Computational molecular engineering by large-scale molecular dynamics simulation

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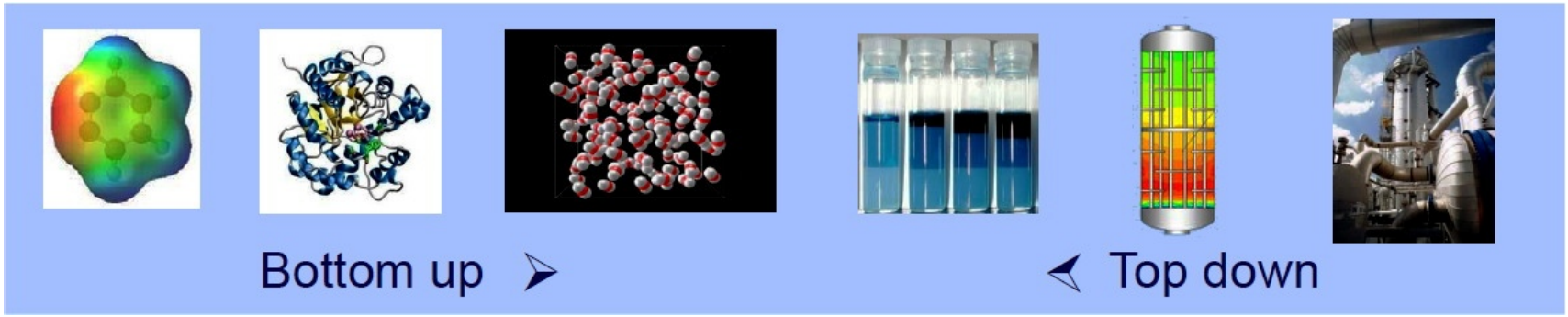
Indo-German Frontiers of Engineering

Computational Molecular Engineering

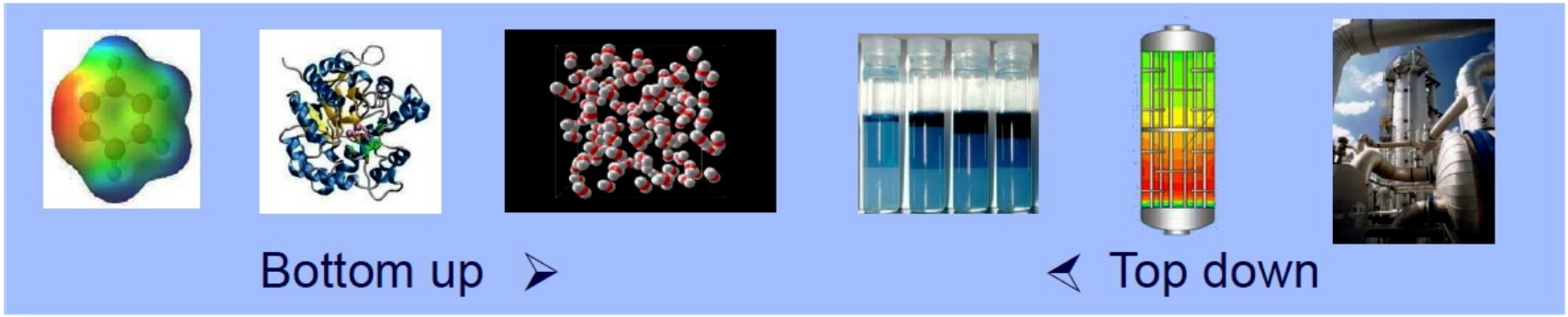
Computational Molecular Engineering



From Physics
(qualitative accuracy)

- Physically realistic modelling of intermolecular interactions
- Separate contributions due to repulsive and dispersive as well as electrostatic interactions

Computational Molecular Engineering



From Physics (qualitative accuracy)

- Physically realistic modelling of intermolecular interactions
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To Engineering (quantitative reliability)

- No blind fitting, but parameters of effective pair potentials are adjusted to experimental data
- Physical realism facilitates reliable interpolation and extrapolation

