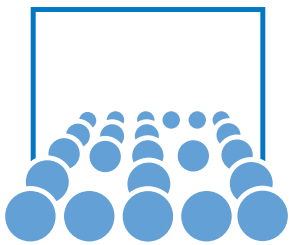
Towards Flexible Adaptive Molecular–Continuum Simulations

ICMMES 2012

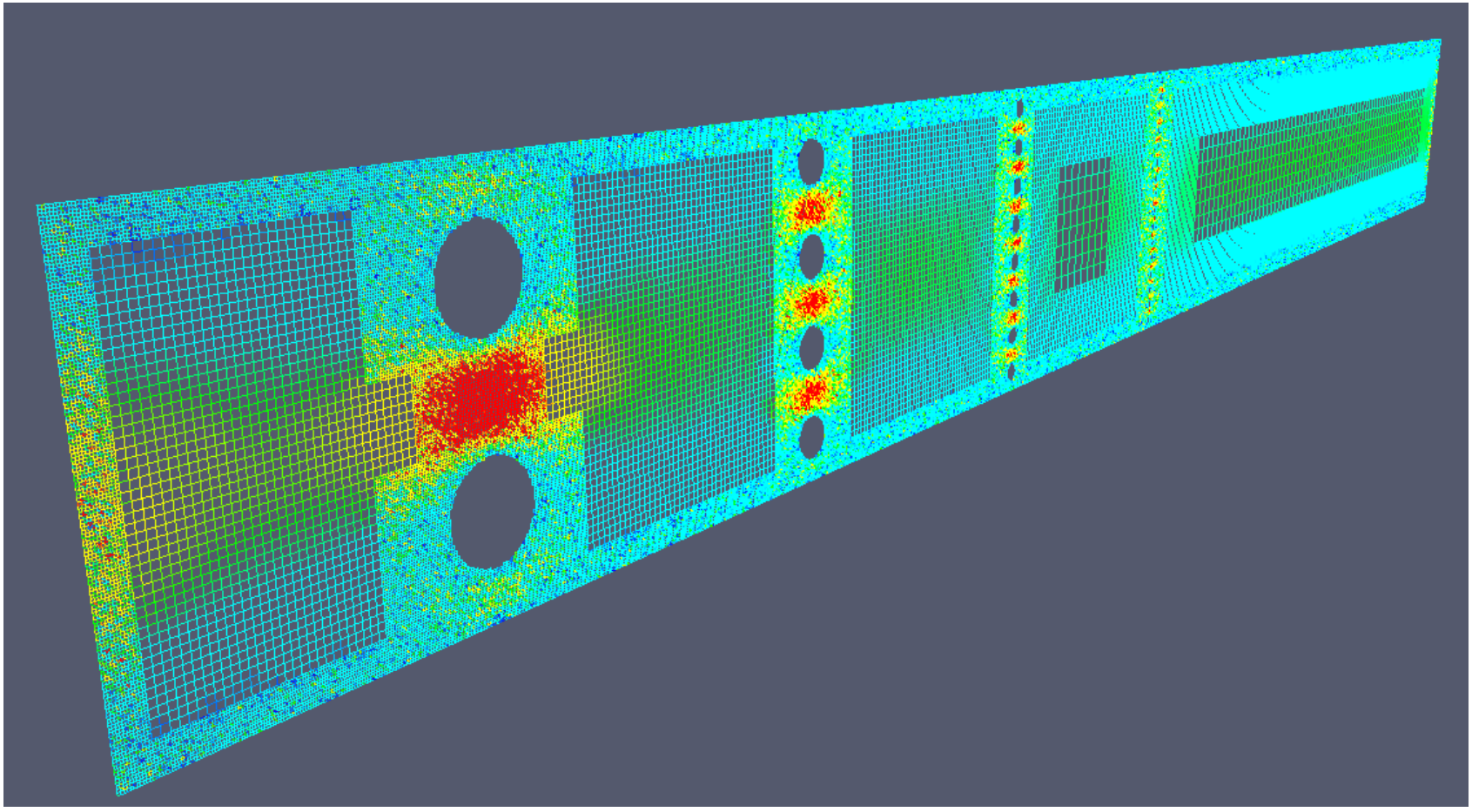
Philipp Neumann and Wolfgang Eckhardt

25.07.2012



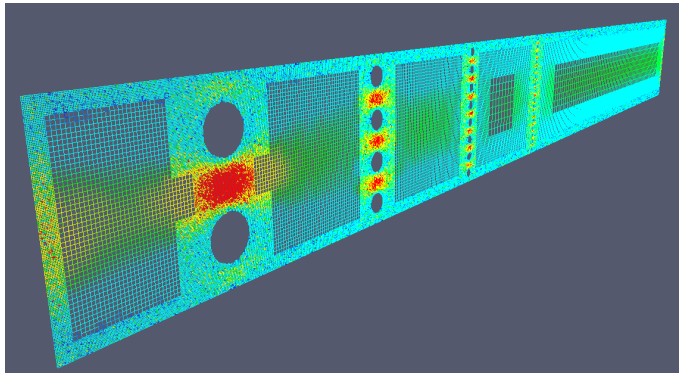
Contents

Hybrid Molecular–Continuum Simulations: Why?



Hybrid Molecular–Continuum Simulations: Why?

- Huge interest in flows at micro- to nanoscale
  $\rightarrow$ Biosensors, micropumps, ...
- Nanoflows: May represent only small part of huge flow system



- Molecular Dynamics (MD) required to capture correct flow behaviour

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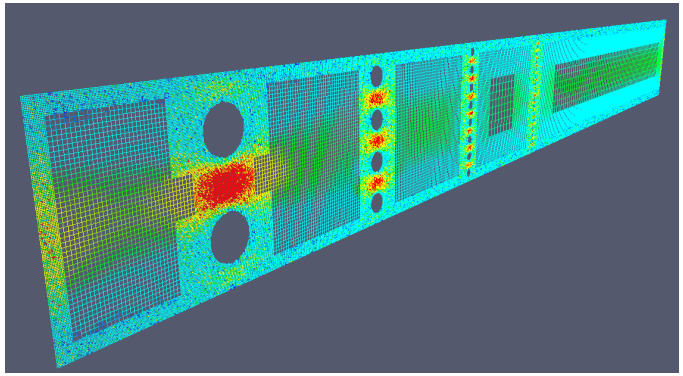
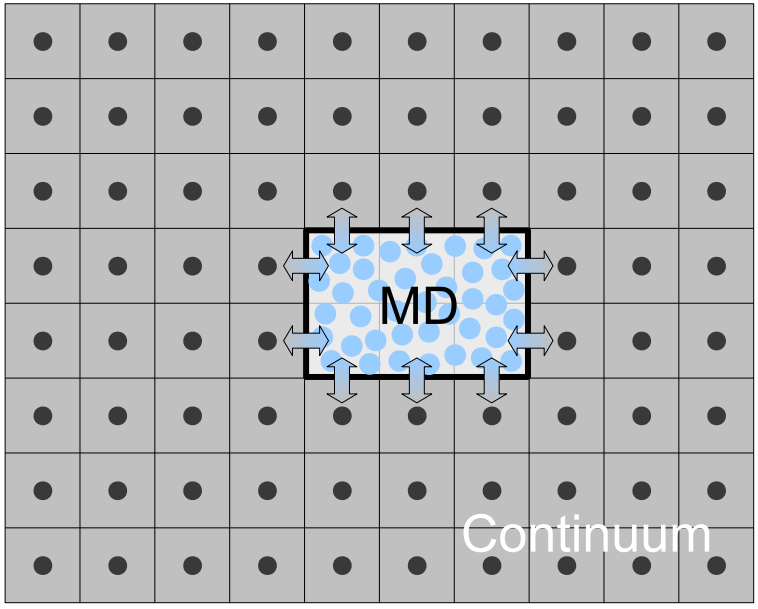


