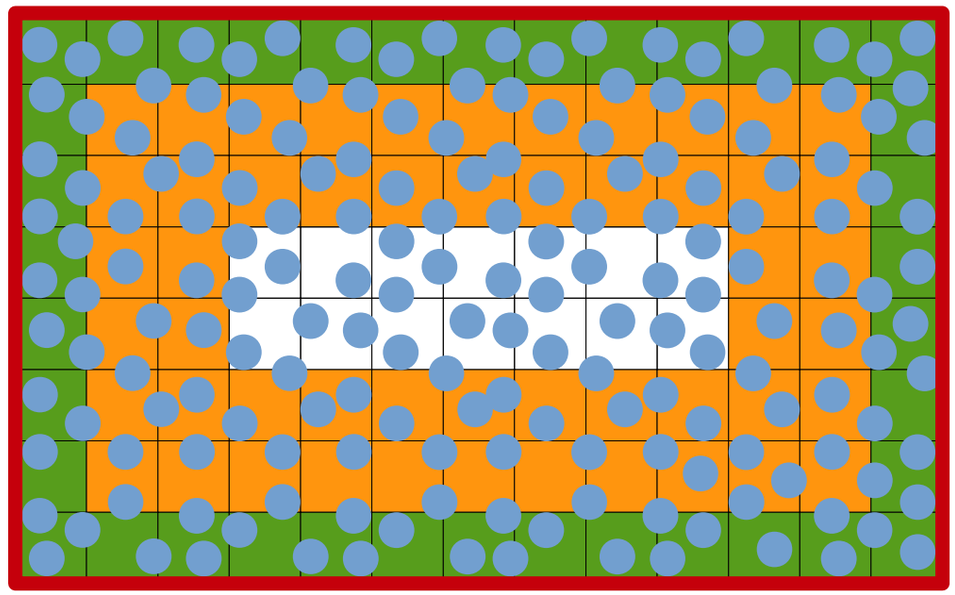
MaMiCo: Transient Coupling

- 3D one-way coupling
  (but two-way communication)
- Continuum → MD: **Momentum imposition**[1]

$$\frac{d^2\mathbf{x}_i}{dt^2} = \frac{1}{m}\mathbf{F}_i - \frac{1}{Nm}\sum_{k=1}^{N}\mathbf{F}_k + \frac{D\mathbf{u}_{LB}}{Dt}$$

- Continuum → MD: **Mass flux imposition**[2,3]
  (USHER scheme)
- MD open boundaries: **Forcing scheme**[4]
- Couette flow: Parameters (MD | DPD)

dx=2.5, dt^{MD}=0.005	dx=1.0, dt^{DPD}=0.005
(ρ,T)=(0.81,1.1)	(ρ,T)=(3.0,1.0)
u_{wall}=1.5, dt^{LB}=0.5	u_{wall}=1.5, dt^{LB}=0.5
H=50.0, H^{MD}=30.0	H=50.0, H^{DPD}=30.0



