Scale-bridging massively-parallel molecular simulation with *ls1 mardyn*

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Computational Molecular Engineering

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Force fields for low-molecular fluids

Geometry

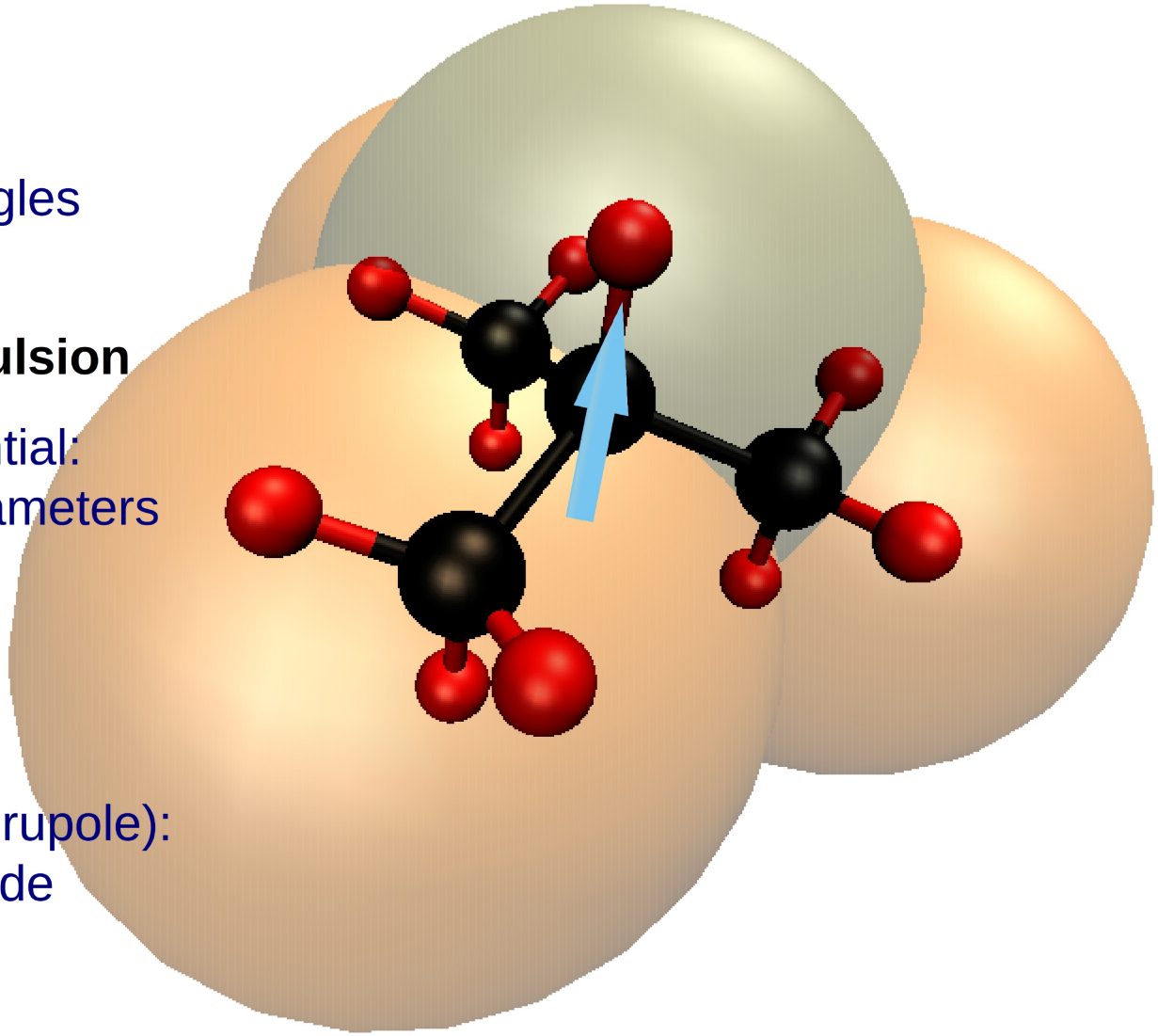
Bond lengths and angles

Dispersion and repulsion

Lennard-Jones potential:
Size and energy parameters

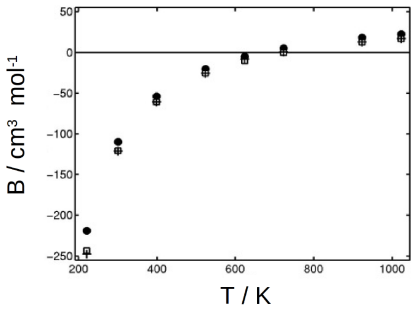
Electrostatics

Point polarities
(charge, dipole, quadrupole):
Position and magnitude

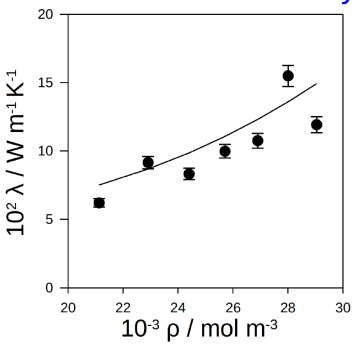


Homogeneous systems in equilibrium: ms2

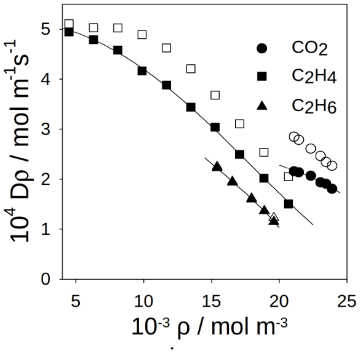
Second virial coefficient



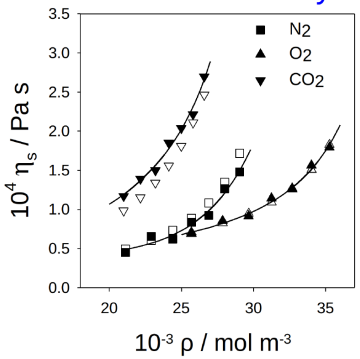
Thermal conductivity



Self-diffusion coefficient