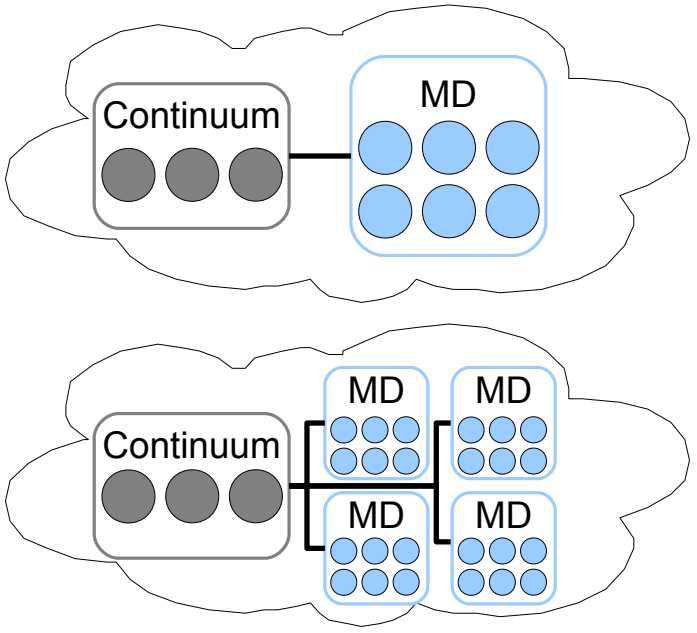
- Molecular Dynamics (MD) required to capture correct flow behaviour

Computationally expensive accurate MD simulations $\Leftrightarrow$ Less accurate computationally cheap continuum simulations

Challenges: Physics & Distributed Computing



- Correct physical description at molecular–continuum interface
- Simple & fast testing of new coupling schemes



- Statistical noise on MD data[1] $\rightarrow$ sampling
- Flexibility
- (Massively) Parallel implementation

N.G. Hadjiconstantinou, A.L. Garcia, M.Z. Bazant and G. He, Statistical error in particle simulations of hydrodynamic phenomena. J. Comput. Phys. 187, pp. 274–297, 2003.

Macro–Micro Coupling: Preparations

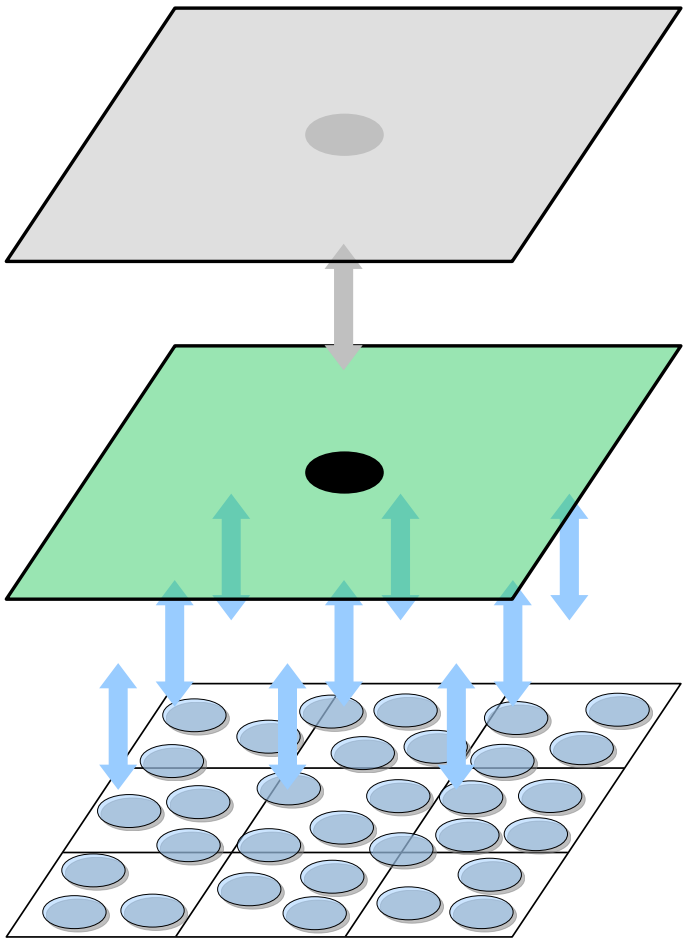
MD → Continuum:

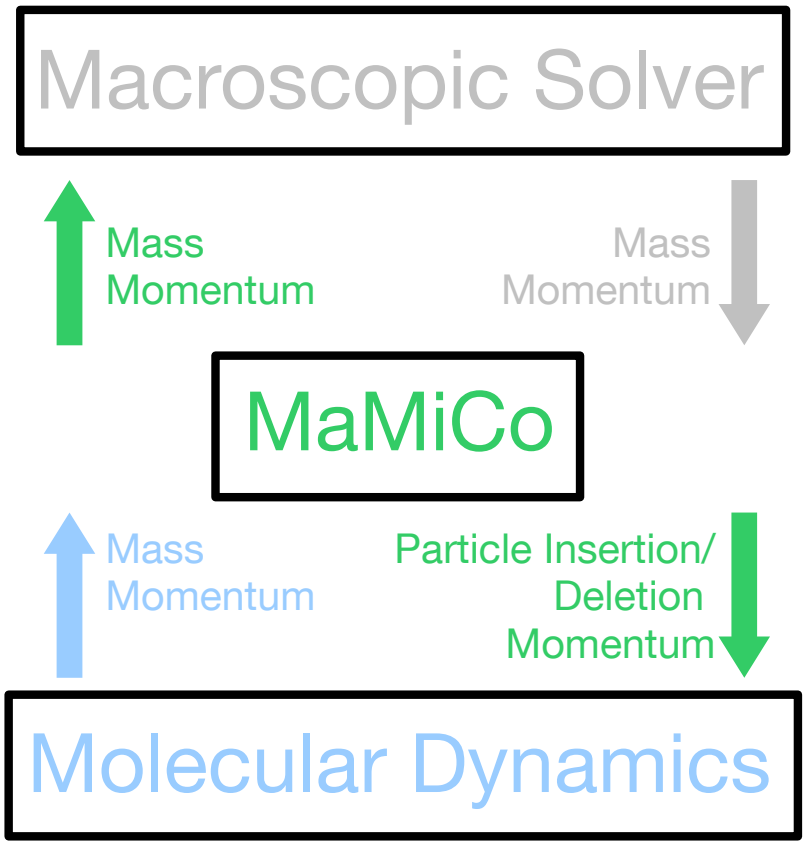
Mass exchange	→	average number of molecules
Momentum exchange	→	average velocities/ momentum of molecules
Energy exchange		

Continuum → MD:

Mass exchange	→	insert/ delete molecules
Momentum exchange	→	in-/ decrease velocities of molecules
Energy exchange		

The Macro–Micro Coupling Tool (MaMiCo) [1]





[1] P. Neumann and N. Tchipev, A Coupling Tool for Parallel Molecular Dynamics–Continuum Simulations. Proceedings of the 11th International Symposium on Distributed and Parallel Computing, München, 2012. Accepted.