1 Nie et al. J Fluid Mech 500:55-64, 2004
2 Delgado-Buscalioni, Coveney. J Chem Phys 119(2): 978-987, 2003
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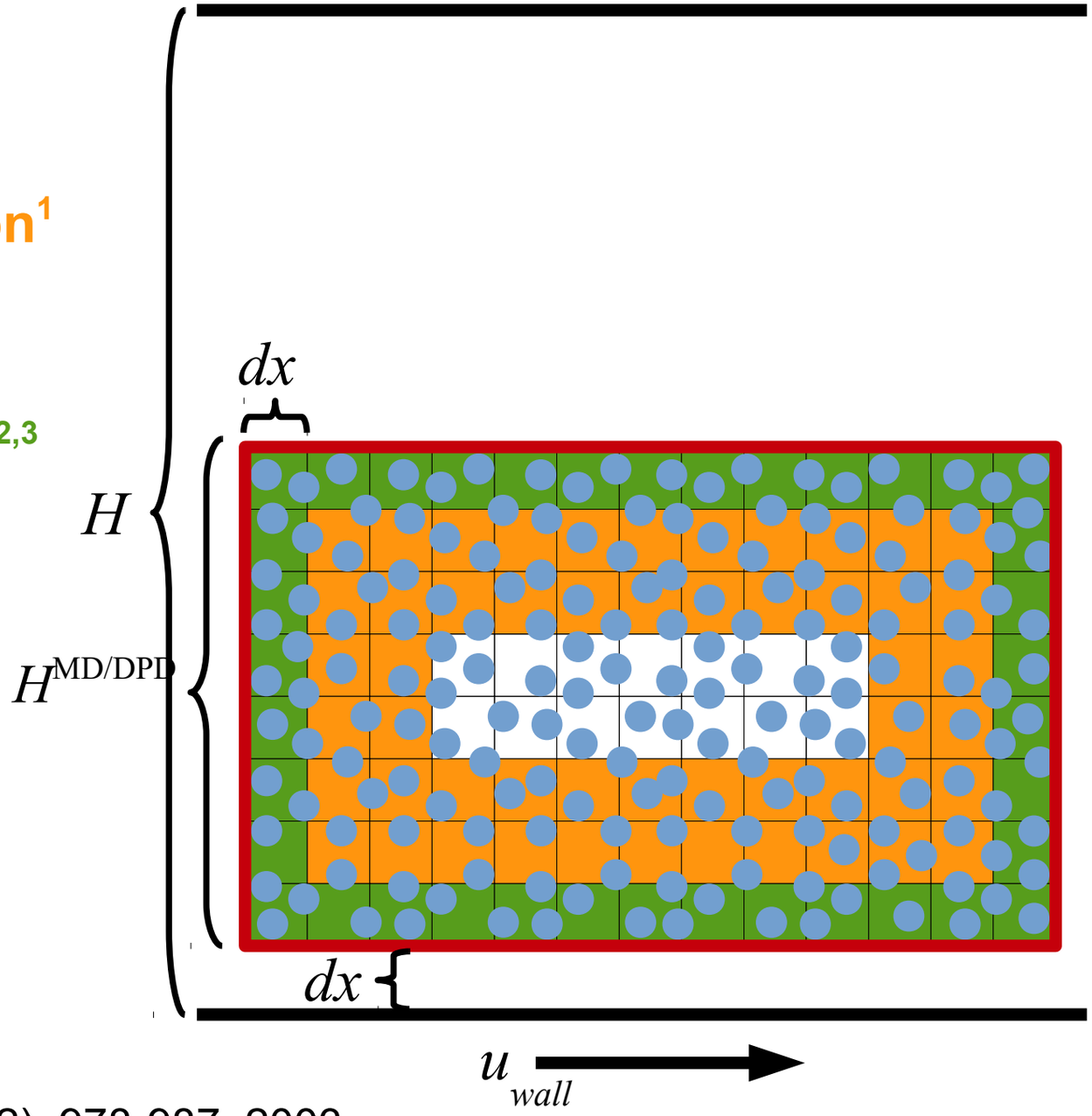