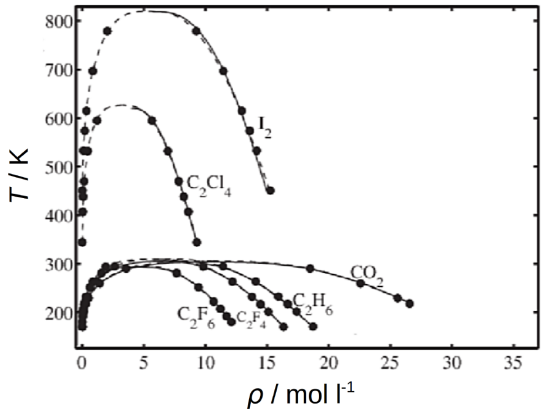


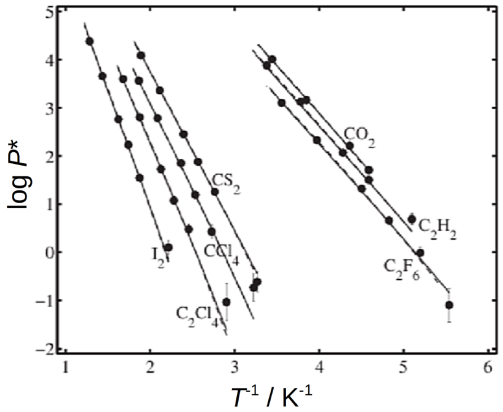
Shear viscosity



transport properties from equilibrium MD simulation

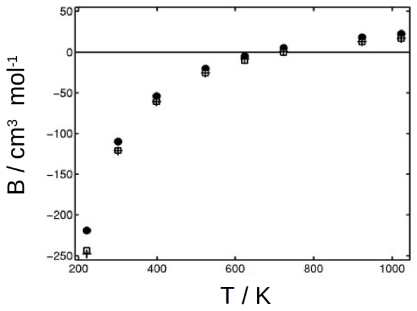
Vapour-liquid equilibira: Saturated densities and vapour pressures



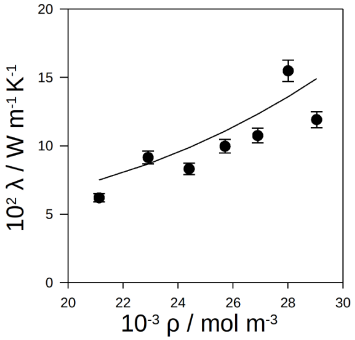


Homogeneous systems in equilibrium: ms2

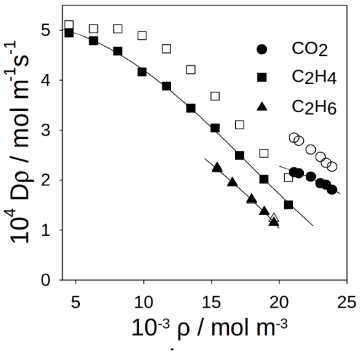
Second virial coefficient



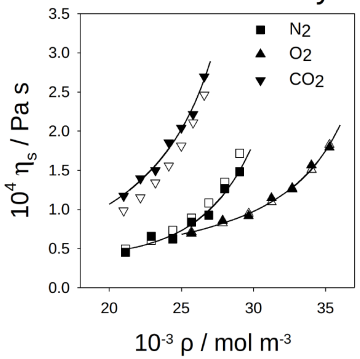
Thermal conductivity



Self-diffusion coefficient

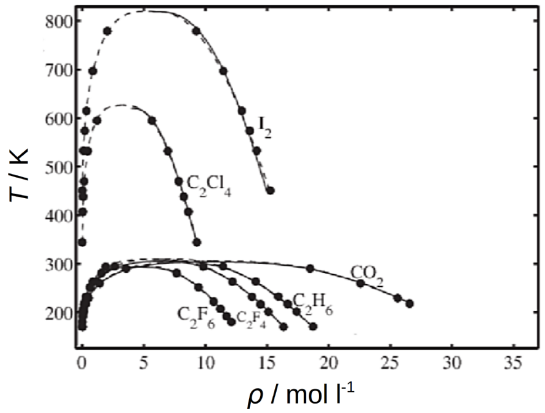


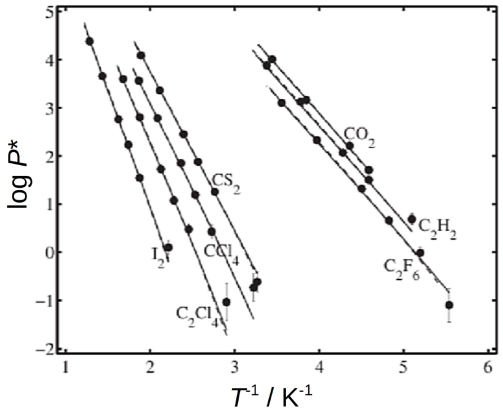
Shear viscosity



ms2 is freely available for academic use – register at http://www.ms-2.de/

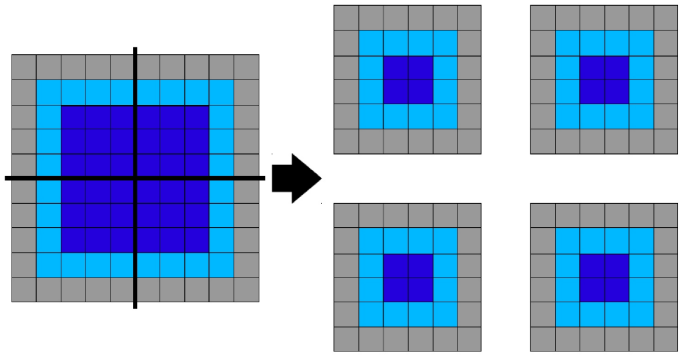
Vapour-liquid equilibira: Saturated densities and vapour pressures