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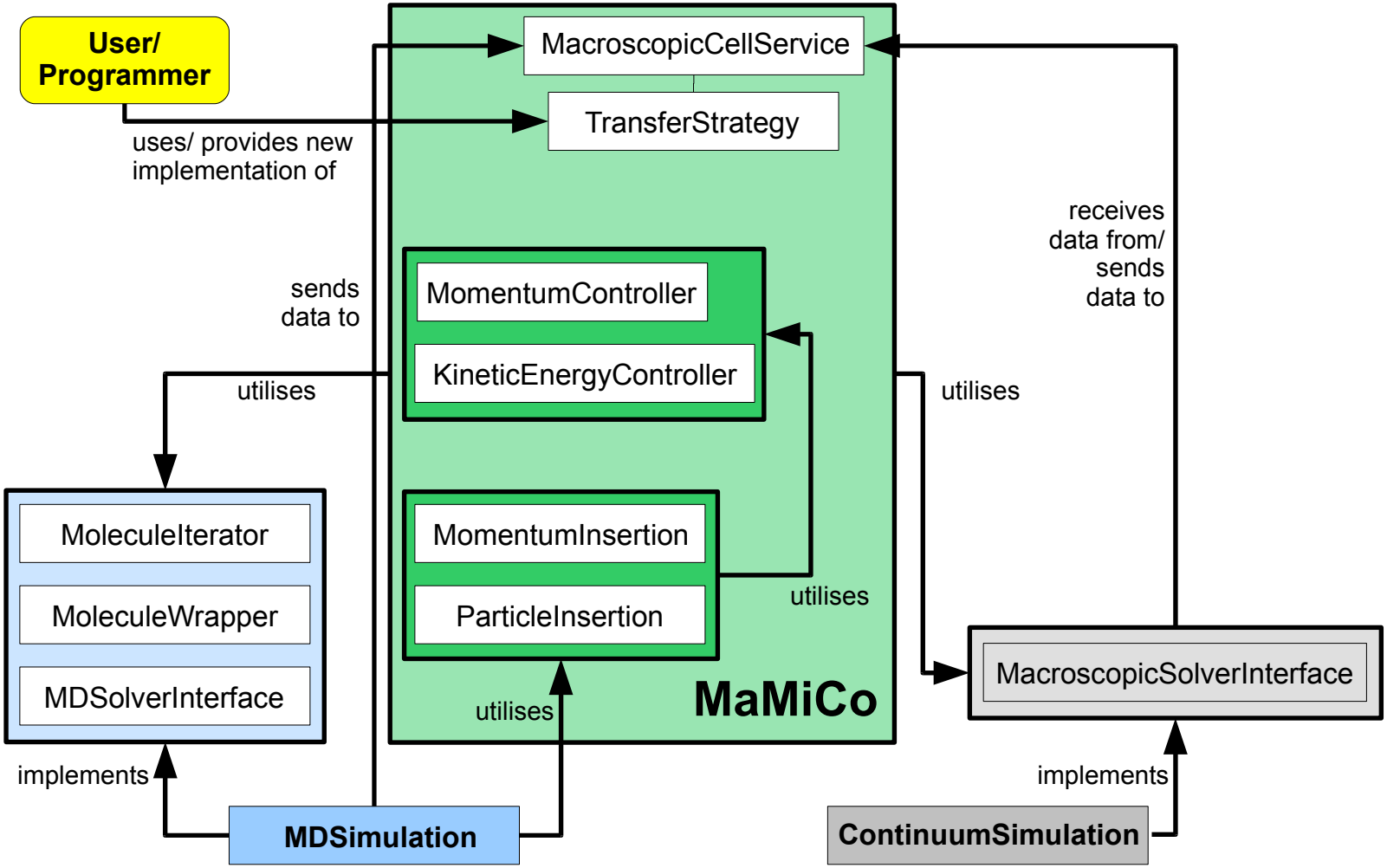
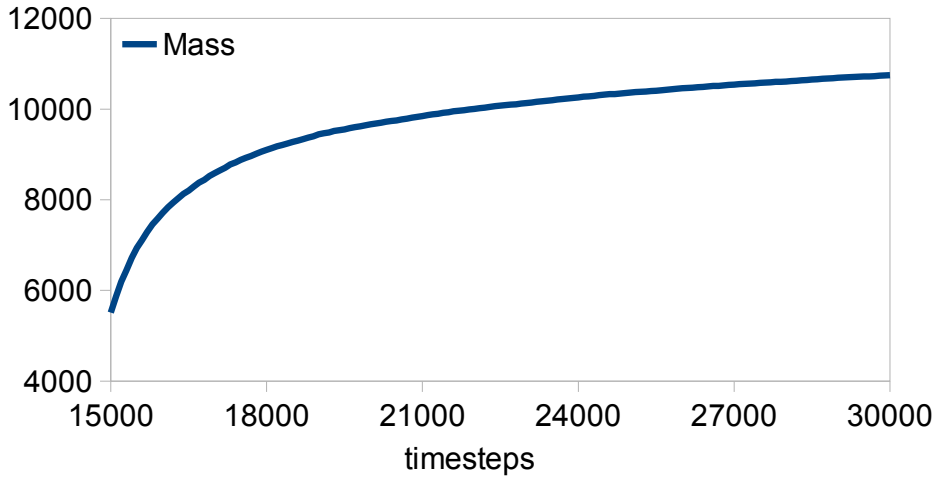
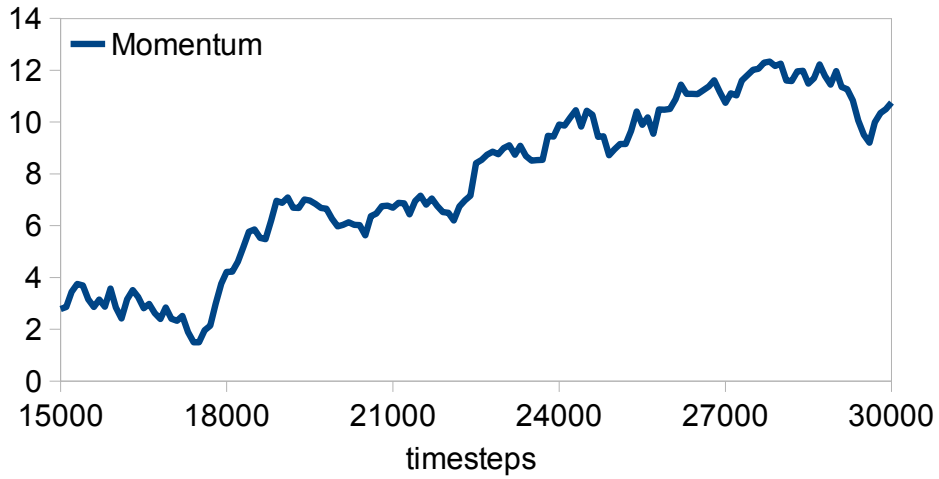
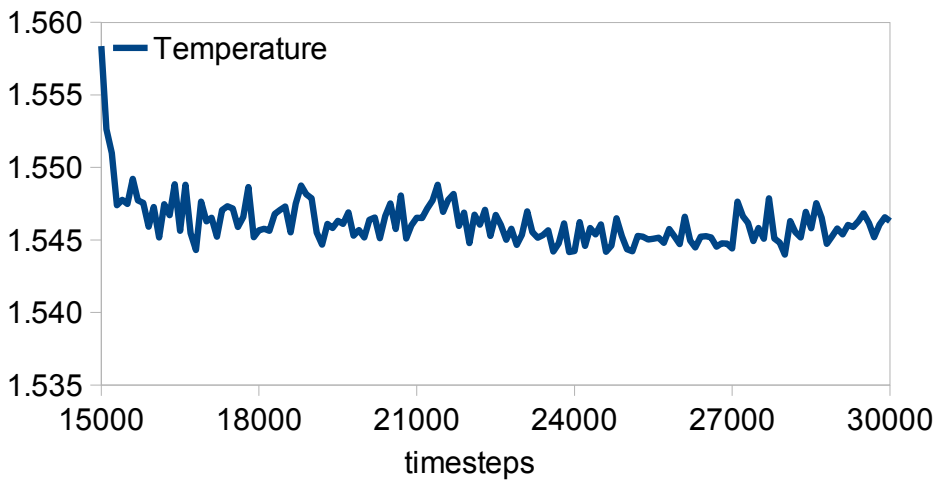


