# Large-scale MD simulation of heterogeneous systems with ls1 mardyn

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Computational Molecular Engineering

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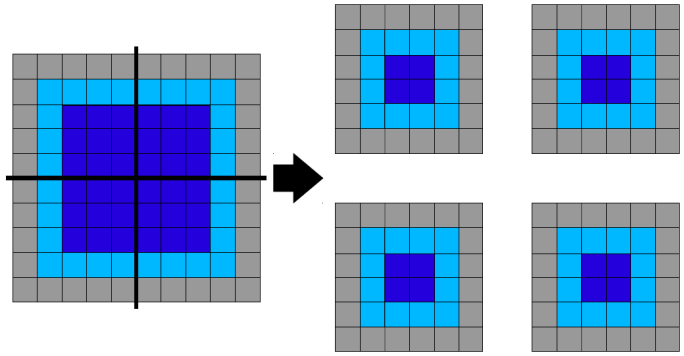
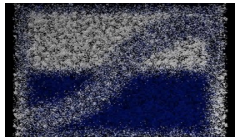
ProcessNet International Workshop MolMod

# Parallelization by volume decomposition

Linked-cell data structure suitable for spatial domain decomposition:



(non-blocking, overlapping MPI send/receive operations)



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UNIVERSITÄT PADERBORN
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HLRS

large systems “1”: molecular dynamics http://www.ls1-mardyn.de/

# Parallelization by volume decomposition

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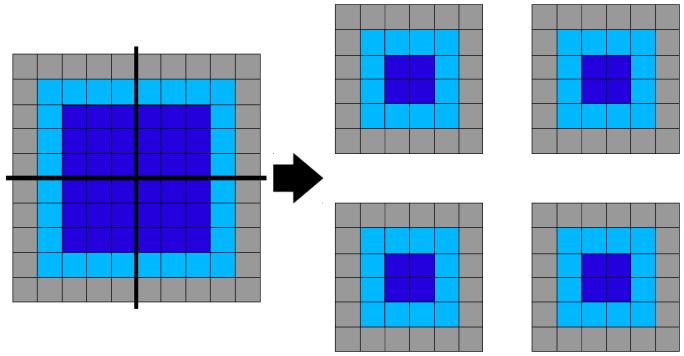

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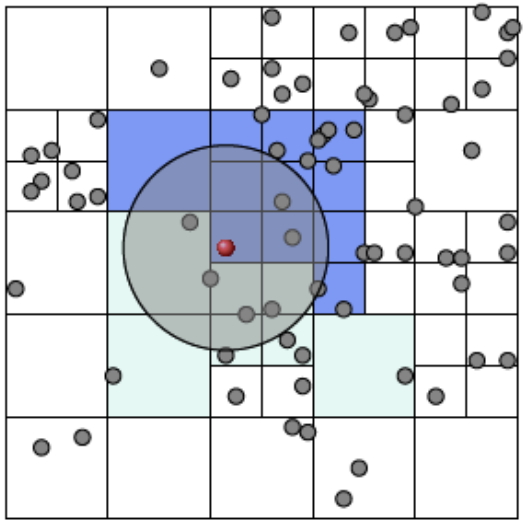
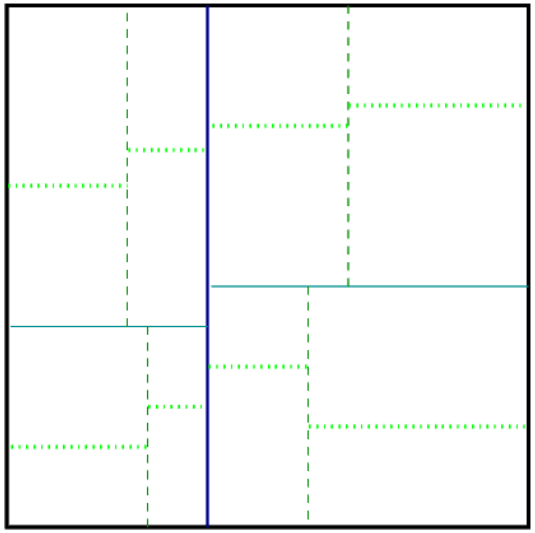
Methods for heterogeneous or fluctuating particle distributions:

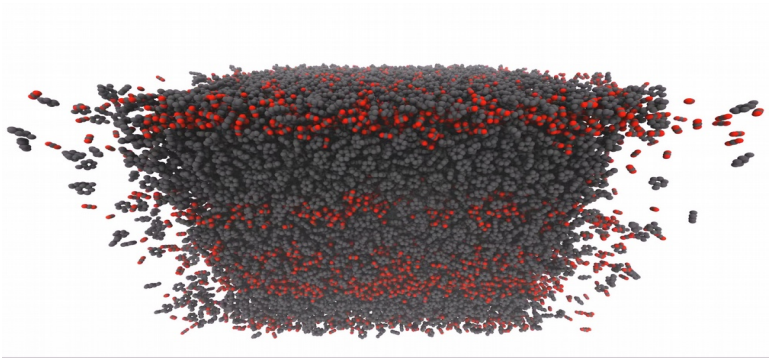


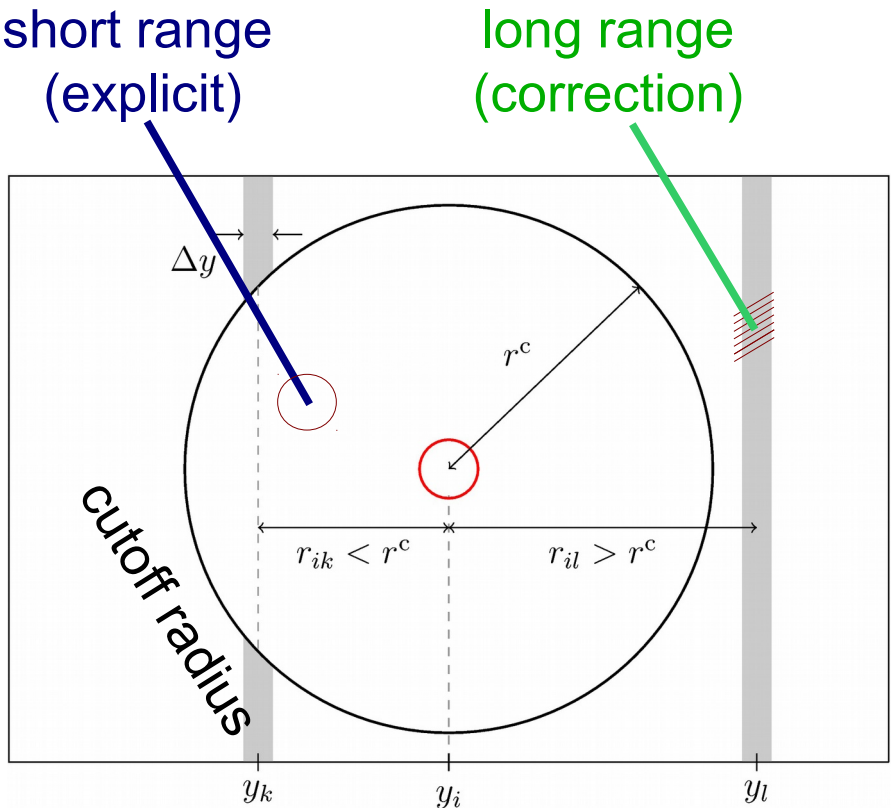


# Scale separation and long-range correction

For planar interfaces:

**Long-range correction** from the density profile, following **Janeček**.






Full evaluation of all pairwise interactions is too expensive ...
... instead, **short-range interactions** are evaluated for **neighbours**.

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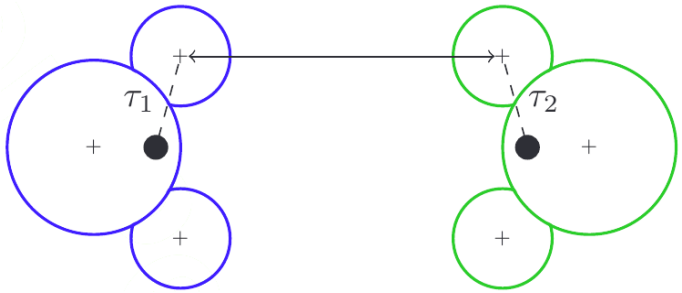
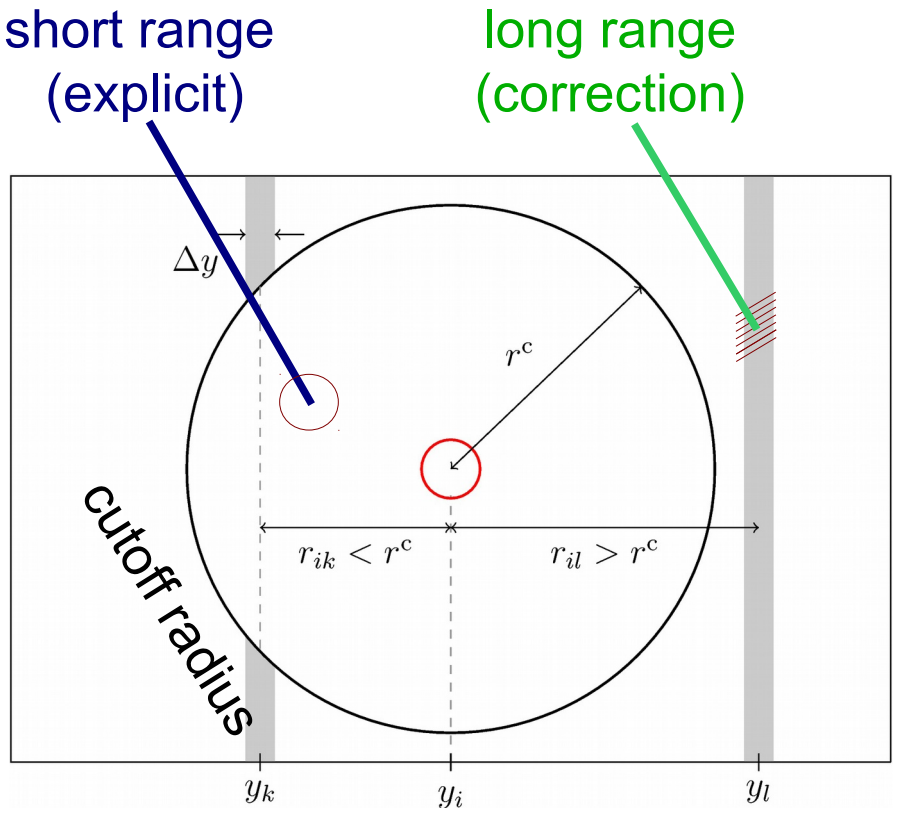



**Angle-averaging** expression for multi-site models, following **Lustig**.

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# Molecular simulation of fluids at interfaces

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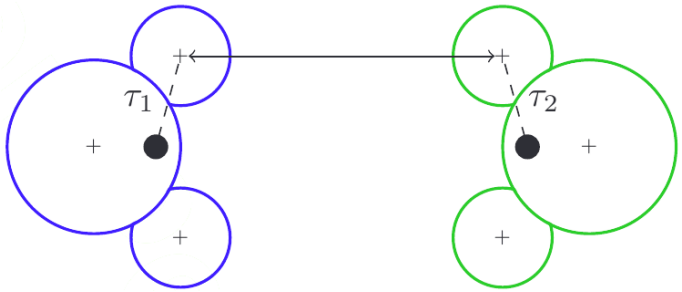