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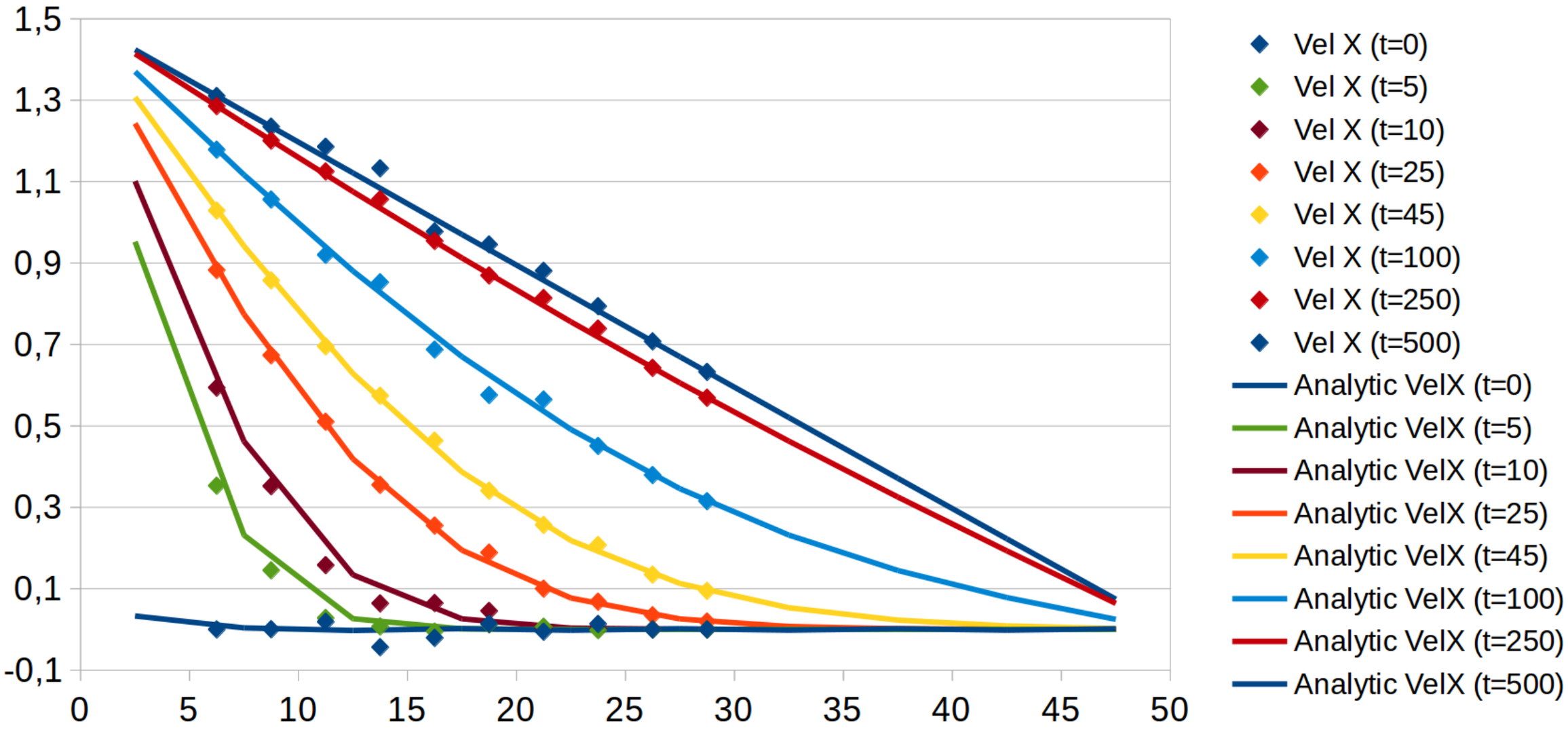
MaMiCo: Couette Flow with SimpleMD



Issue 1: Sampled over all inner cells → 144 samples per z-layer
Issue 2: Mol-cont limited in scalability → MD domain size limited