Validation: Mass Insertion



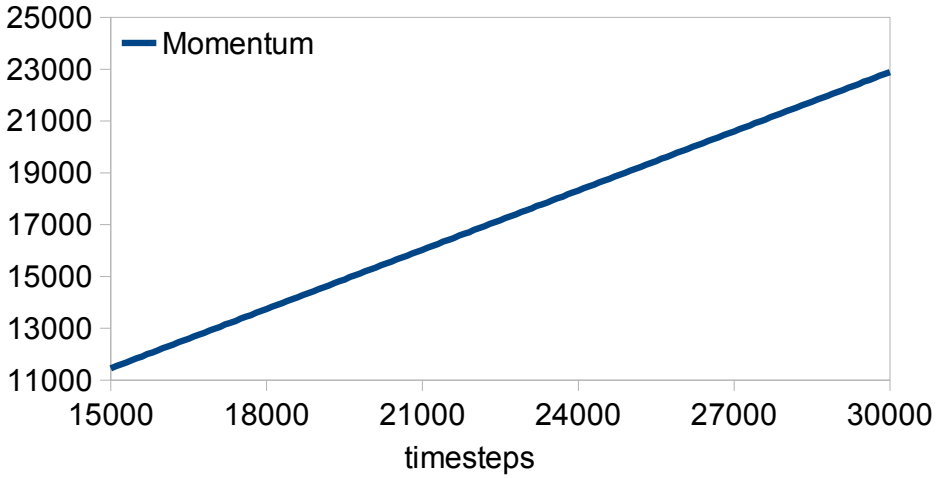


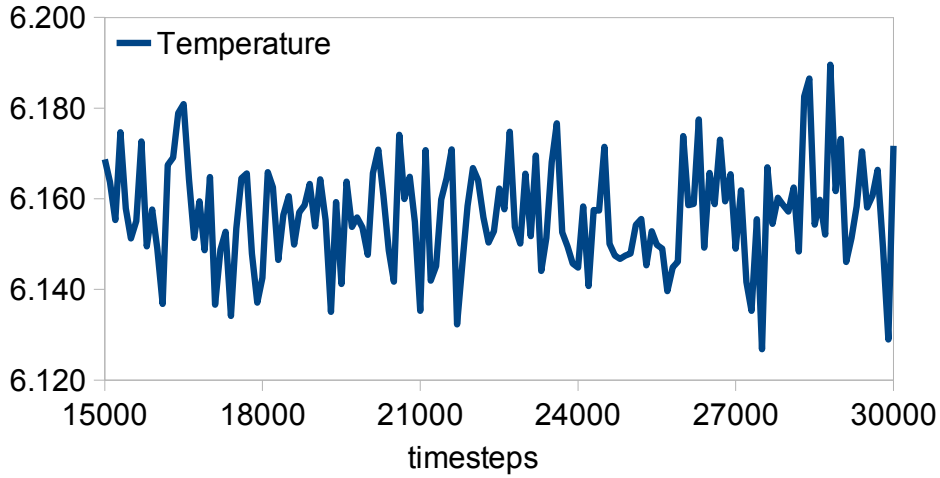


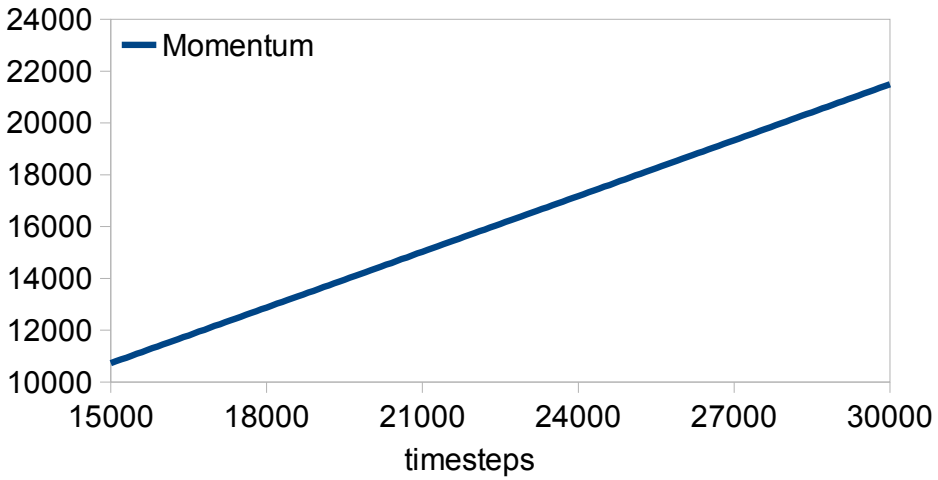
Experiment:

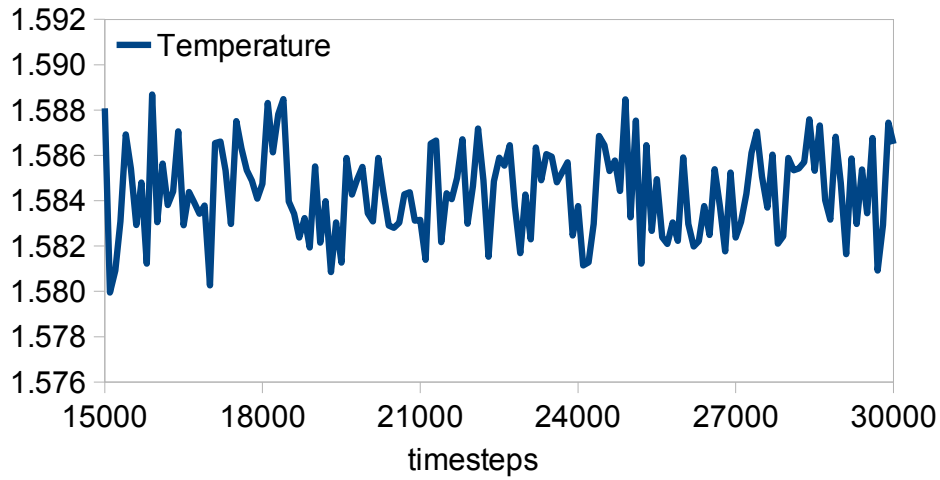
- Equilibrate MD system
- Double *number of molecules*
  or
  momentum
- Keep *momentum and temperature*
  or
  temperature constant