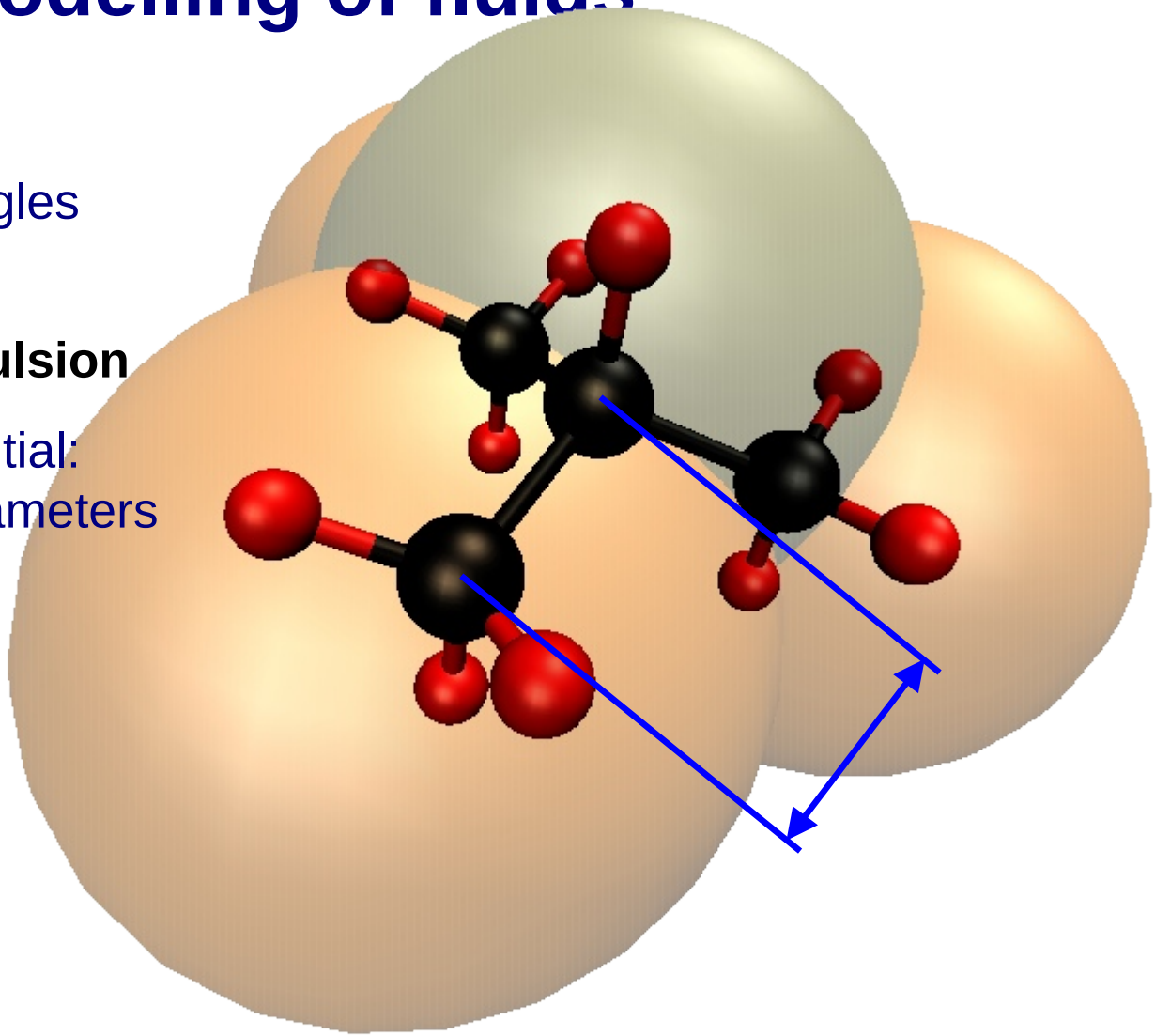
Molecular modelling of fluids

Geometry

Bond lengths and angles

Dispersion and repulsion

Lennard-Jones potential:
Size and energy parameters



Molecular modelling of fluids

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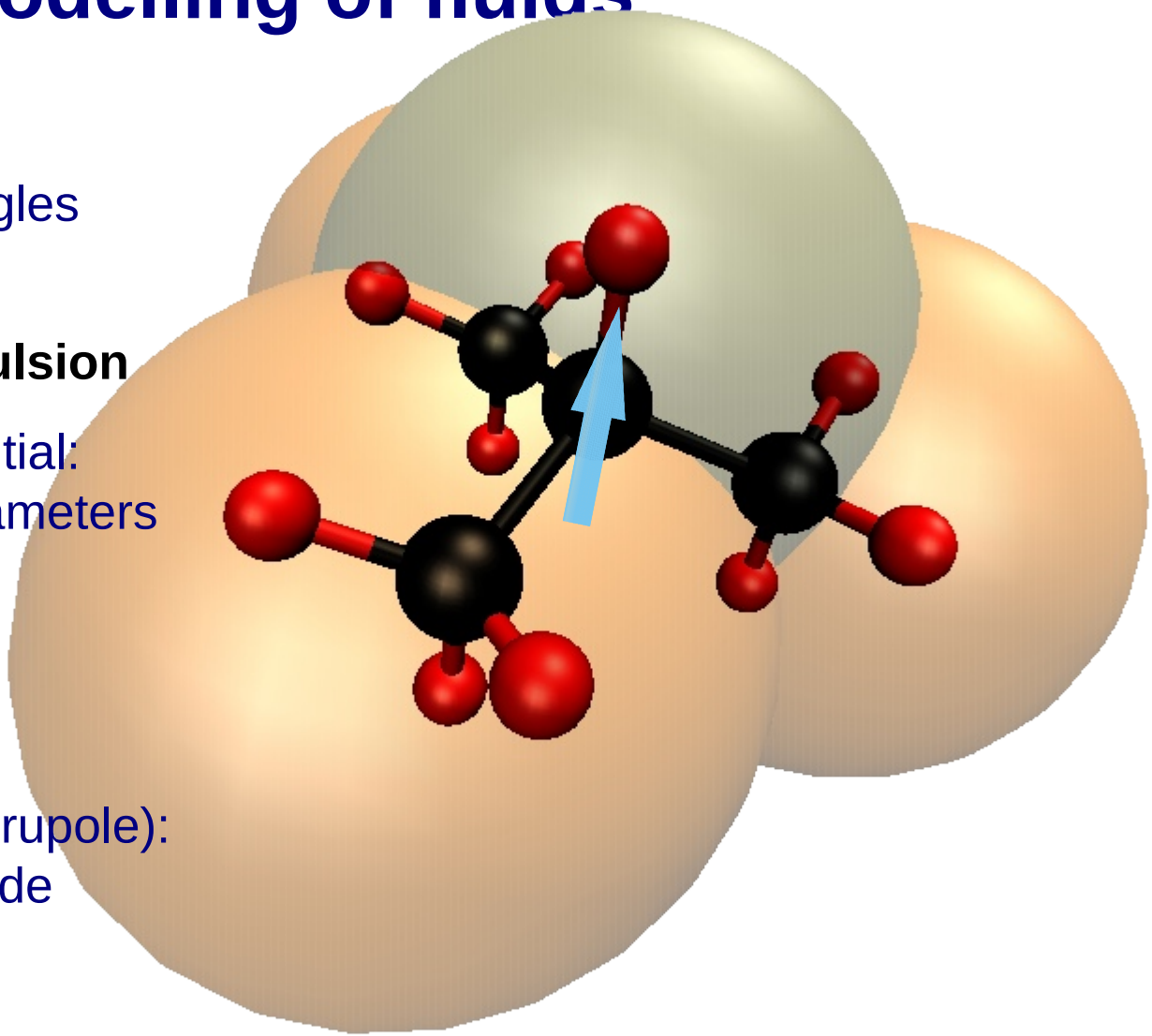
Dispersion and repulsion