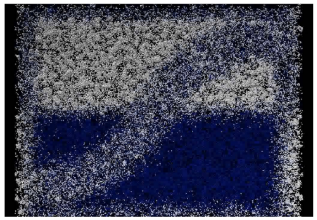


Efficient simulation of large systems

Linked-cell data structure suitable for spatial domain decomposition:



(non-blocking, over-lapping MPI send/ receive operations)



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H L R S

large systems “1”: molecular dynamics

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

Efficient simulation of large systems

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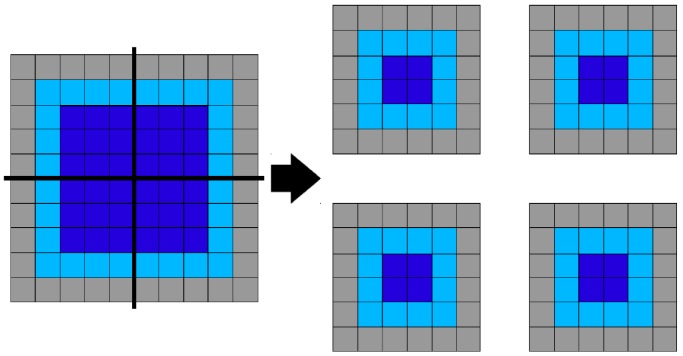
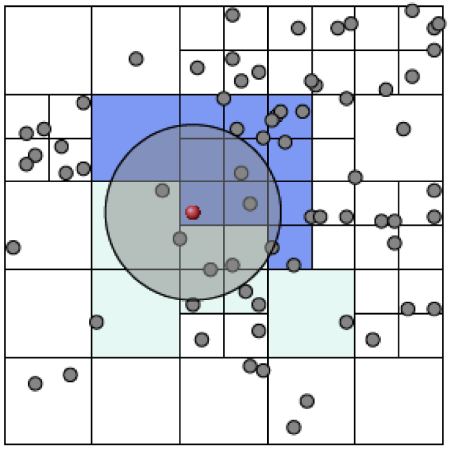
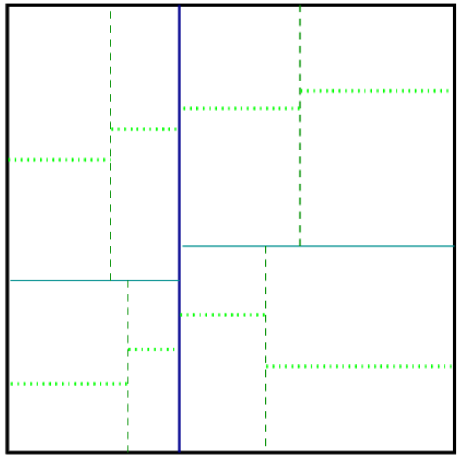


(non-blocking, over-lapping MPI send/ receive operations)

Methods for heterogeneous or fluctuating particle distributions:



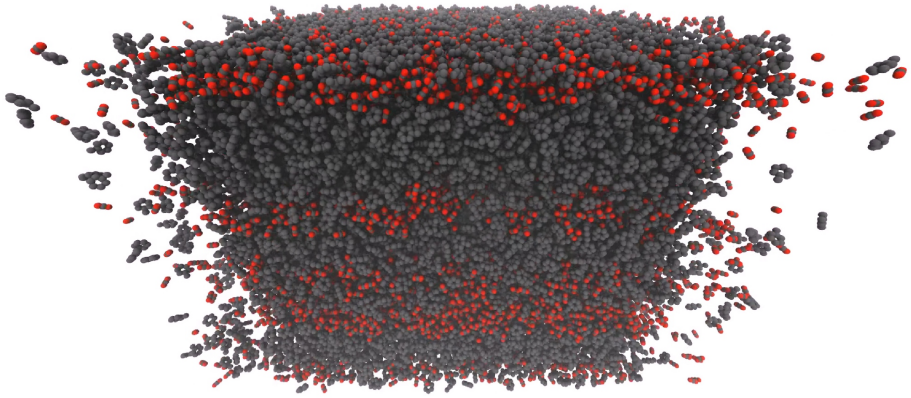


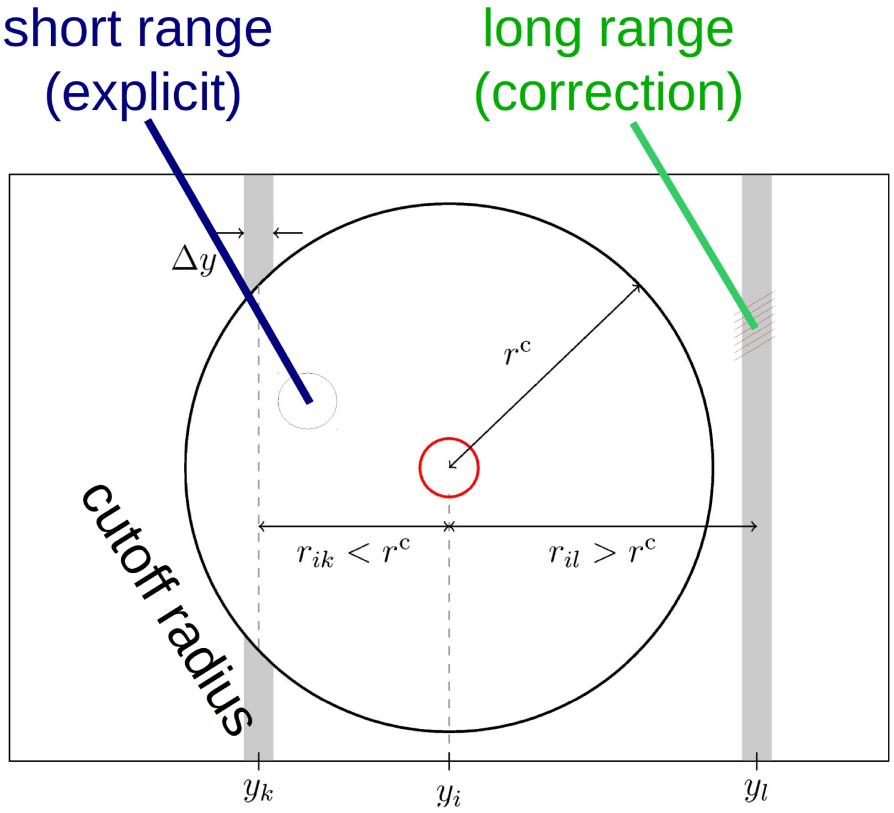
large systems “1”: molecular dynamics **http://www.ls1-mardyn.de/**

Efficient simulation of fluids at interfaces

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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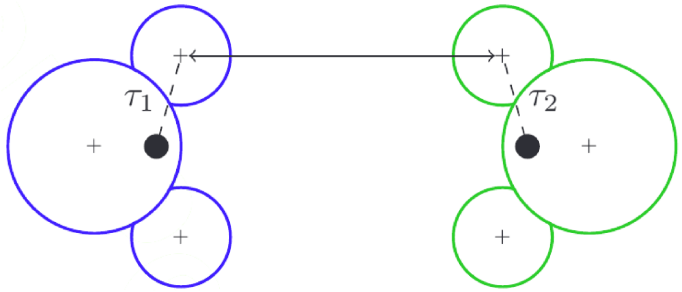
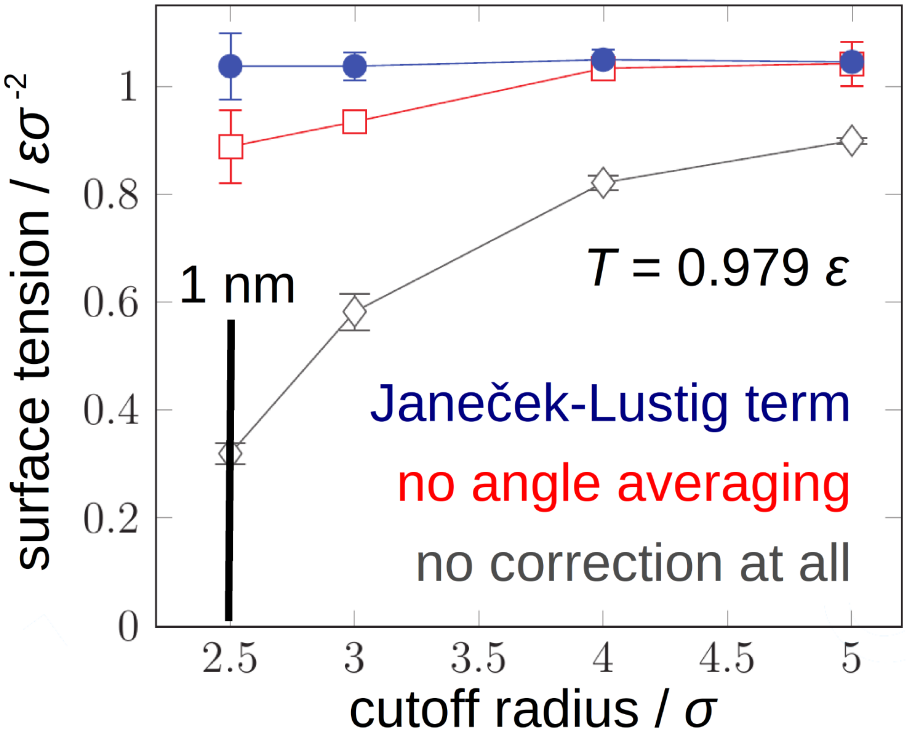


Angle-averaging expression for multi-site models, following **Lustig**.

Two-centre LJ fluid (2CLJ)



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

Efficient simulation of large systems

Memory-efficient implementation based on the linked-cell data structure:

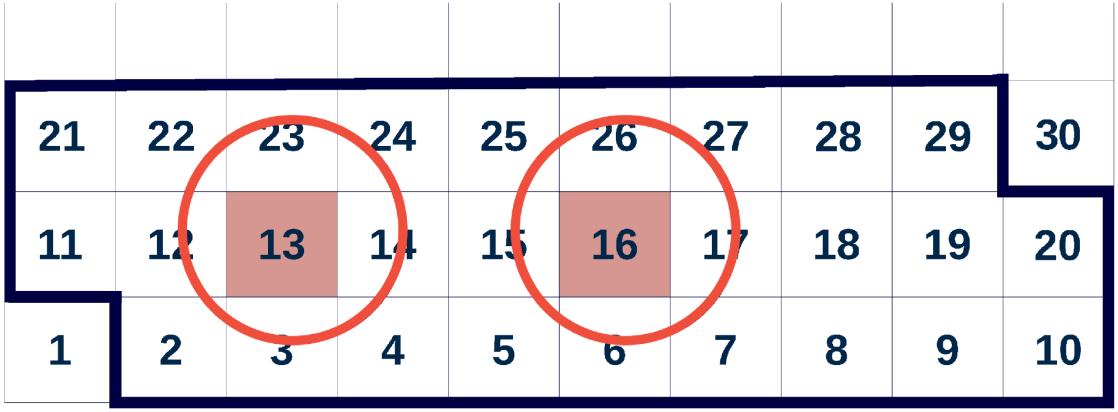
sliding window

Optionally, forces acting on molecules are only stored until their cell leaves the sliding window.