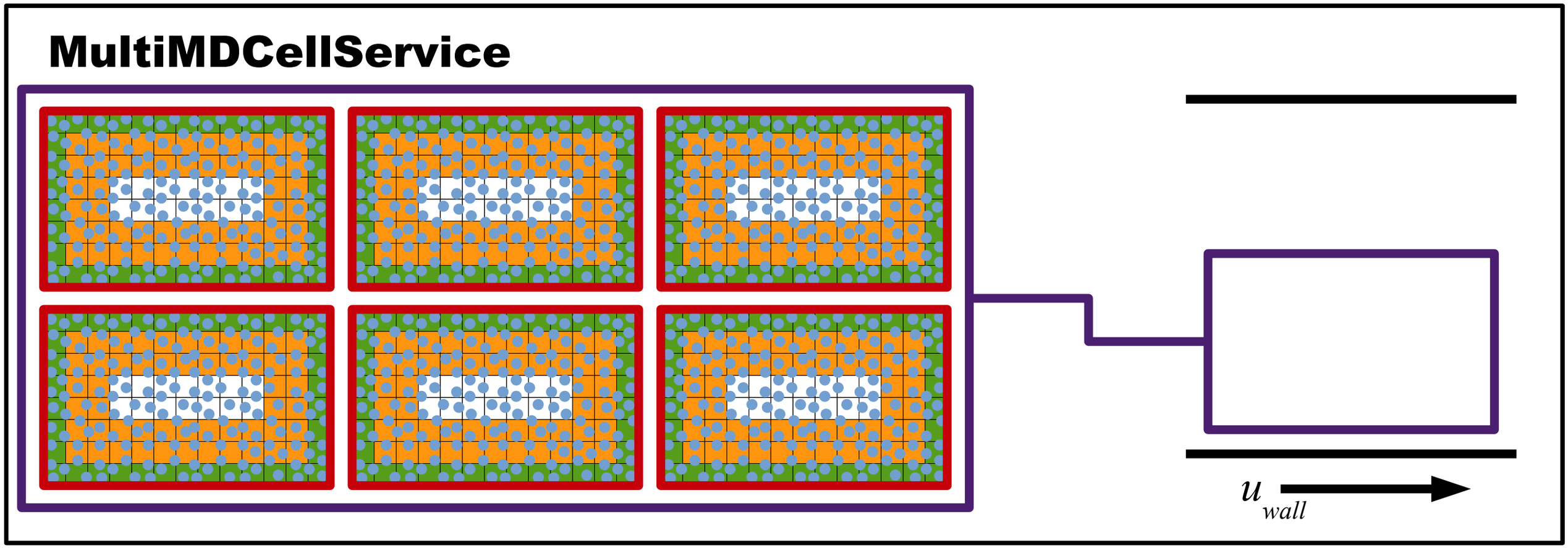
Increasing Parallelism for Sampling

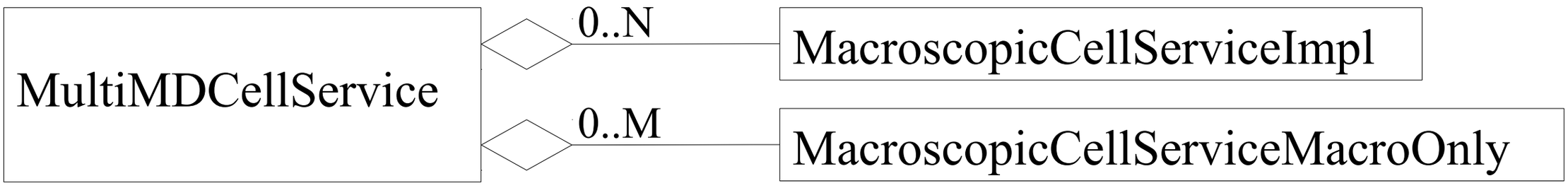
madeinbrazil.welt.de

Increasing Parallelism for Sampling