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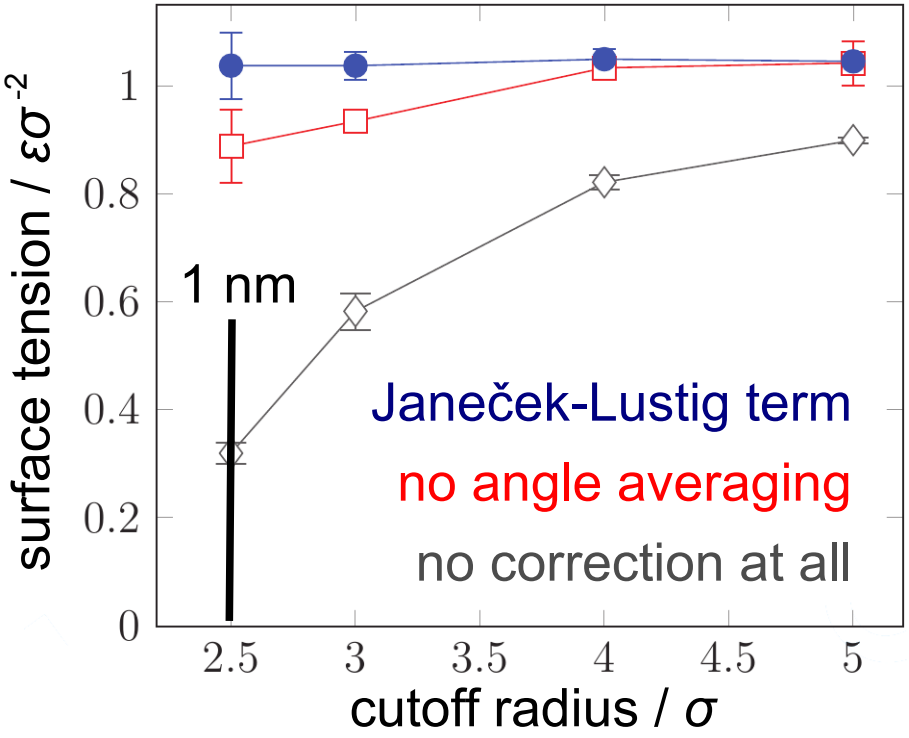
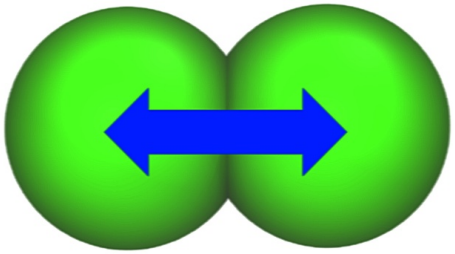
Two-centre LJ fluid (2CLJ)




For arbitrary geometries, e.g. the fast multipole method can be employed.

# Molecular simulation of fluids at interfaces



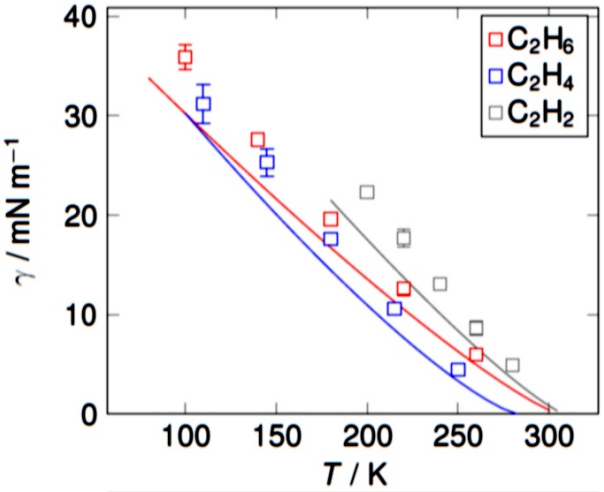
2CLJQ models:

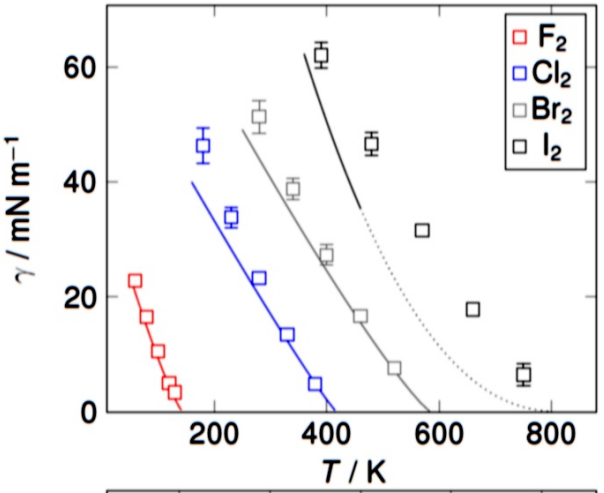
- 2 LJ centres
- Quadrupole

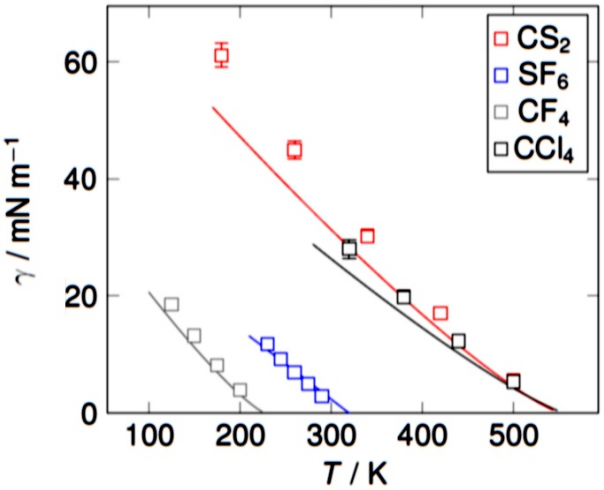
Test of predictivity for interfacial properties