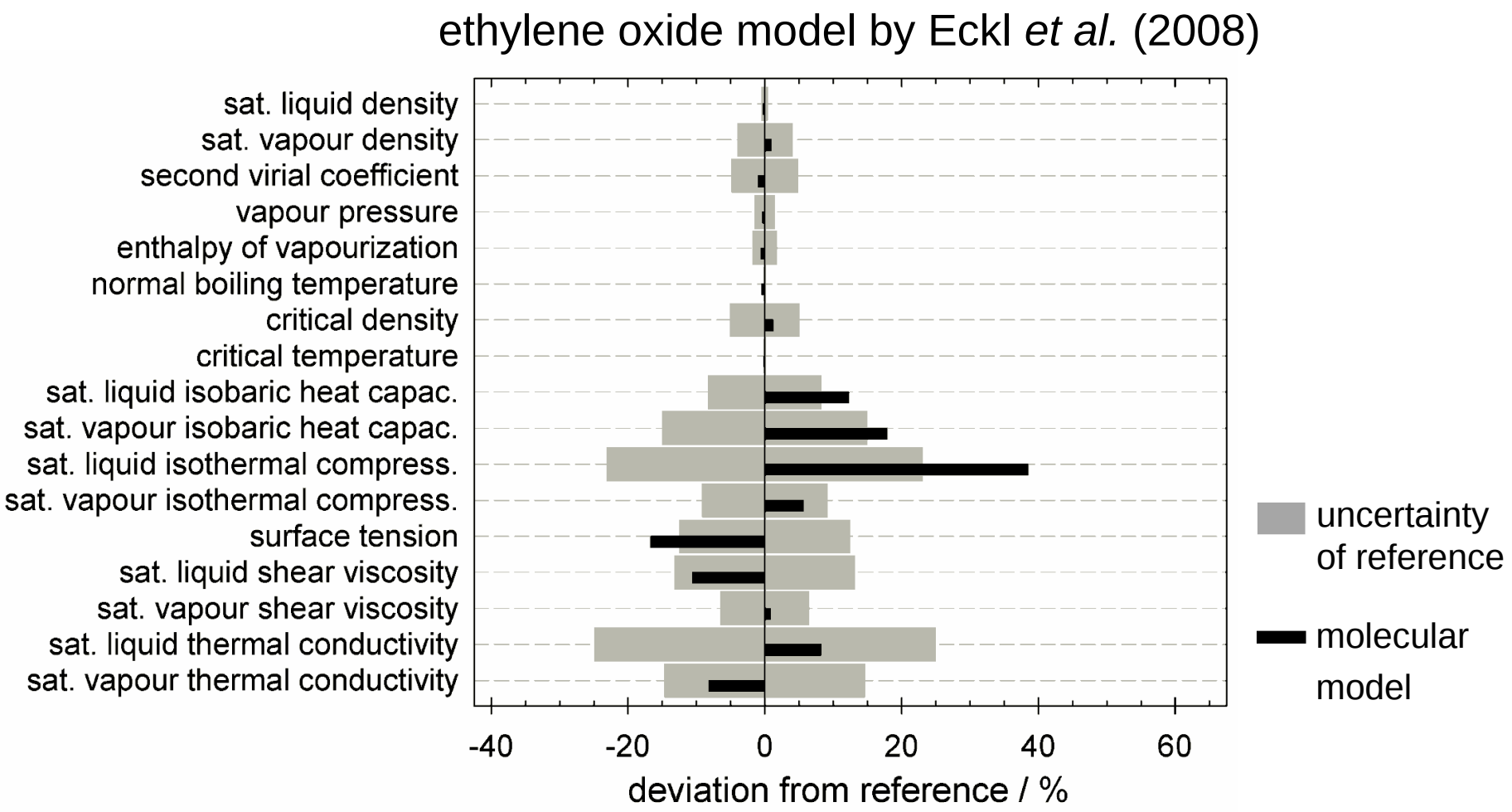
Lennard-Jones potential:
Size and energy parameters