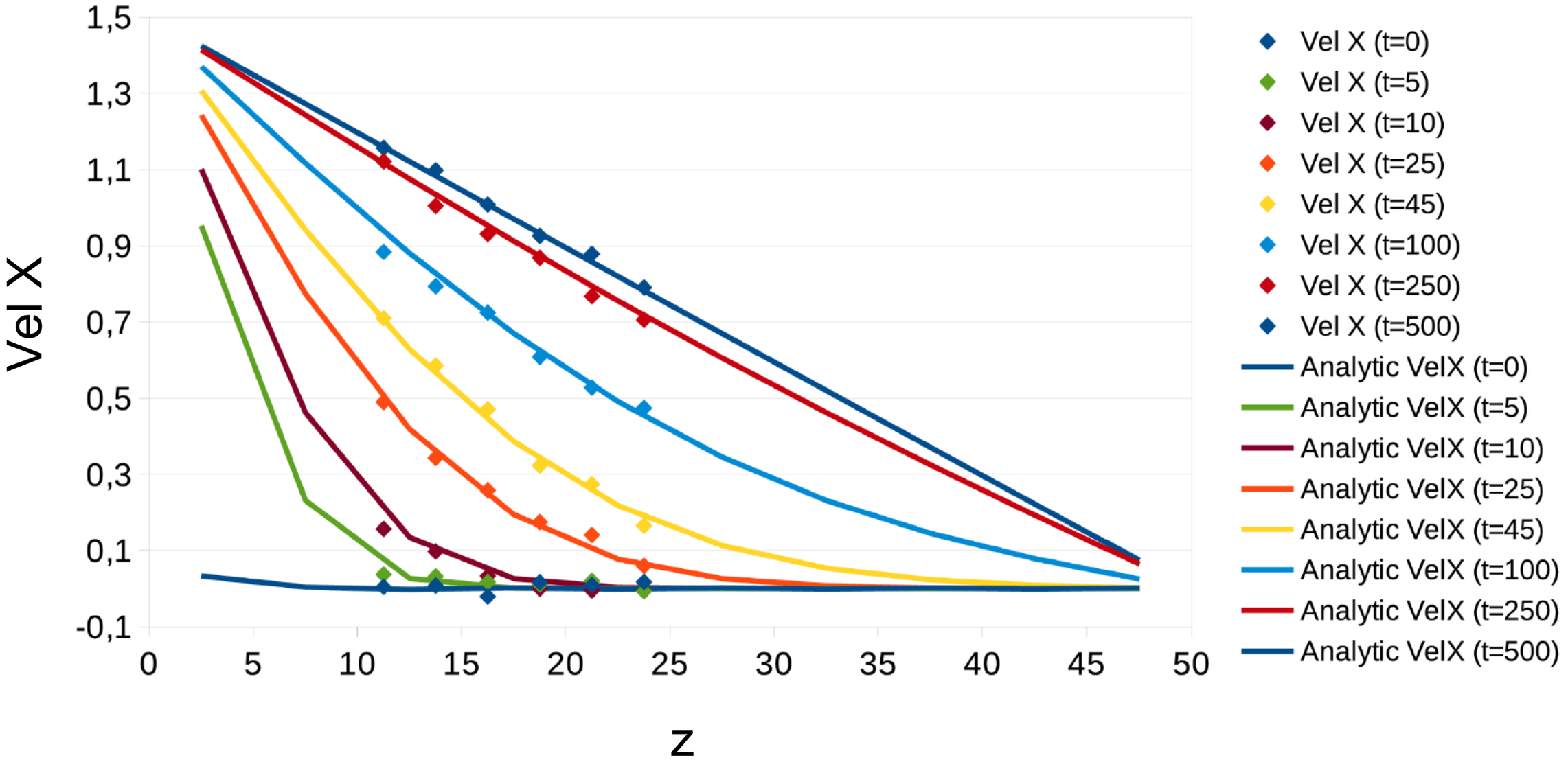
boerse.ard.de

Multi-Instance Coupling



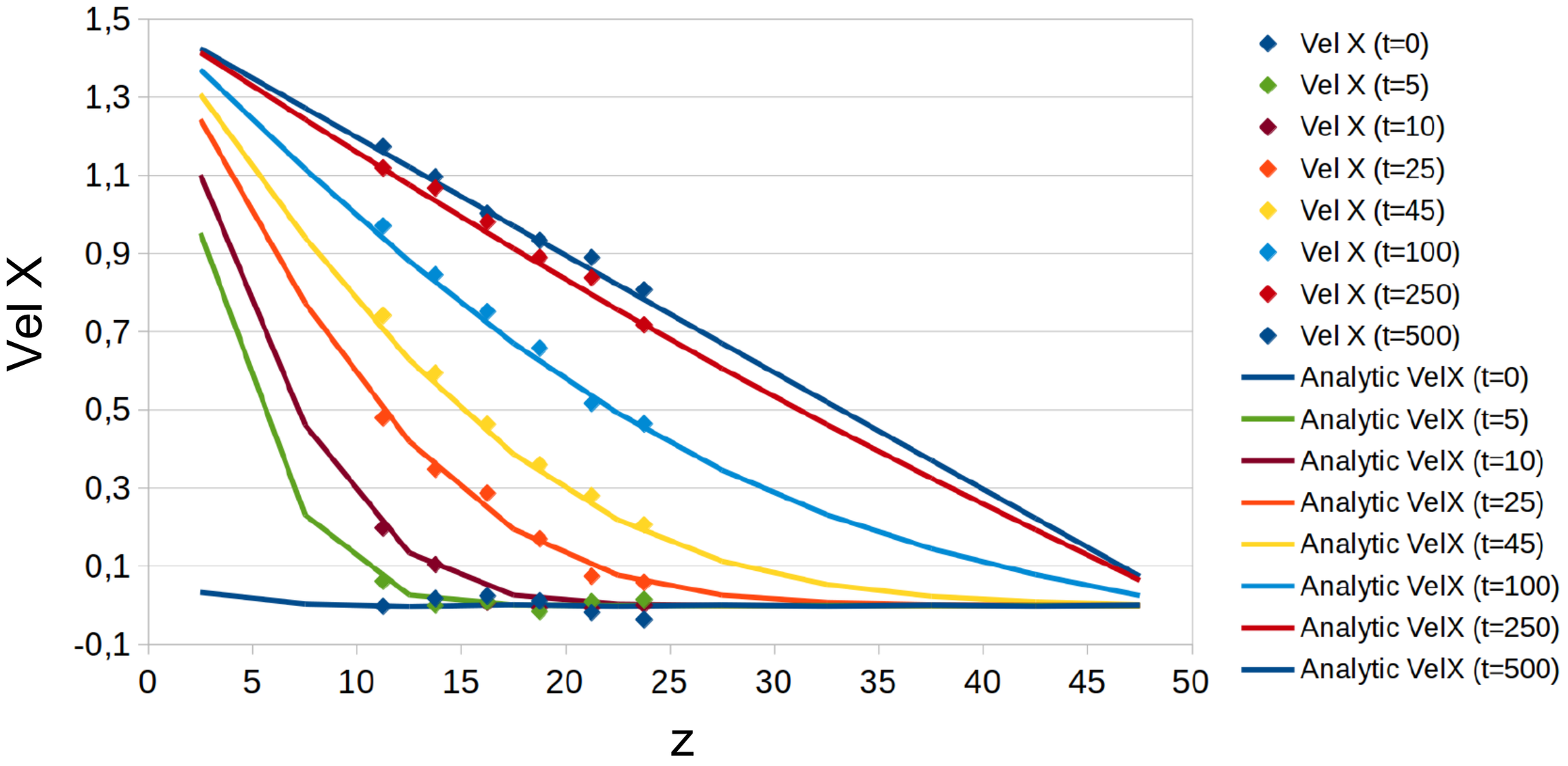


Transient Multi-Instance Coupling: Couette Flow with SimpleMD (MD-30)



144 MD samples → “cell-local” sampling
→ exploit embarrassing parallelism

Transient Multi-Instance Coupling: Couette Flow with LAMMPS (MD-30)