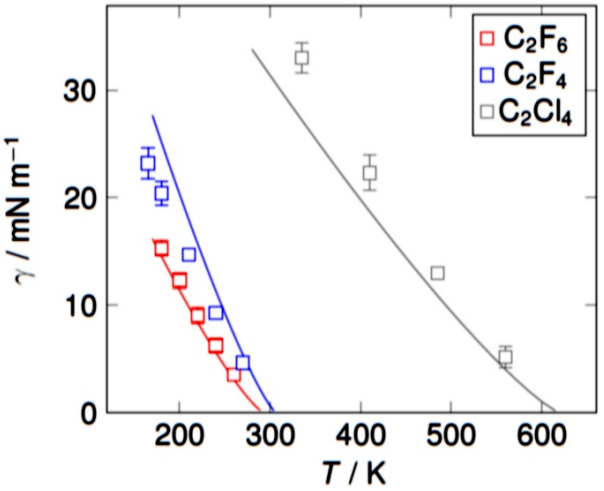
↓

Model validation and optimization



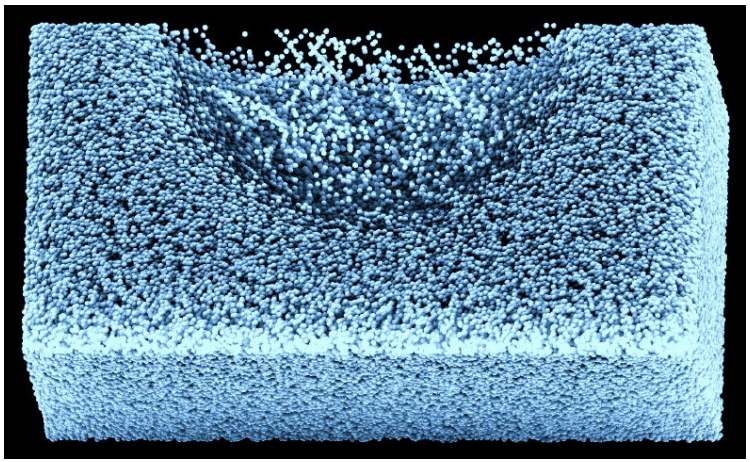



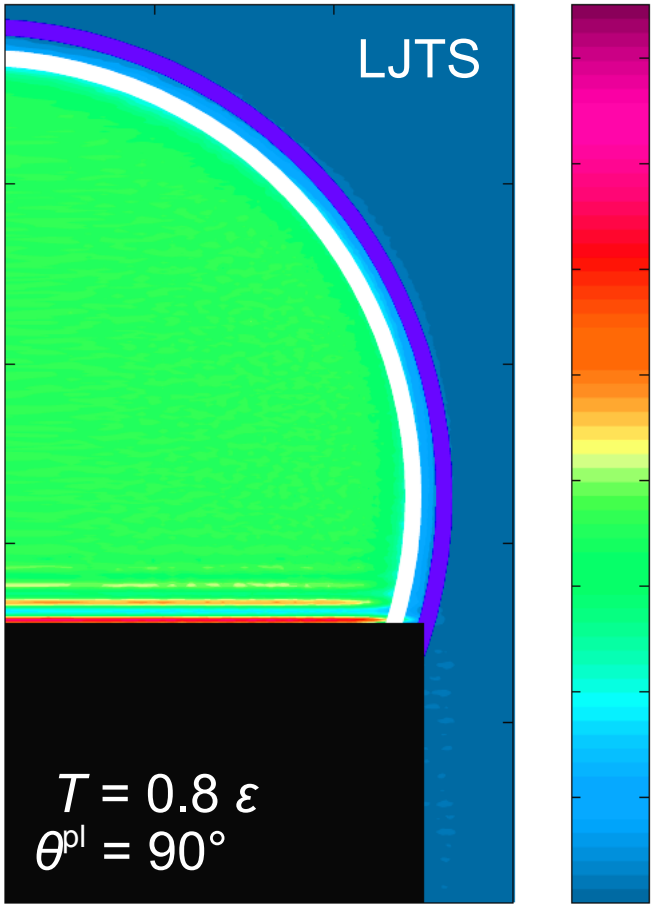



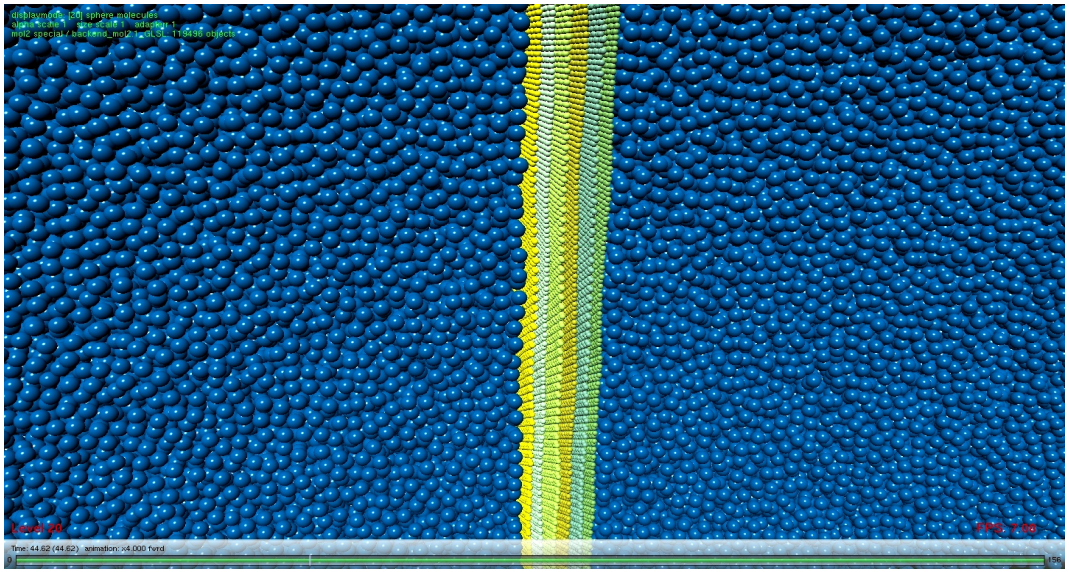
# Molecular simulation of fluids at interfaces

- Adsorption (fluid-fluid and fluid-solid)
- Vapour-liquid surface tension
- Curved vapour-liquid interfaces
- Contact angle and contact line pinning