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

Efficient simulation of large systems

Memory-efficient implementation based on the linked-cell data structure:



hyperthreaded sliding window

Optionally, forces acting on molecules are only stored until their cell leaves the sliding window.

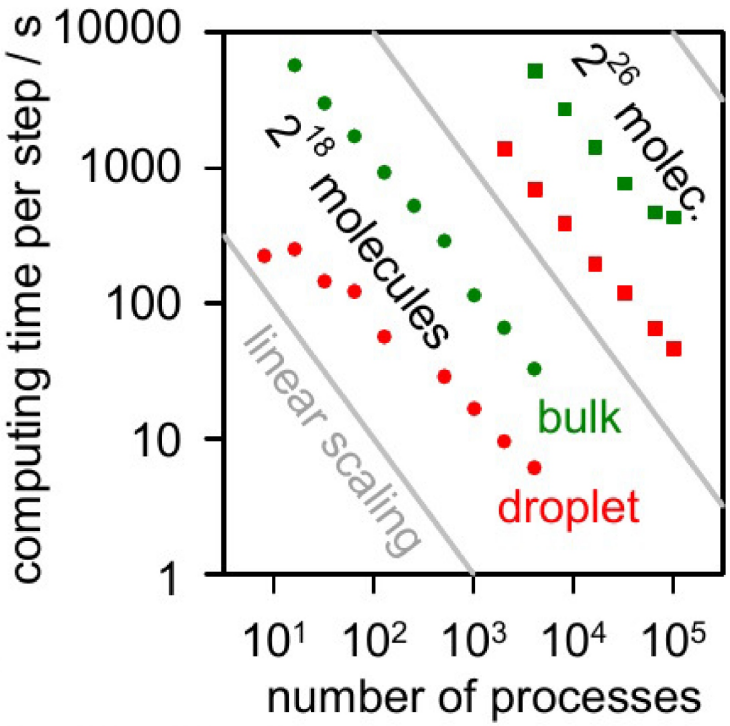
Efficient vectorization:

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

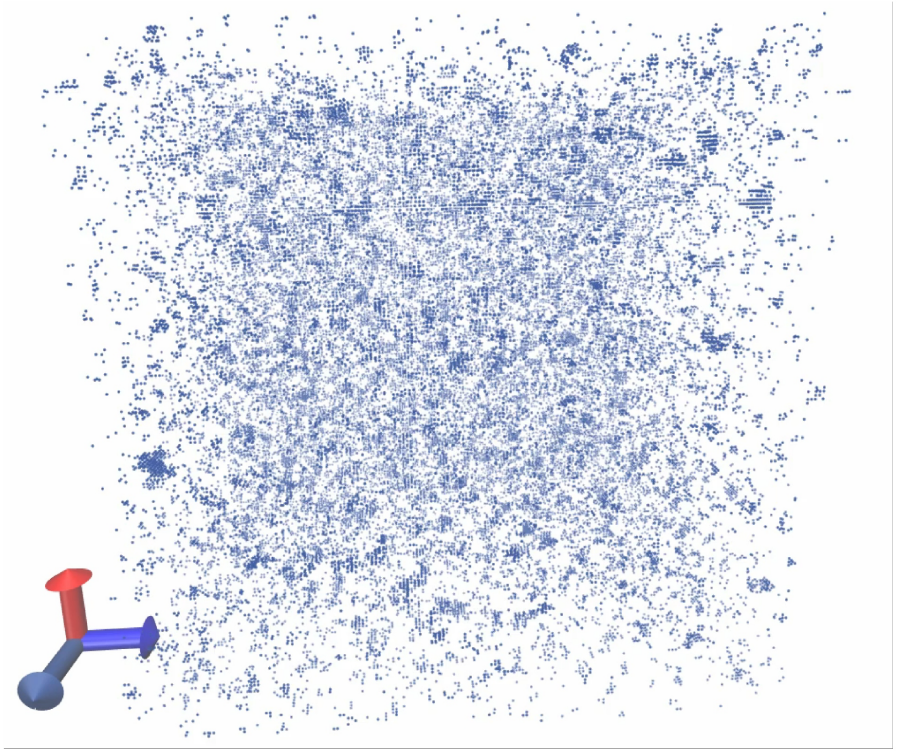
large systems “1”: molecular dynamics **http://www.ls1-mardyn.de/**

Large-scale MD simulation on hermit

strong scaling (Amdahl)