Validation: Momentum Insertion





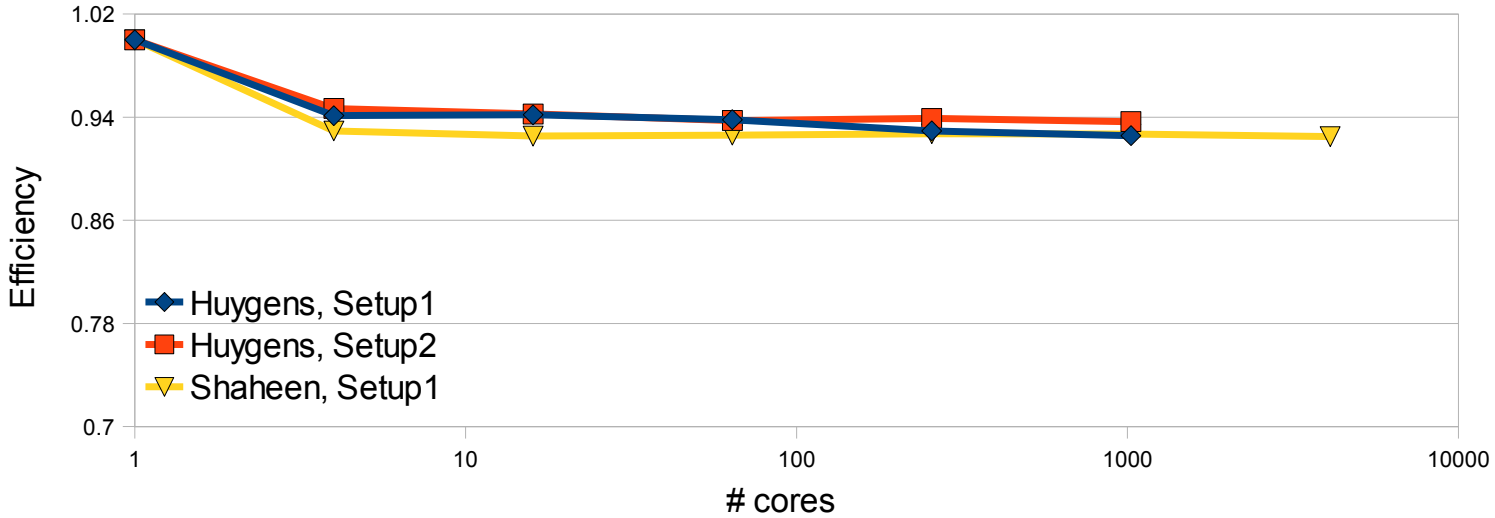


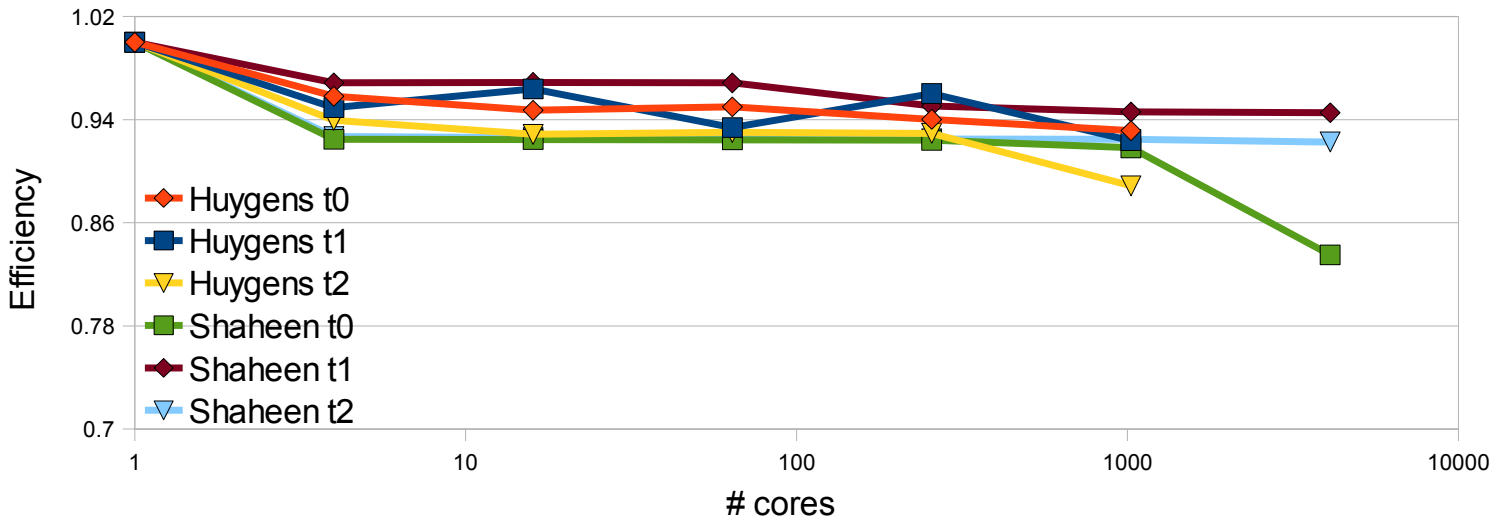


Runtimes

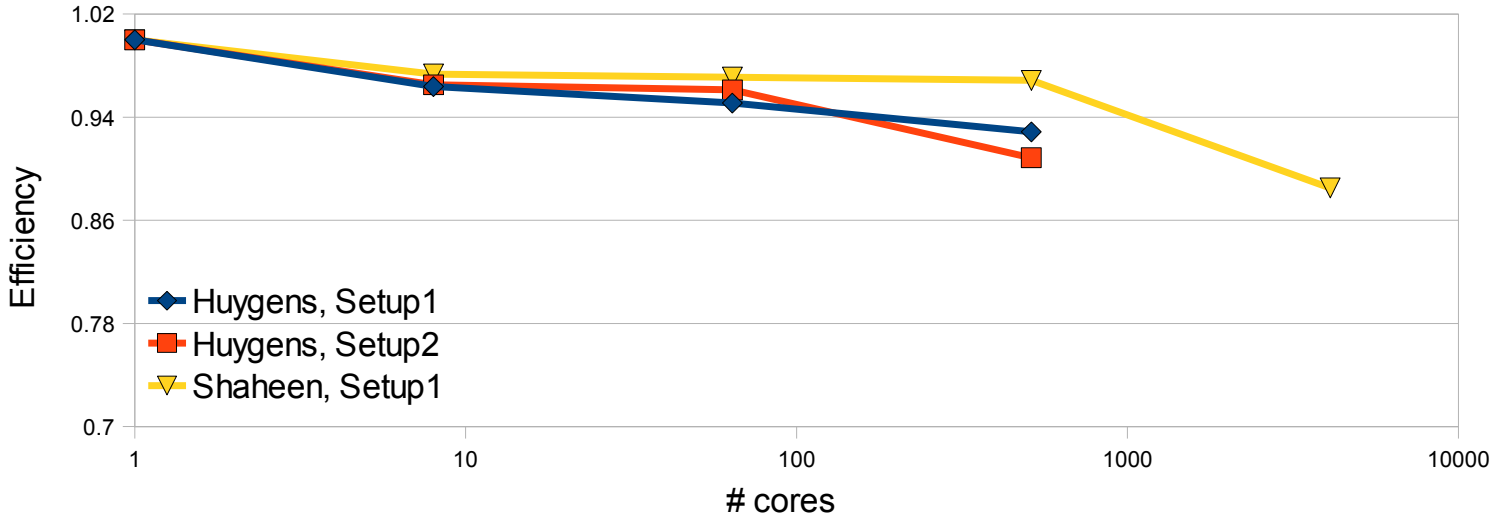
Scenario	Runtime (s)	Timesteps/ Particle insertion	Timesteps/ Momentum insertion
MD($n = 0.40$) (2D)	23.5	0	0
MD($n = 0.78$) (2D)	46.6	0	0
Test A (2D)	55.9	30	0
MD($n = 0.80$) (2D)	48.0	0	0
Test B ($n = 0.80$) (2D)	54.8	0	30
MD($n = 0.40$) (3D)	92.1	0	0
MD($n = 0.78$) (3D)	166.7	0	0
Test A (3D)	268.4	15	0
MD($n = 0.80$) (3D)	167.7	0	0
Test B ($n = 0.80$) (3D)	175.2	0	15