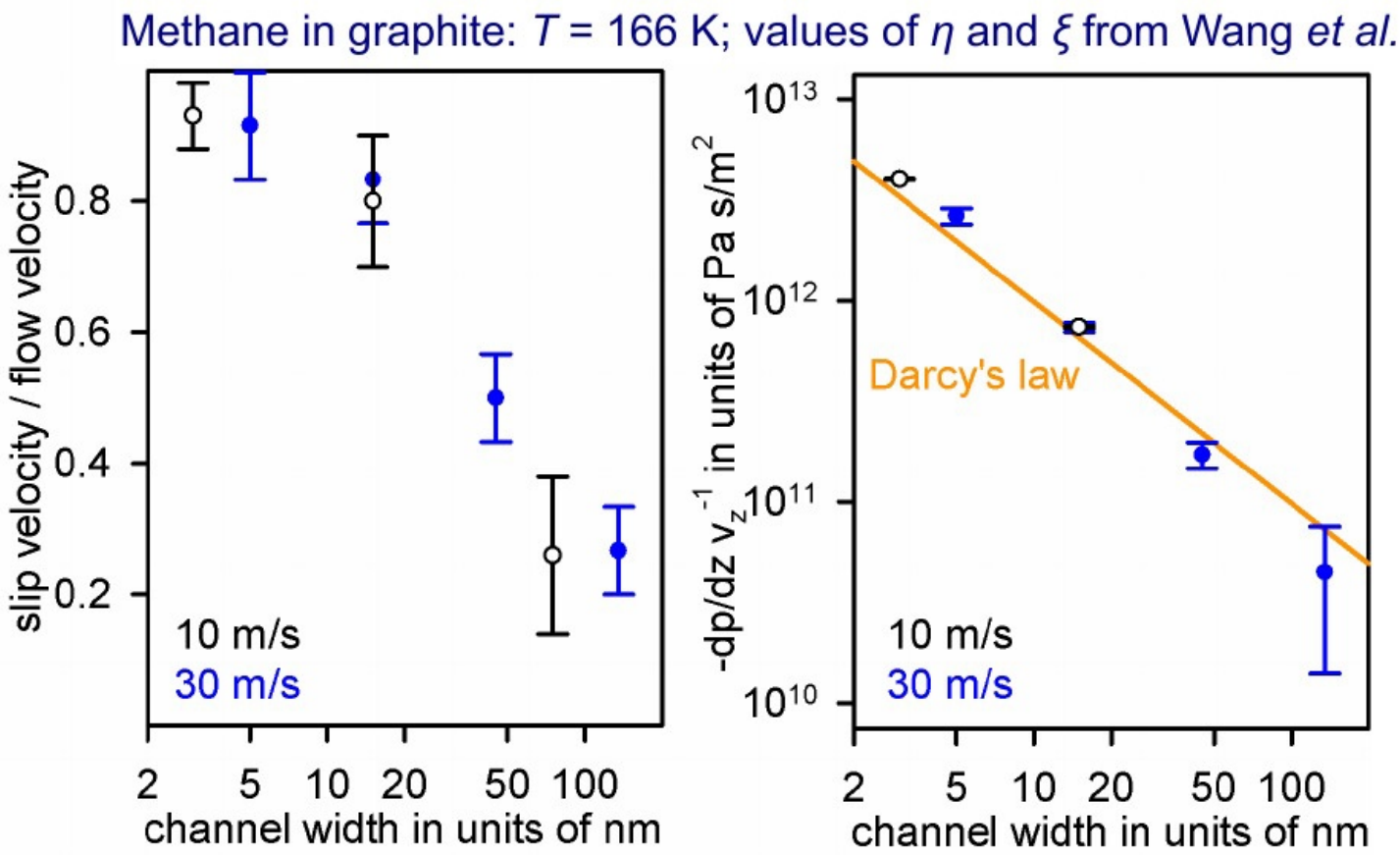




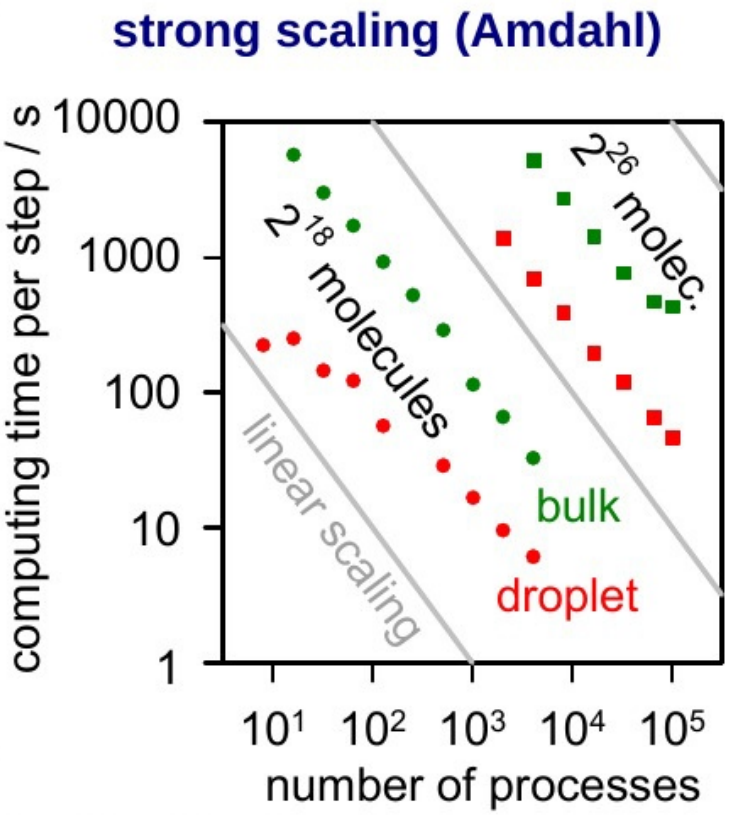
# MD simulation of nanofluidics

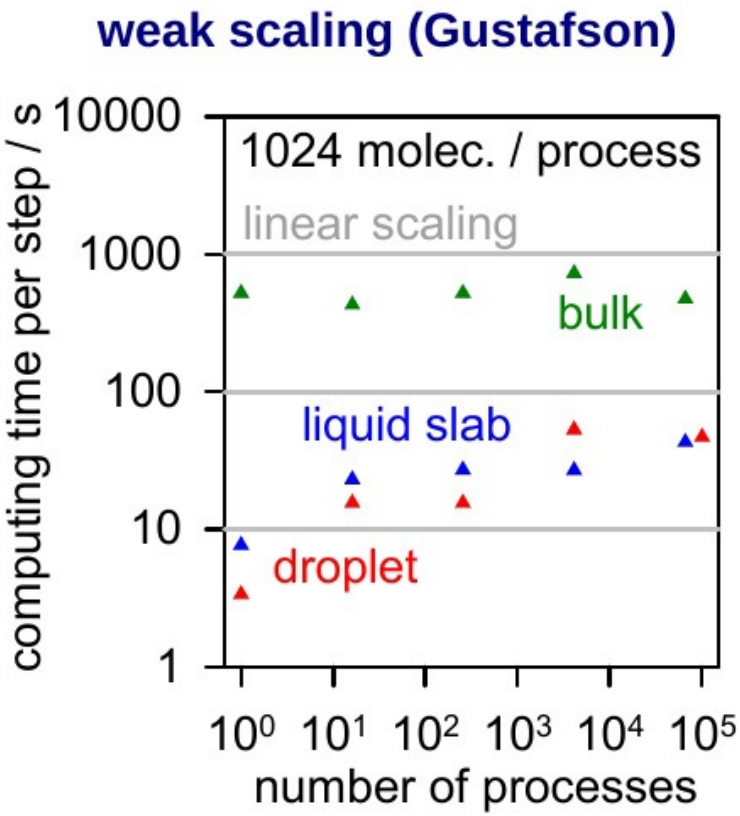


# Scale bridging from nano- to microfluidics



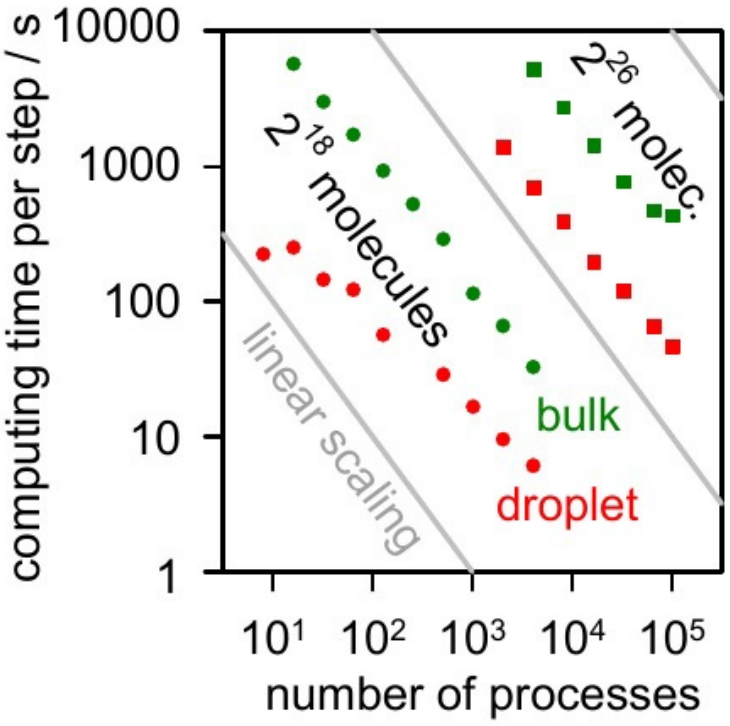