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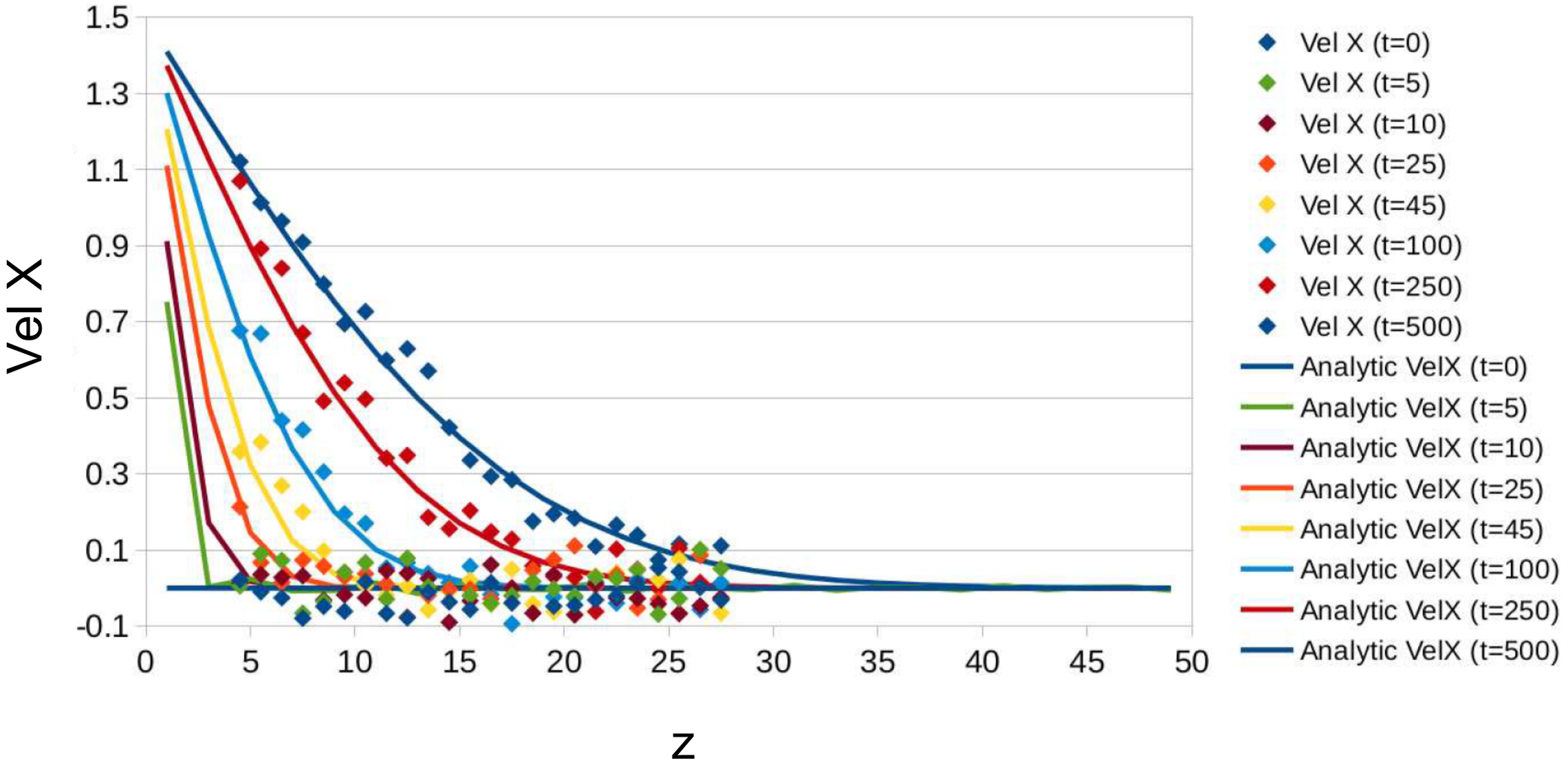
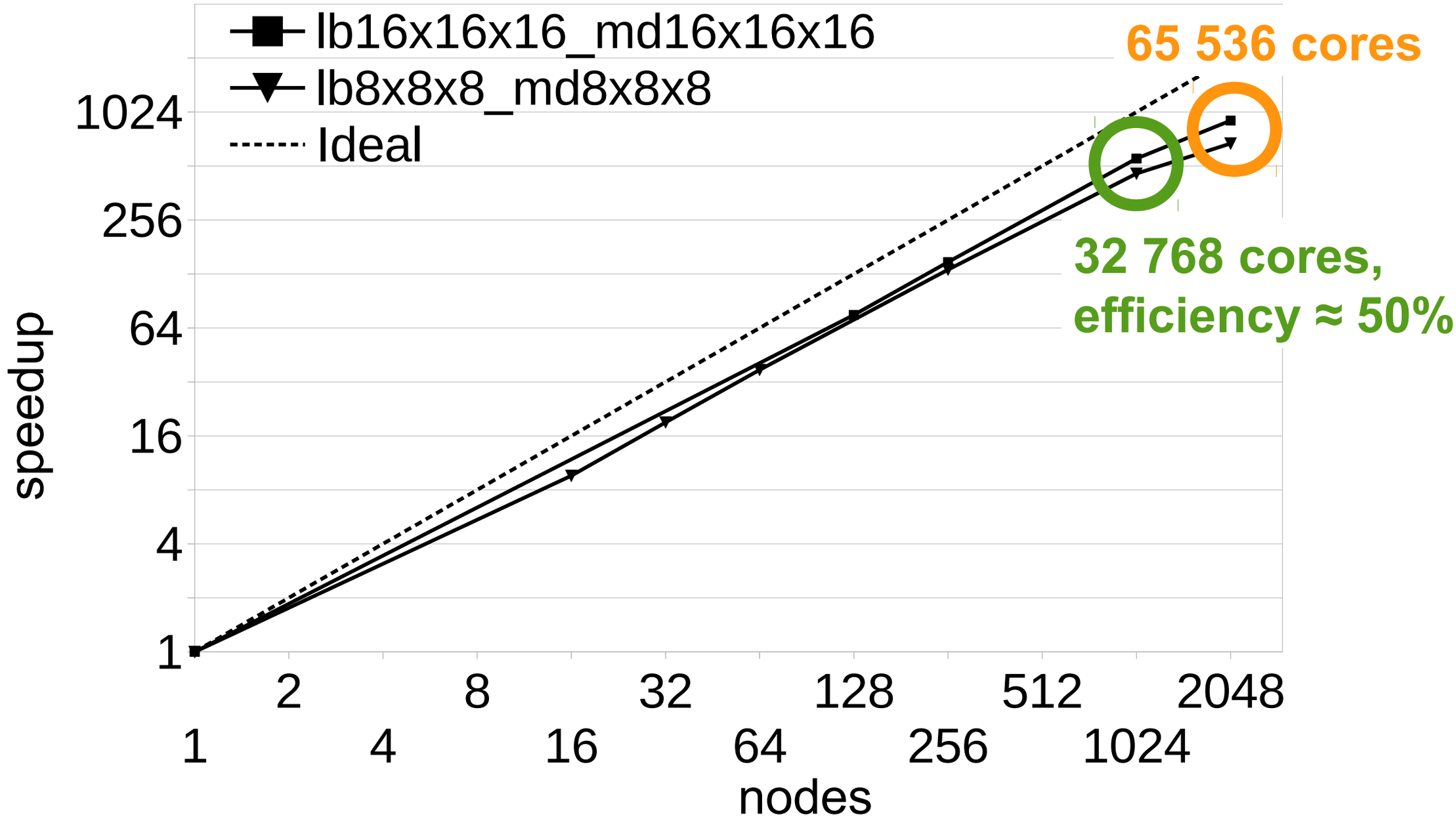
Transient Multi-Instance Coupling: Couette Flow with LAMMPS-DPD (DPD-30)