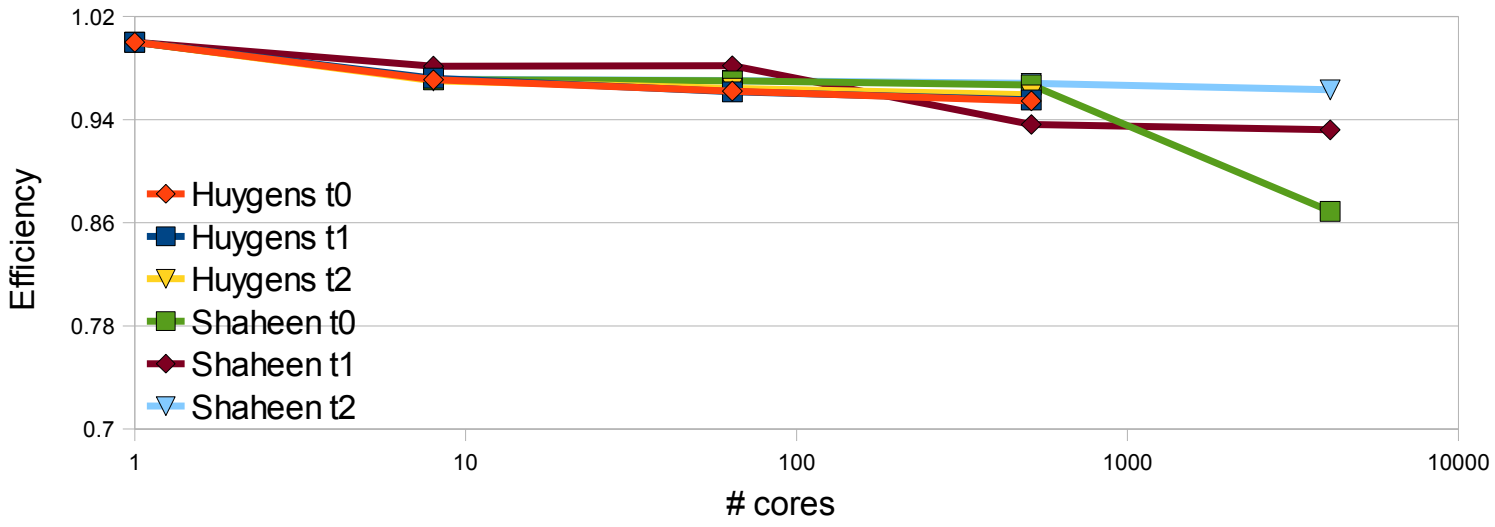
Parallel Particle Insertion: Results (2D)





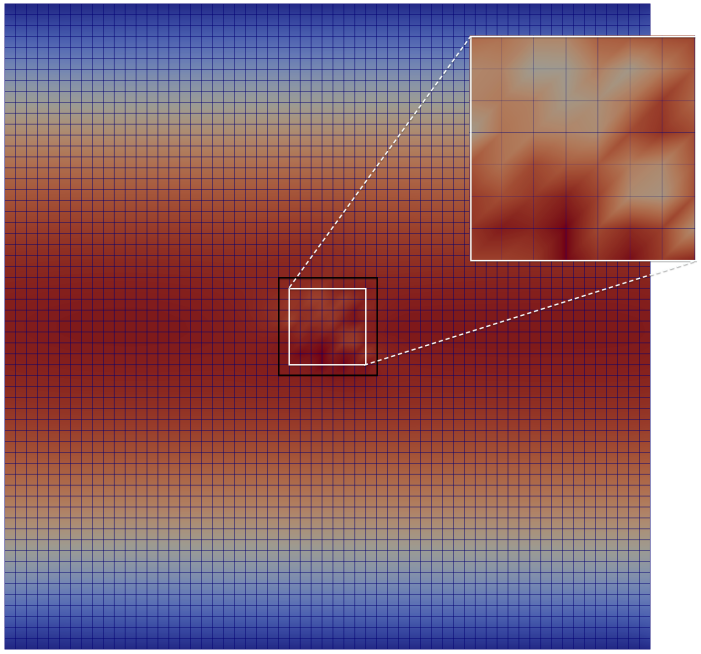
Parallel Particle Insertion: Results (3D)





LB–MD Coupling: Prototype

- Coupling between Mardyn[1] and Peano's Lattice Boltzmann component[2]
- Following the coupling approaches from Dupuis et al.[3] and Werder et al.[4]
  - MD: 3D, LB: 2D
  - MD: Velocity relaxation in overlap regions
  - MD: RDF-based boundary forces
  - LB: Forcing terms for momentum exchange
- Fluctuations agree with theory



[1] M. Buchholz, Framework zur Parallelisierung von Molekulardynamiksimulationen in verfahrenstechnischen Anwendungen. PhD thesis. Institut für Informatik, Technische Universität München. Verlag Dr. Hut, München, 2010.

[2] P. Neumann and T. Neckel, A dynamic mesh refinement technique for Lattice Boltzmann simulations on octree-like grids. Comput. Mech., DOI 10.1007/s00466-012-0721-y, 2012. Published online.

[3] A. Dupuis, E.M. Kotsalis and P. Koumoutsakos, Coupling lattice Boltzmann and molecular dynamics models for dense fluids. Phys. Rev. E 75 (046704), 2007.

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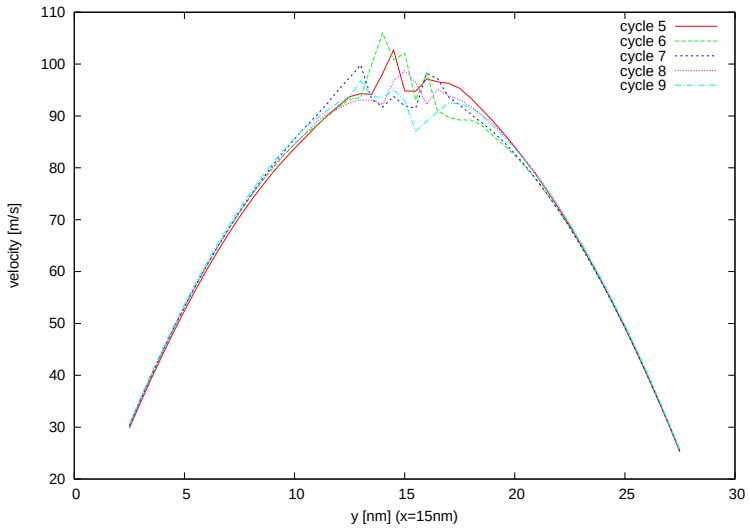