# Scaling of ls1 mardyn on hermit



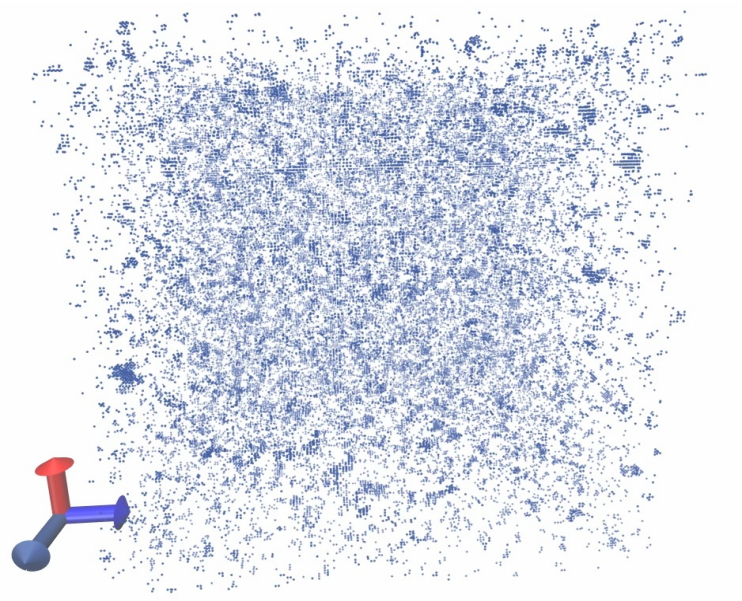



# Scaling of ls1 mardyn on hermit

## strong scaling (Amdahl)



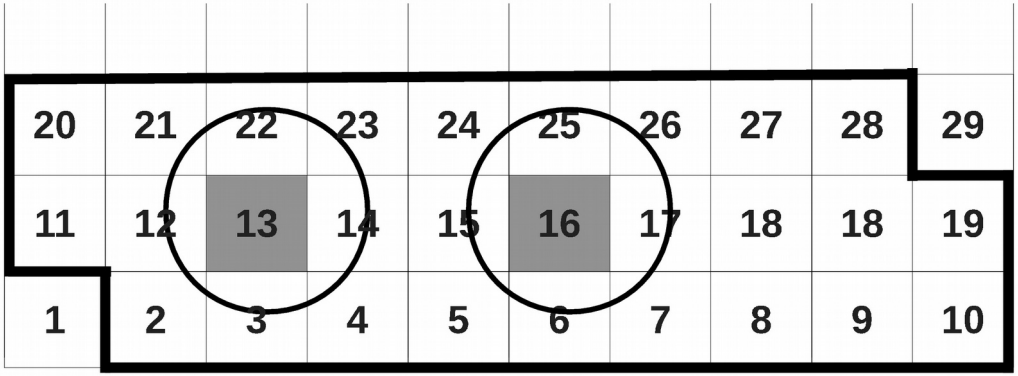

## homogeneous cavitation



$CO_2$ ($T$ = 280 K and $\rho$ = 17.2 mol/l), 3CLJQ
25 million molecules on 110 592 cores