64 MD samples → “cell-local” sampling
→ exploit embarrassing parallelism

Transient Multi-Instance Coupling: Strong Scalability (SimpleMD MD-120)



Platform: KAUST Shaheen II, Intel Haswell, 1 node: 2x 16 cores

Summary

Molecular Dynamics:

- Limited in applicability, despite trillion atom run
- Towards auto-tuning → BMBF project TaLPas

MaMiCo:

- Enabling modular, flexible, fully 3D, transient mol-cont coupling
- Incorporation of data analytics (noise filters, error estimators,…)

Outlook: PIRE-DFG-NSF Revival

- (German) Partner: Mathias Krause, KIT
- Load balanced particle-fluid simulation of filtration processes
  → particles at sub-grid scale (similar to mol-cont setting)
  → particle clustering and arising computational load imbalances
  → large particle systems (high-performance computing!)
  → Re-submission of proposal soon

Thanks to

- **People:**
  - SCCS: Nikola Tchipev, Steffen Seckler
  - The *TaLPas* crew
  - Brown Univ: Xin Bian
  - Students: Hanno Flohr, Rahul Arora, Piet Jarmatz, Sergey Zakharov
- **Funding:**
  - BMBF, project *Task-Based Load Balancing and Auto-Tuning for Particle Simulations (TaLPas)*
  - BayFOR BayIntAn, project *Molecular-Continuum Simulations on Supercomputers*
- **Supercomputing projects:**
  - KAUST Supercomputing Lab, project *Hybrid Multiscale Flow Simulation*
  - LRZ, project *Massively Parallel Multiscale Simulation of Nanoflows*
  - HLRS, project *Extreme-Scale MD Simulation of Droplet Coalescence*
- **...and you for your attention!**