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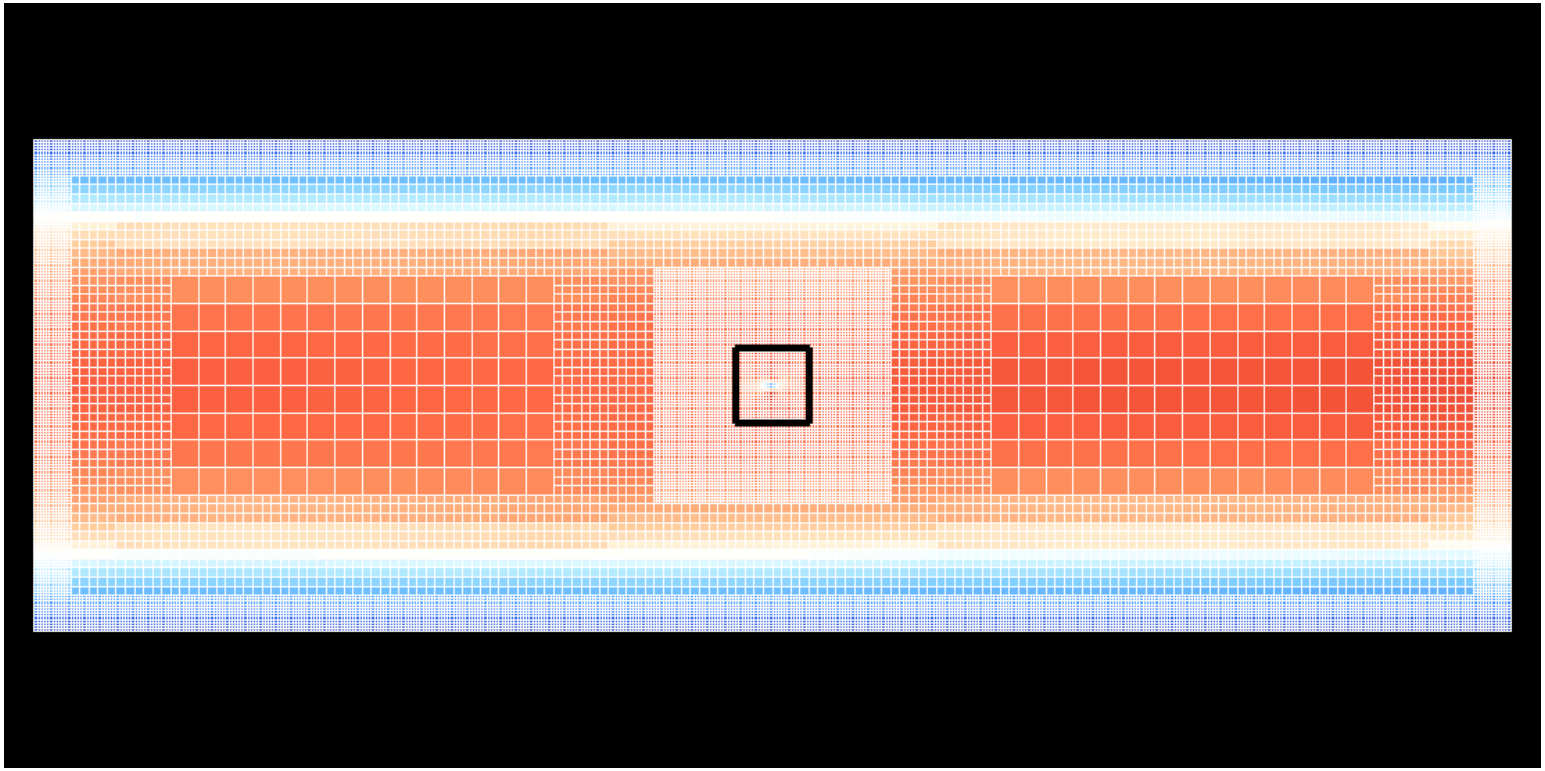
LB–MD Coupling: Flow around CNT



- Extension to adaptive grids
- Steady-state coupling:

  22 000 MD iterations $\Leftrightarrow$
  500 LB iterations

- MD: $n = 0.6$, $T = 1.8$
- 8000 single-centered LJ-atoms
- LB: Three grid levels, $Ma = 0.052$

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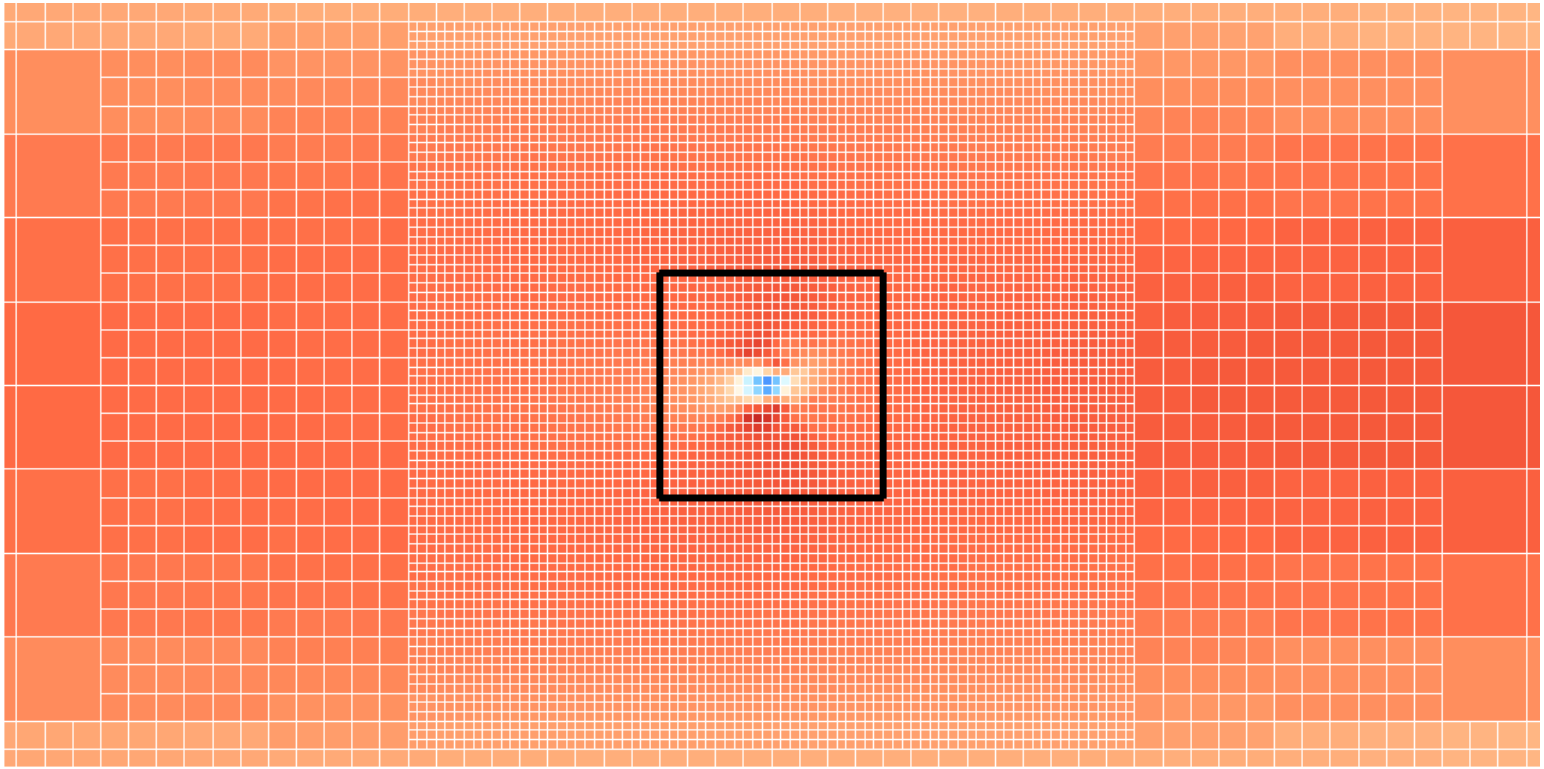