# Optimization of ls1 mardyn for SuperMUC

SuperMUC (LRZ Garching): 3 PFLOPS Intel Xeon Sandy Bridge cluster.




hyperthreaded sliding window

**forces** acting on molecules are only stored while the cell is inside the sliding window

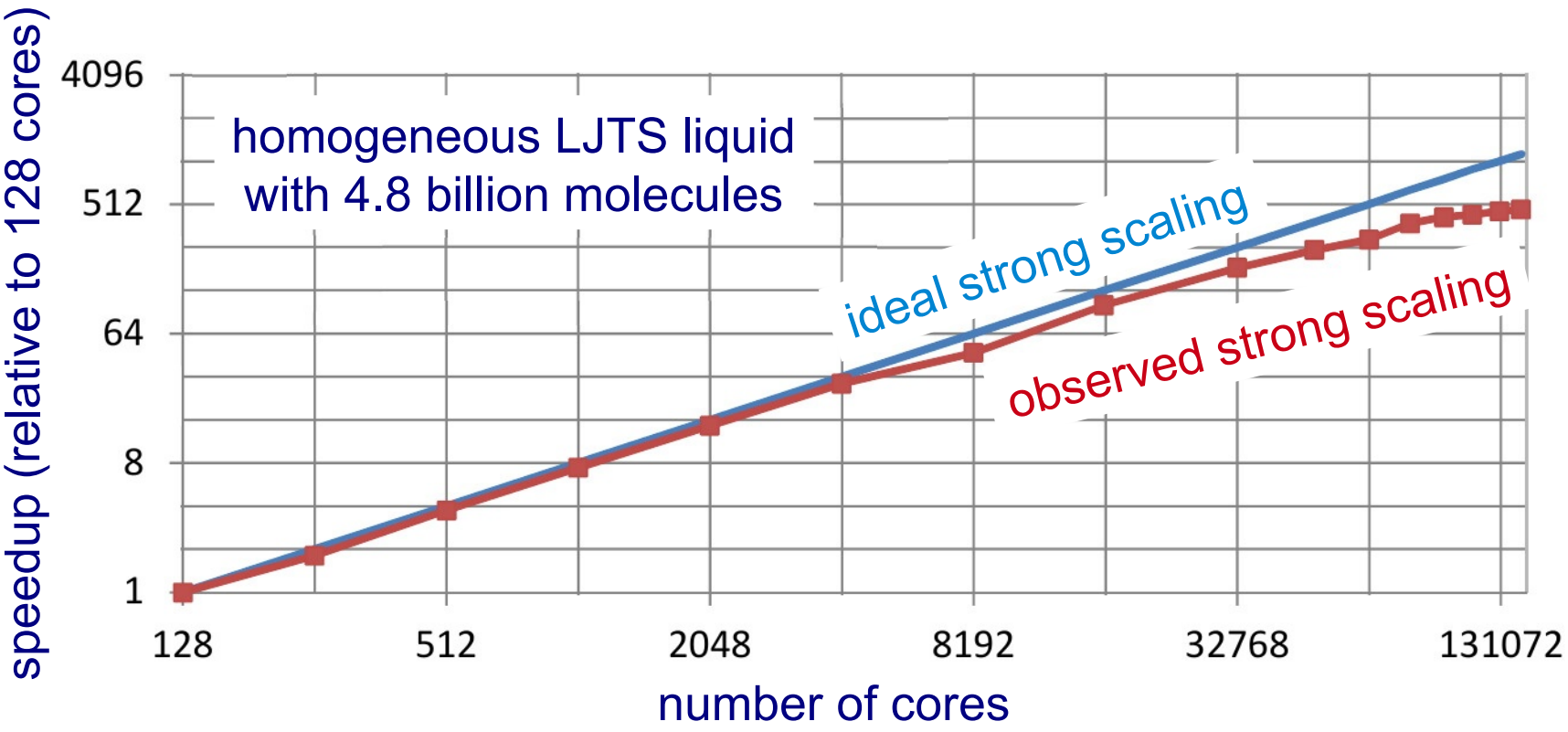
Efficient vectorization:

- Optimization by hand, using advanced vector extensions (AVX).
- Conversion from array of structures (AoS) to structure of arrays (SoA).

Discussed in detail by Nikola Tchipev tomorrow.