Electrostatics

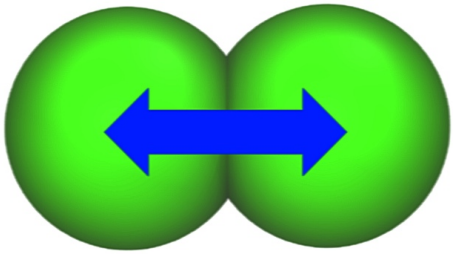
Point polarities
(charge, dipole, quadrupole):
Position and magnitude



Quantitatively reliable molecular models



Molecular models: Parameterization



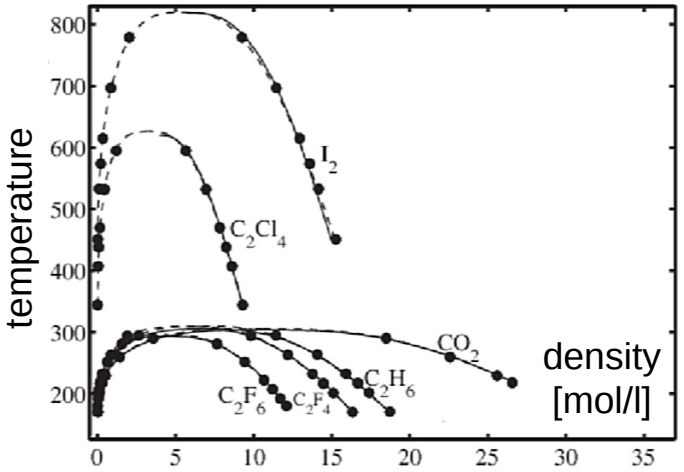
2CLJQ models:

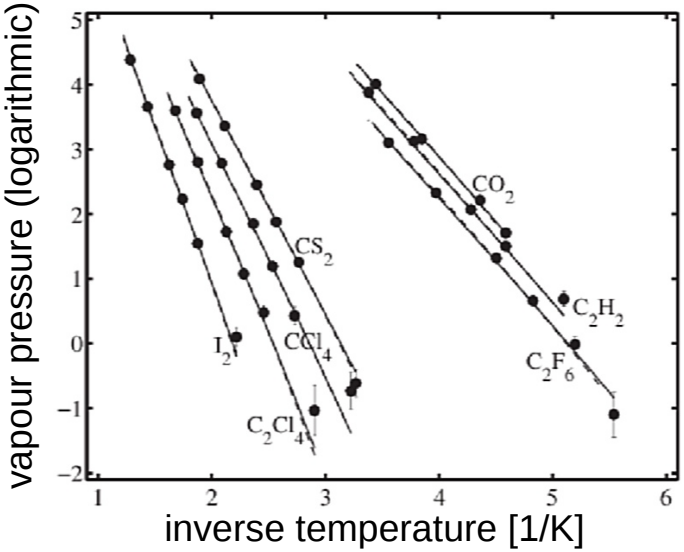
- 2 LJ centres
- Quadrupole

Fit of parameters σ, ε, L, Q to VLE data of 29 fluids by Stoll *et al.*

Deviation:

- $\delta\rho' \approx 1$ %
- $\delta P^{sat} \approx 5$ %

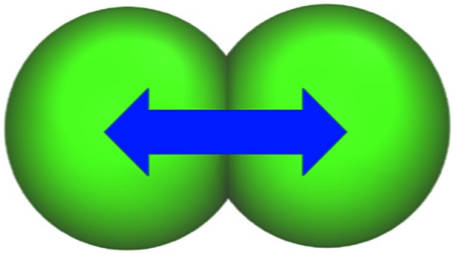




- simulation
— DIPPR correlation

No interfacial properties were considered for the parameterization.