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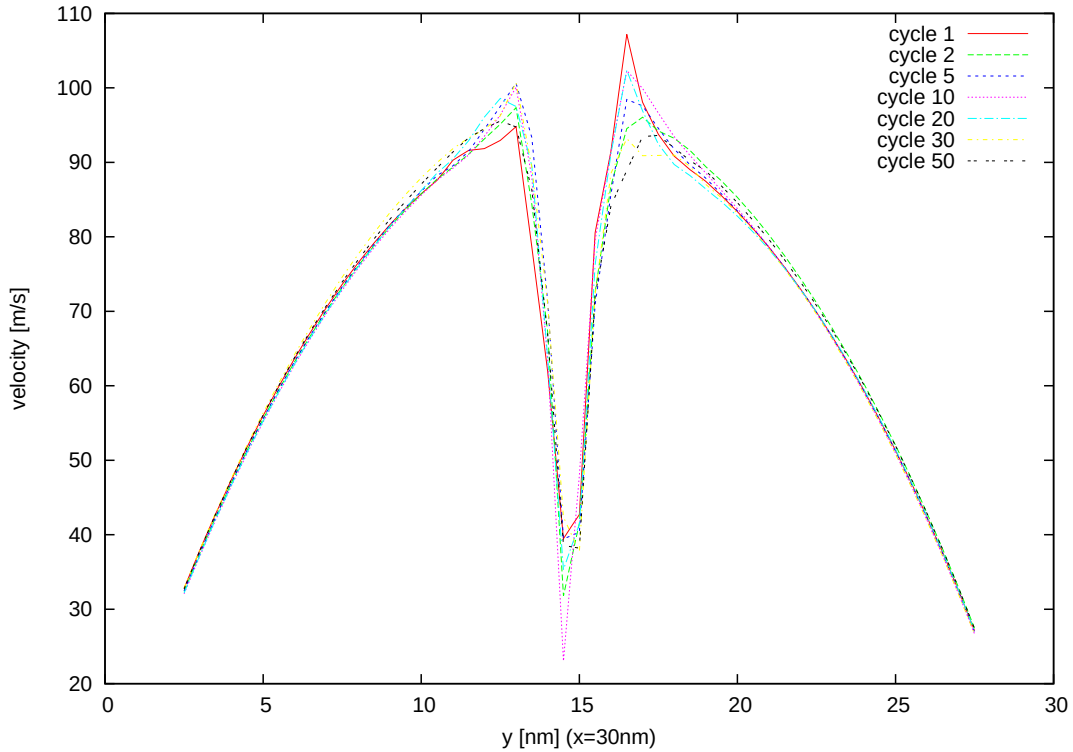

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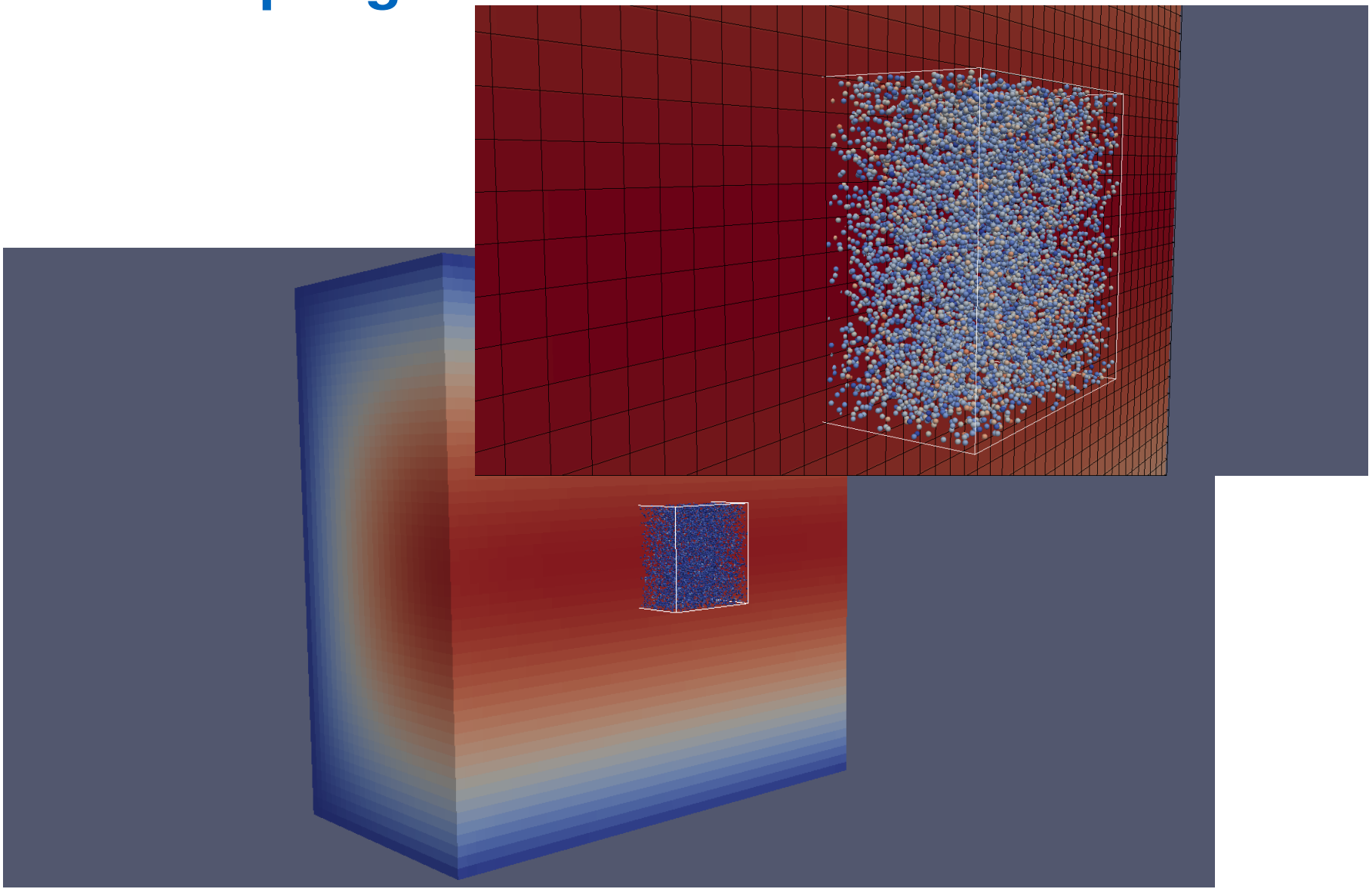

Conclusion & Outlook

Conclusion:

- Tool for hybrid molecular–continuum simulations (MaMiCo)
- 2D/ 3D support
- Distributed memory parallelisation

Outlook: From tests to parallel coupling algorithms

Thanks to:
Peter Hoffmann
Nikola Tchipev