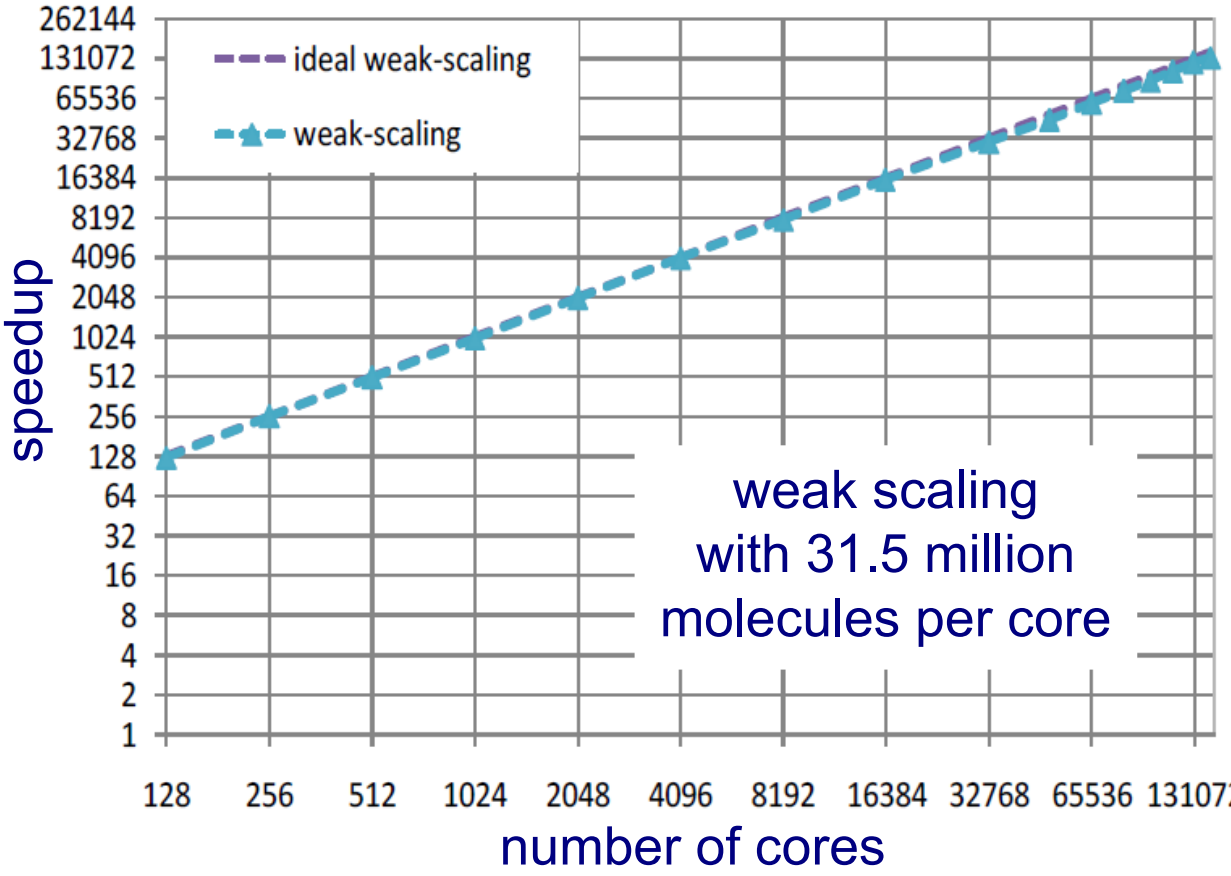
# Large-scale MD simulations on SuperMUC

Scaling of ls1 mardyn examined on up to 146 016 cores, i.e. the whole SuperMUC, by Wolfgang Eckhardt and Alexander Heinecke in 2013.

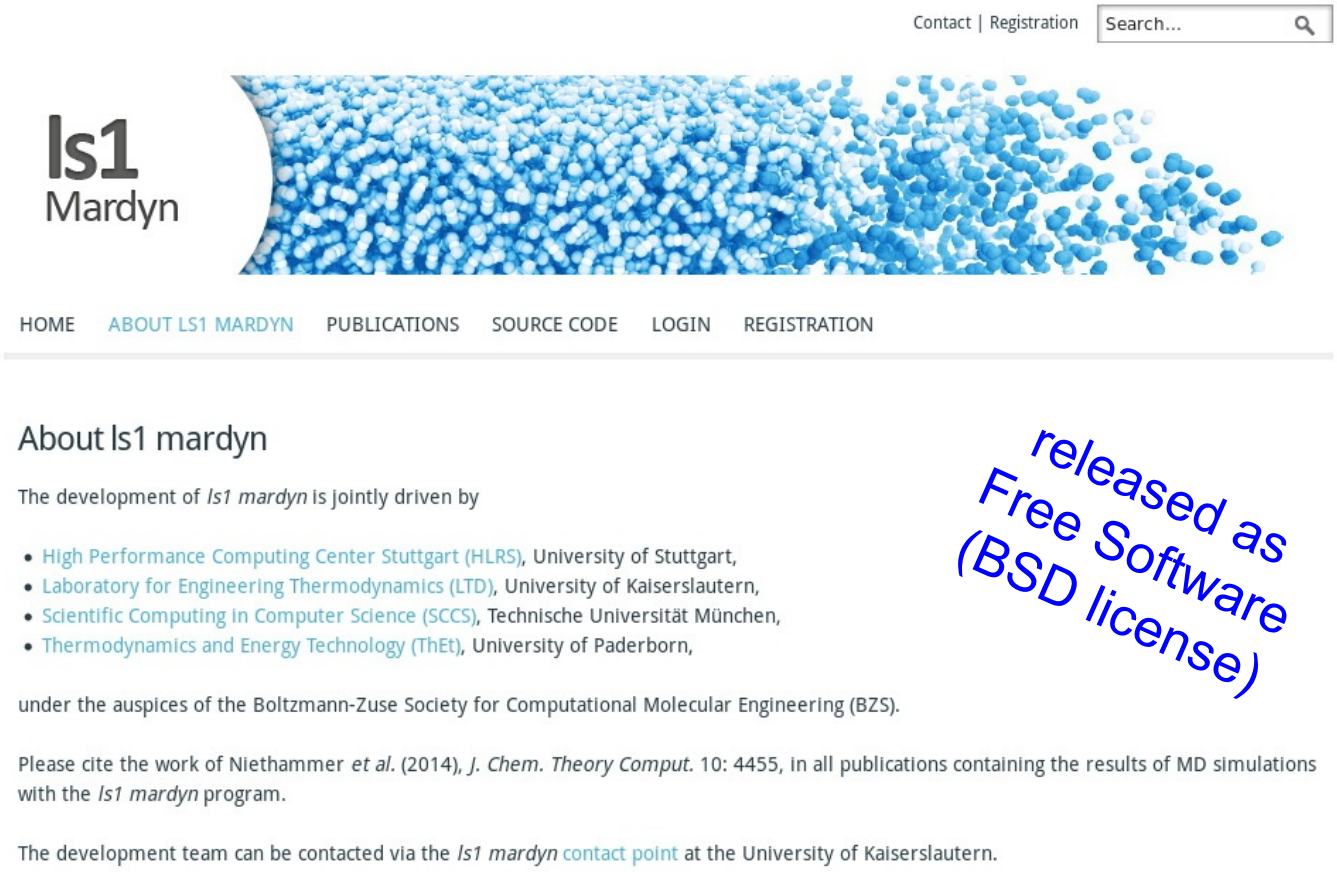


# Large-scale MD simulations on SuperMUC

Up to $N = 4 \cdot 10^{12}$ molecules on *SuperMUC*




# Release of ls1 mardyn




released as Free Software (BSD license)

Free registration for ls1 mardyn at http://www.ls1-mardyn.de/