Molecular models: Prediction and validation



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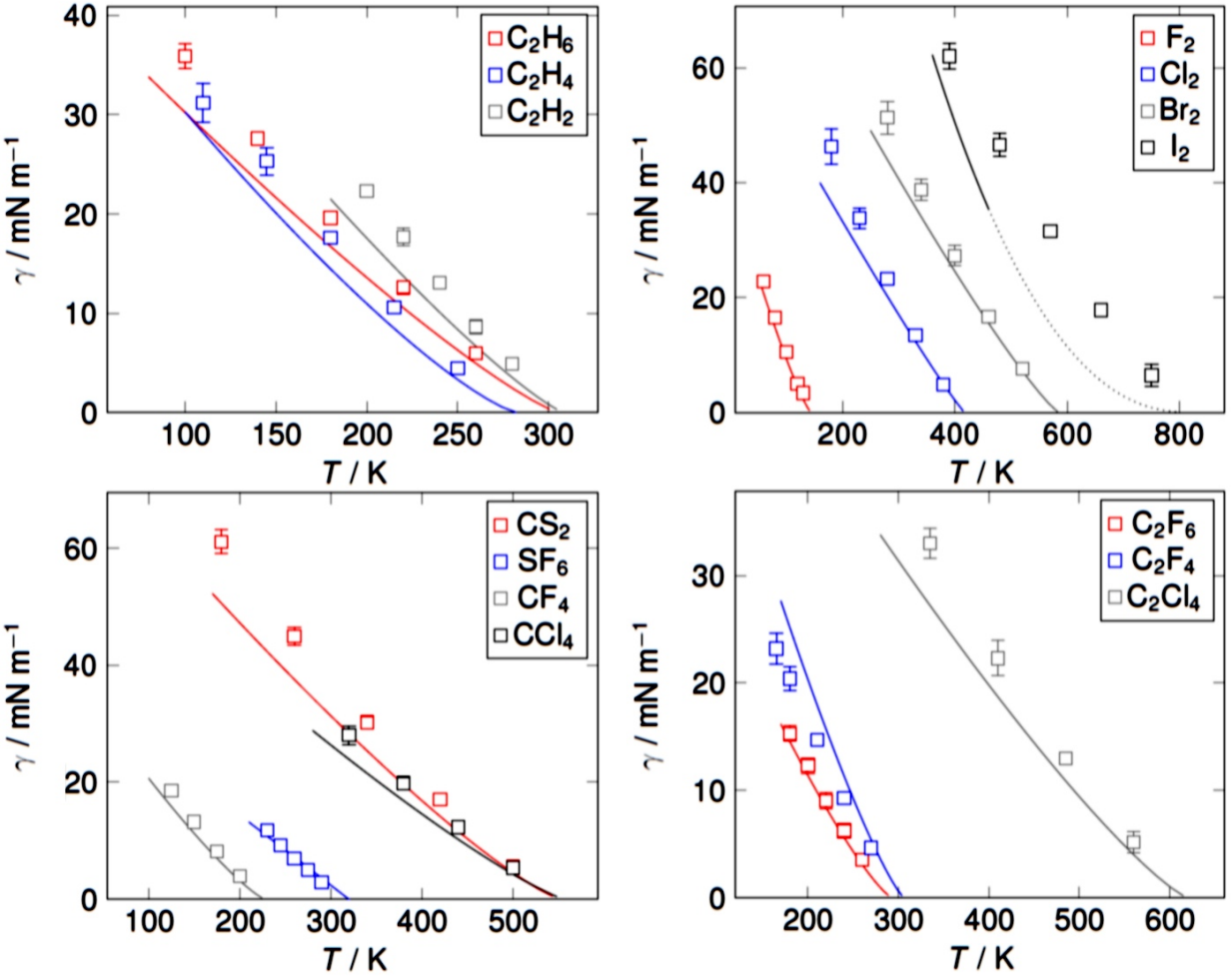
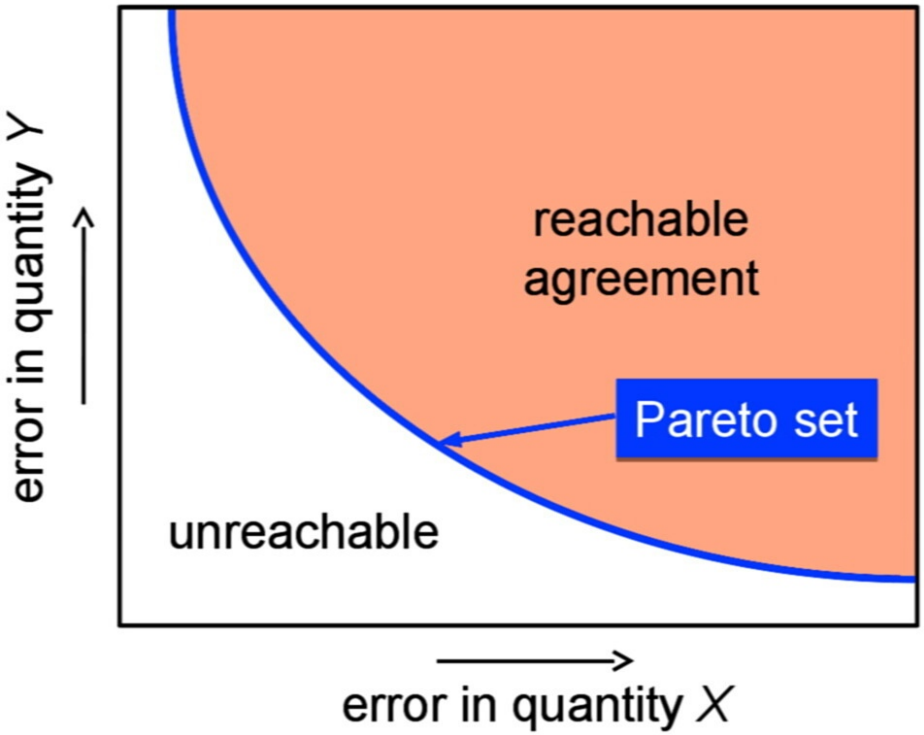
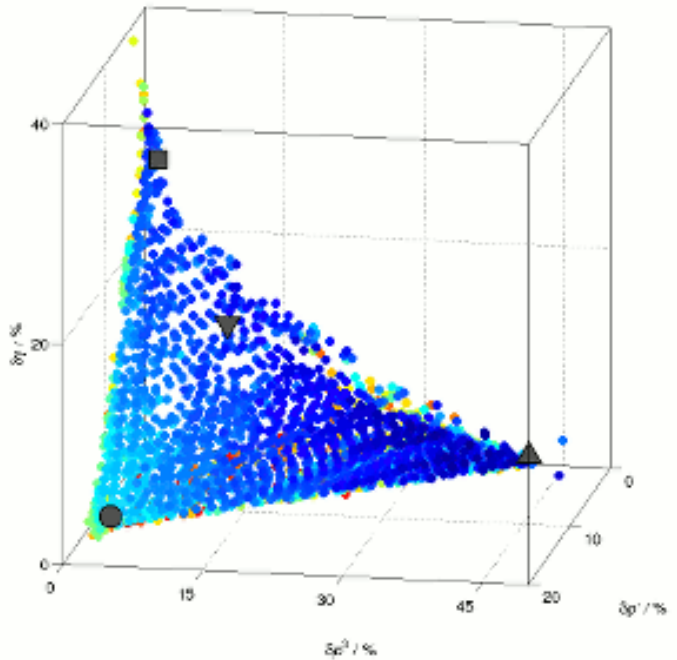