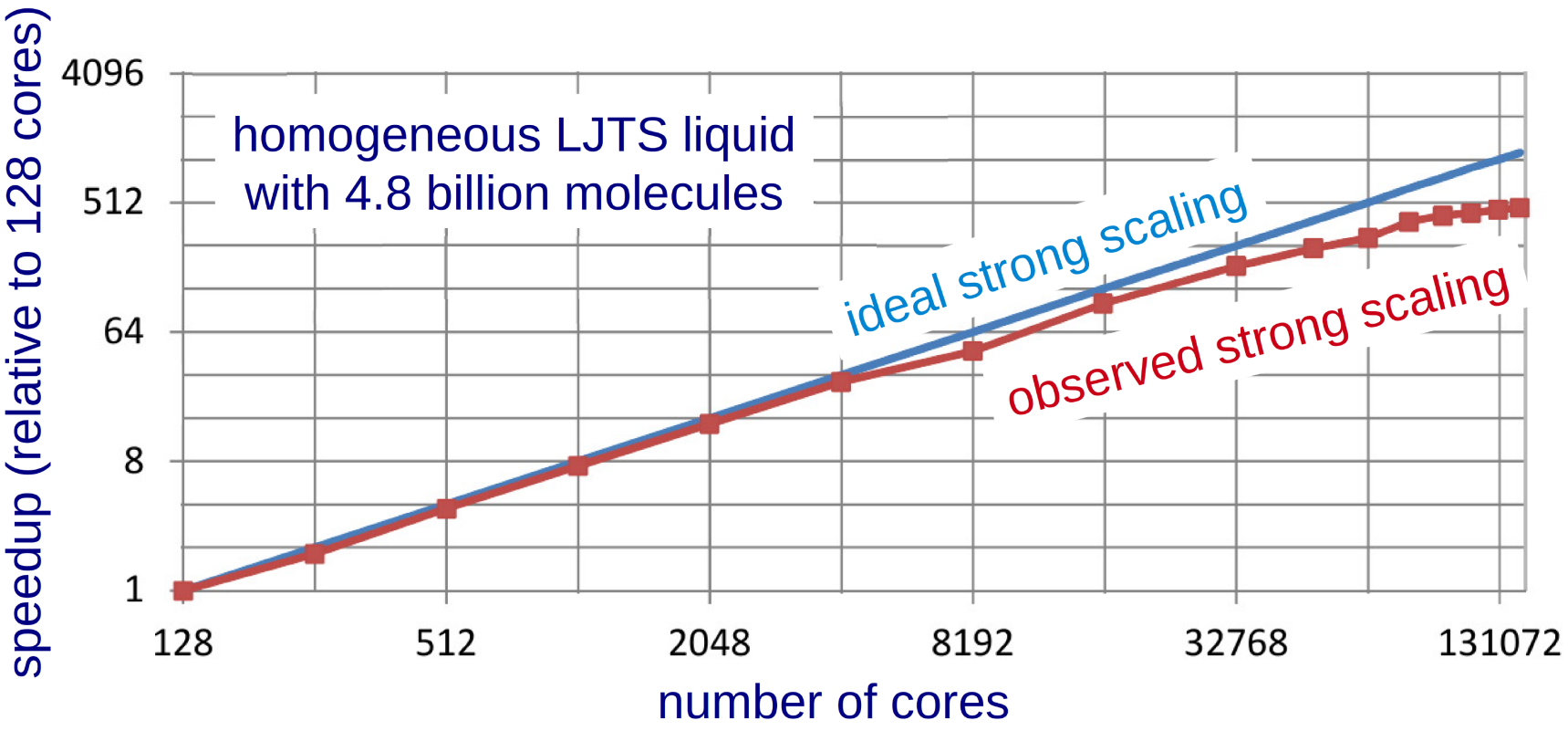
homogeneous cavitation



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

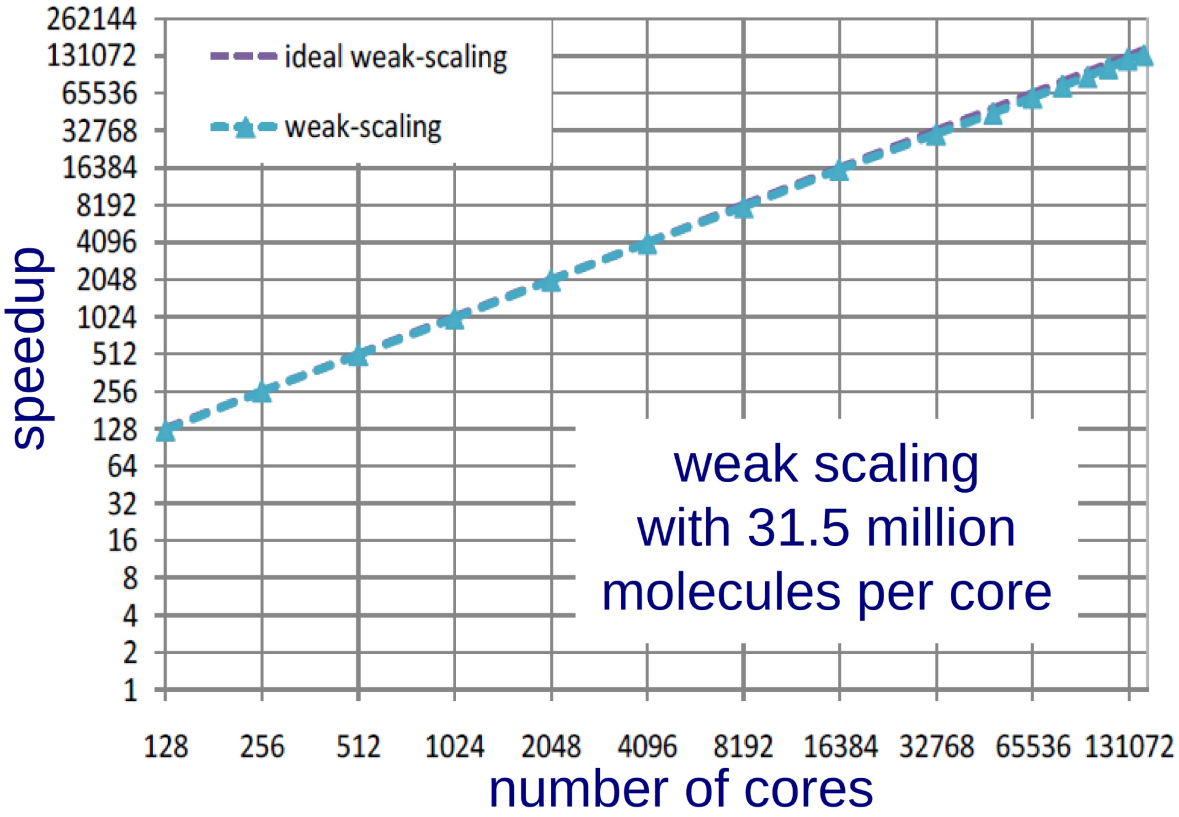
Large-scale MD simulation on SuperMUC

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 simulation on SuperMUC

