Large-scale MD simulation of heterogeneous systems with ls1 mardyn


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ProcessNet International Workshop MolMod
Parallelization by volume decomposition

Linked-cell data structure suitable for spatial domain decomposition:

Large systems “1”: molecular dynamics

http://www.ls1-mardyn.de/

Horsch, Srivastava, Werth, Niethammer, Glass, Eckhardt, Heinecke, Tchipev, Bungartz, Eckelsbach, Vrabec and Hasse
Parallelization by volume decomposition

Linked-cell data structure suitable for spatial domain decomposition:

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.
Scale separation and long-range correction

For planar interfaces:

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

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

Full evaluation of all pairwise interactions is too expensive ...

... instead, short-range interactions are evaluated for neighbours.
Molecular simulation of fluids at interfaces

For planar interfaces:

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

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

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

$T = 0.8 \varepsilon$
$
\theta_{pl} = 90^\circ$

Horsch, Srivastava, Werth, Niethammer, Glass, Eckhardt, Heinecke, Tchipev, Bungartz, Eckelsbach, Vrabec and Hasse
MD simulation of nanofluidics
Scale bridging from nano- to microfluidics

Methane in graphite: $T = 166$ K; values of $\eta$ and $\xi$ from Wang et al.

- $\text{slip velocity / flow velocity}$
  - $10 \text{ m/s}$
  - $30 \text{ m/s}$

- $\frac{-dp}{dz} v_z^{-1}$ in units of $\text{Pa s/m}^2$
  - $10 \text{ m/s}$
  - $30 \text{ m/s}$

Darcy's law
Scaling of ls1 mardyn on hermit

**strong scaling (Amdahl)**

**weak scaling (Gustafson)**

![Graph showing strong and weak scaling](image-url)
Scaling of ls1 mardyn on hermit

**strong scaling (Amdahl)**

<table>
<thead>
<tr>
<th>Computing time per step / s</th>
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<td>$10^2$</td>
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</table>

- $2^{18}$ molecules
- $2^{26}$ molecules
- bulk
- droplet

**homogeneous cavitation**

$\text{CO}_2$ ($T = 280 \, \text{K}$ and $\rho = 17.2 \, \text{mol/l}$), 3CLJQ

25 million molecules on 110 592 cores
Optimization of ls1 mardyn for SuperMUC

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

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.

Graph showing speedup relative to 128 cores versus number of cores. The graph includes a line indicating ideal strong scaling and another line indicating observed strong scaling. The homogeneous LJTS liquid with 4.8 billion molecules is also mentioned.
Large-scale MD simulations on SuperMUC

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

speedup

weak scaling
with 31.5 million molecules per core

number of cores

2013
Release of ls1 mardyn

About ls1 mardyn

The development of ls1 mardyn is jointly driven by

- High Performance Computing Center Stuttgart (HLRS), University of Stuttgart,
- Laboratory for Engineering Thermodynamics (LTD), University of Kaiserslautern,
- Scientific Computing in Computer Science (SCCS), Technische Universität München,
- Thermodynamics and Energy Technology (ThET), University of Paderborn,

under the auspices of the Boltzmann-Zuse Society for Computational Molecular Engineering (BZS).

Please cite the work of Niethammer et al. (2014), J. Chem. Theory Comput. 10: 4455, in all publications containing the results of MD simulations with the ls1 mardyn program.

The development team can be contacted via the ls1 mardyn contact point at the University of Kaiserslautern.

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