Molecular models: Multicriteria optimization

Pareto optimality criterion



Pareto set for carbon dioxide

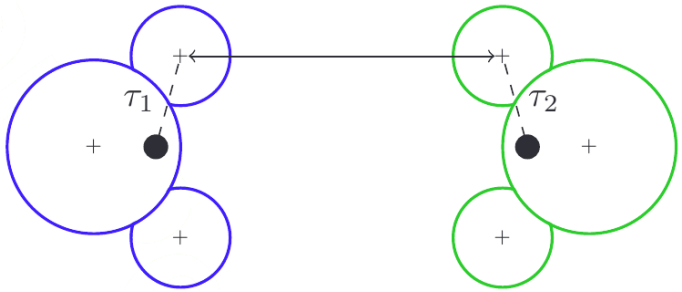


Multicriteria optimization requires massively-parallel molecular modelling.

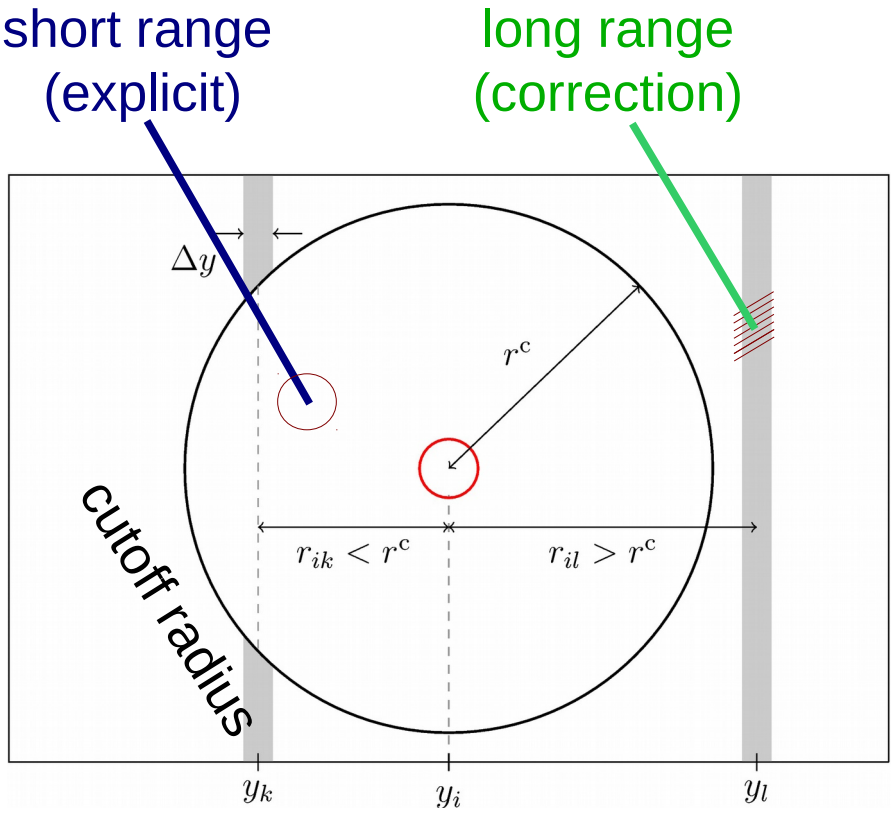
Separation of length scales for simulation

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**.