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



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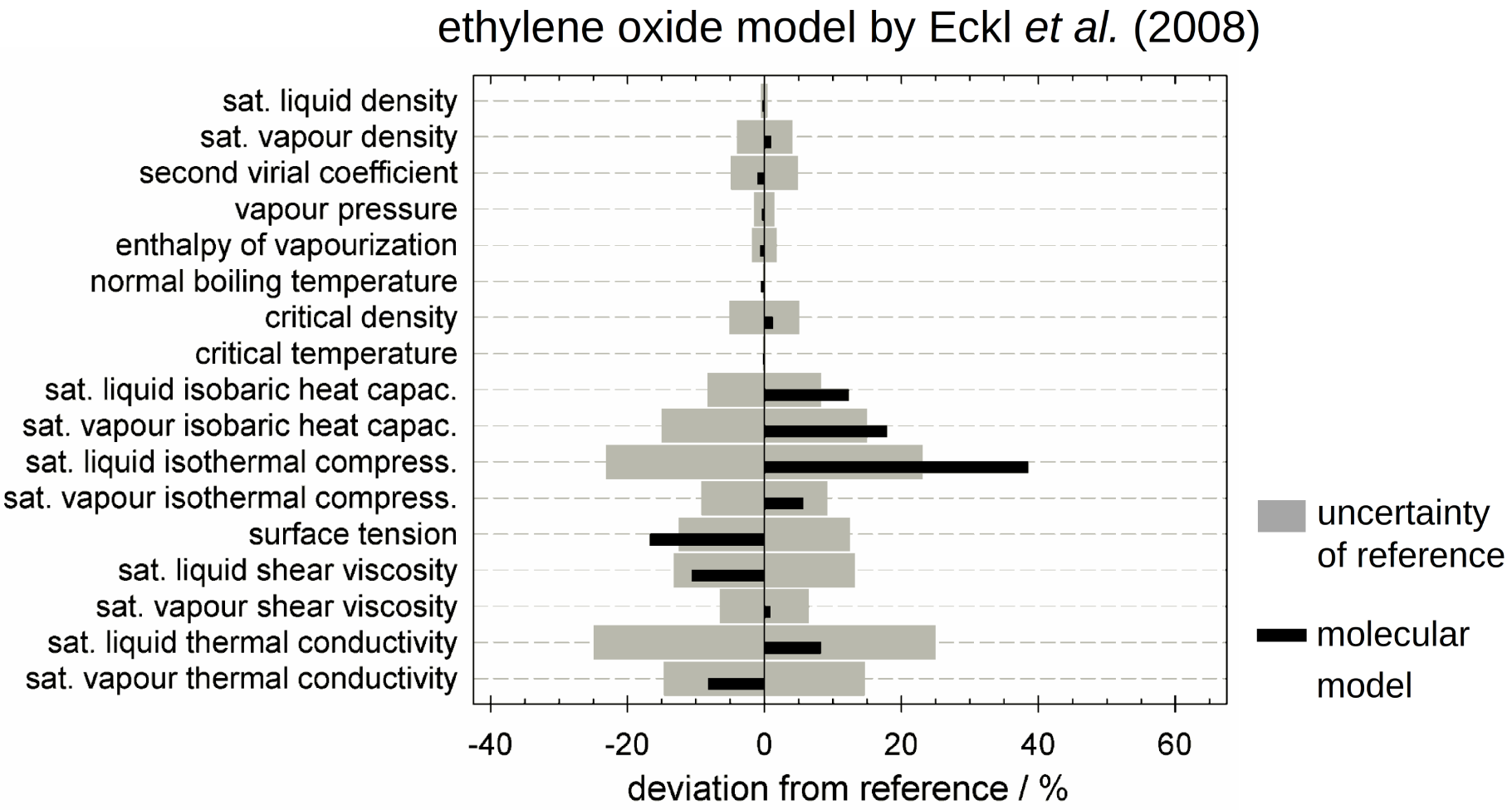
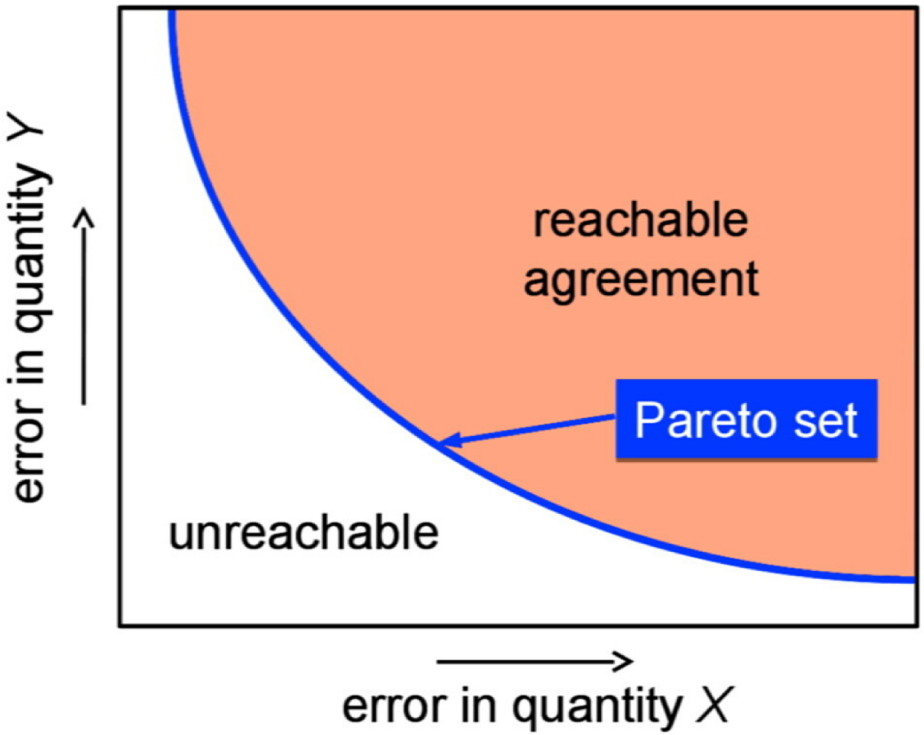
Quantitative reliability of molecular models