Separation of length scales for simulation

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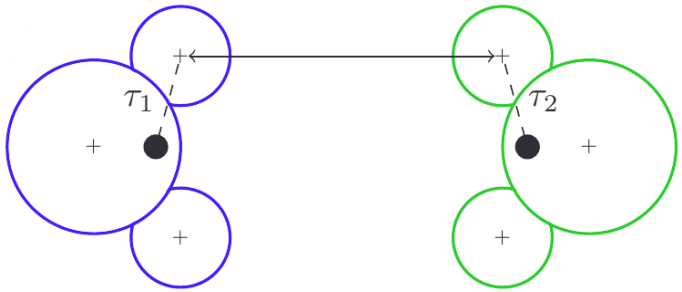

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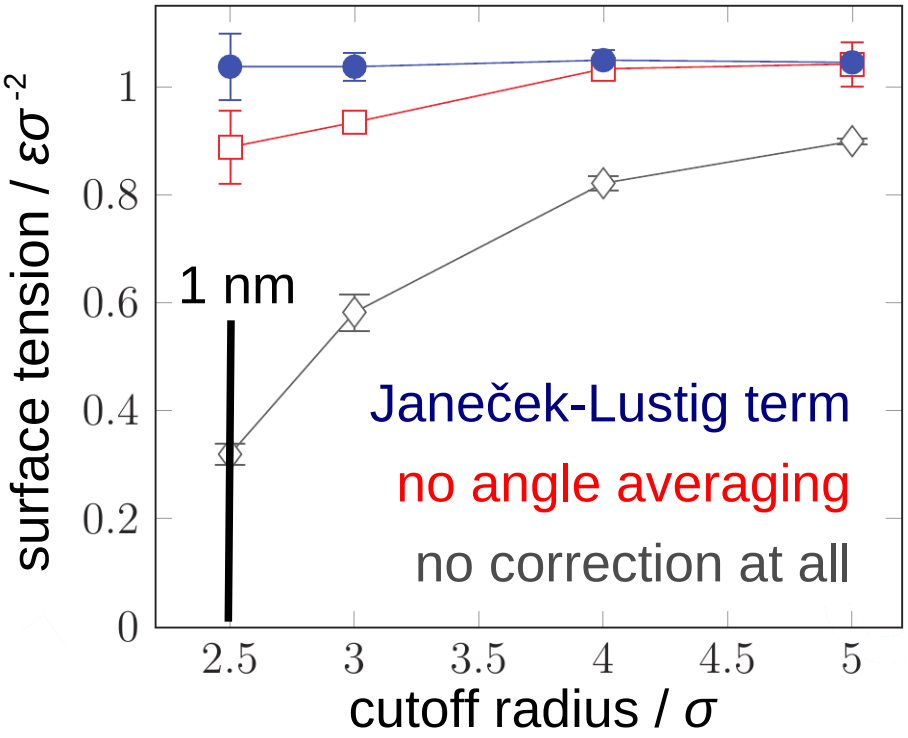
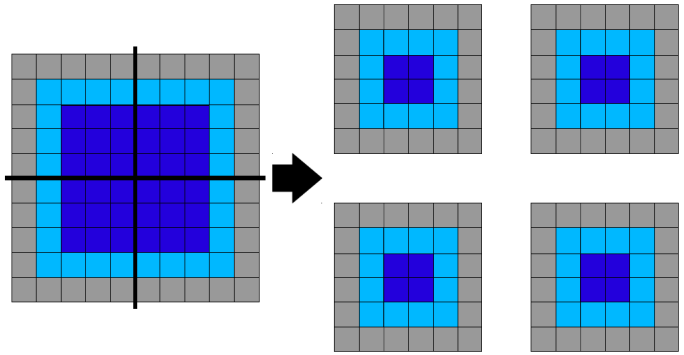
Two-centre LJ fluid (2CLJ)



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

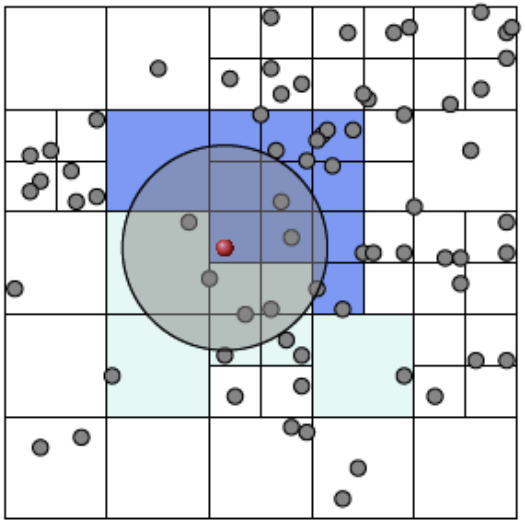
Scalable data structures for large systems