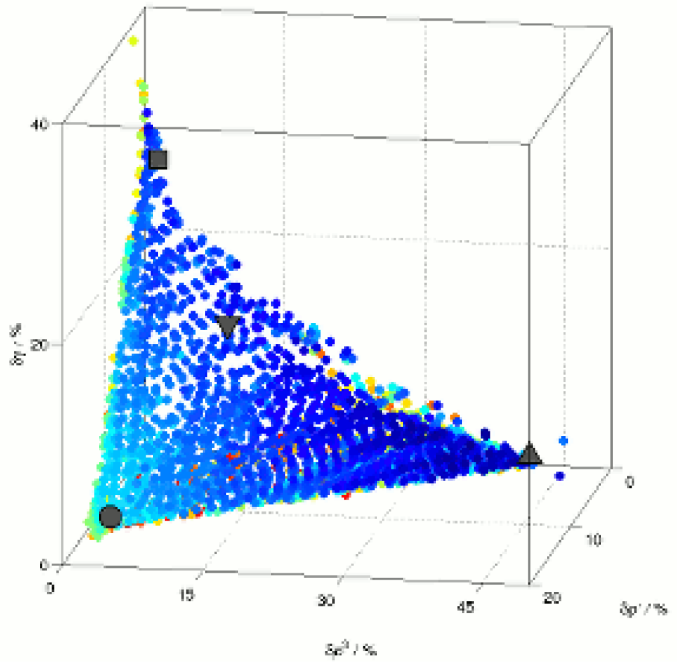


Model tailoring by multicriteria optimization

Pareto optimality criterion



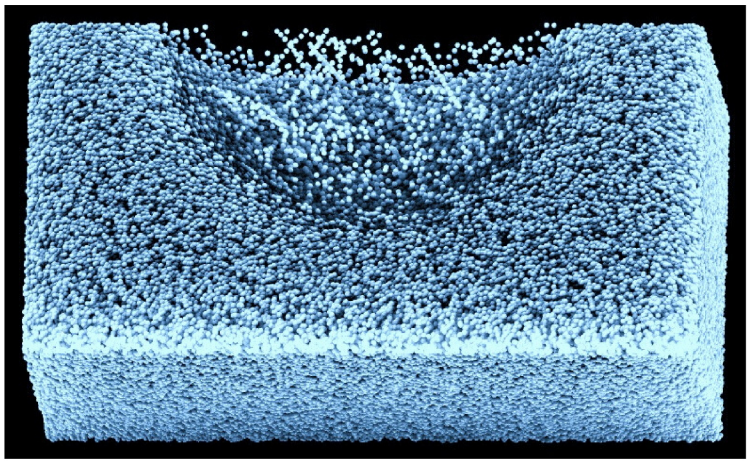
Pareto set for carbon dioxide

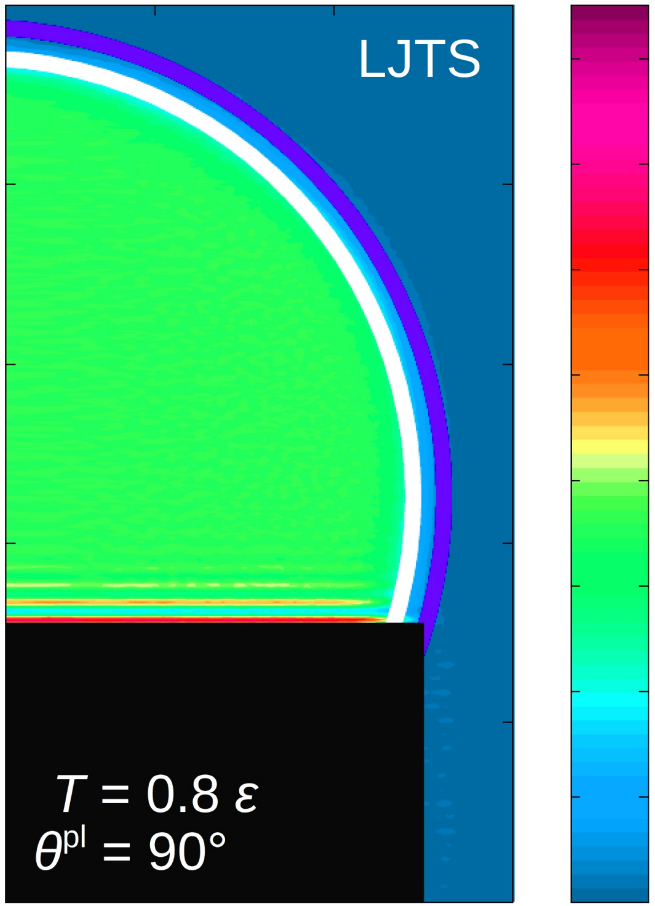


Multicriteria optimization requires massively-parallel molecular modelling.

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





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