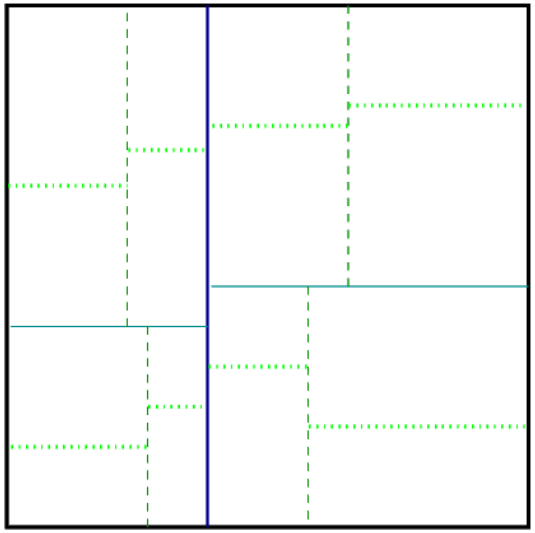
Linked-cell data structure suitable for spatial domain decomposition:



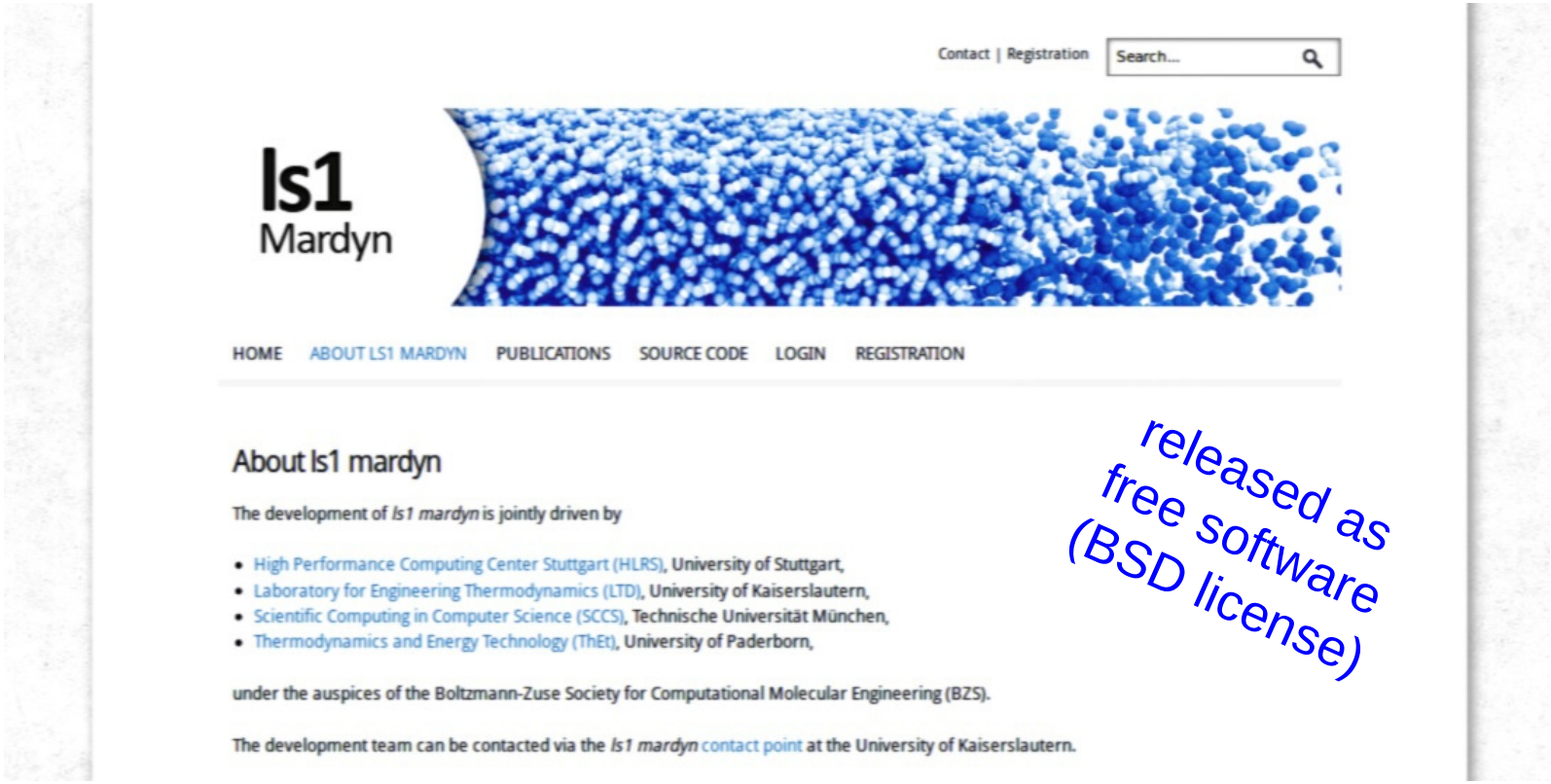
(non-blocking, overlapping MPI send/receive operations)

Methods for heterogeneous or fluctuating particle distributions:





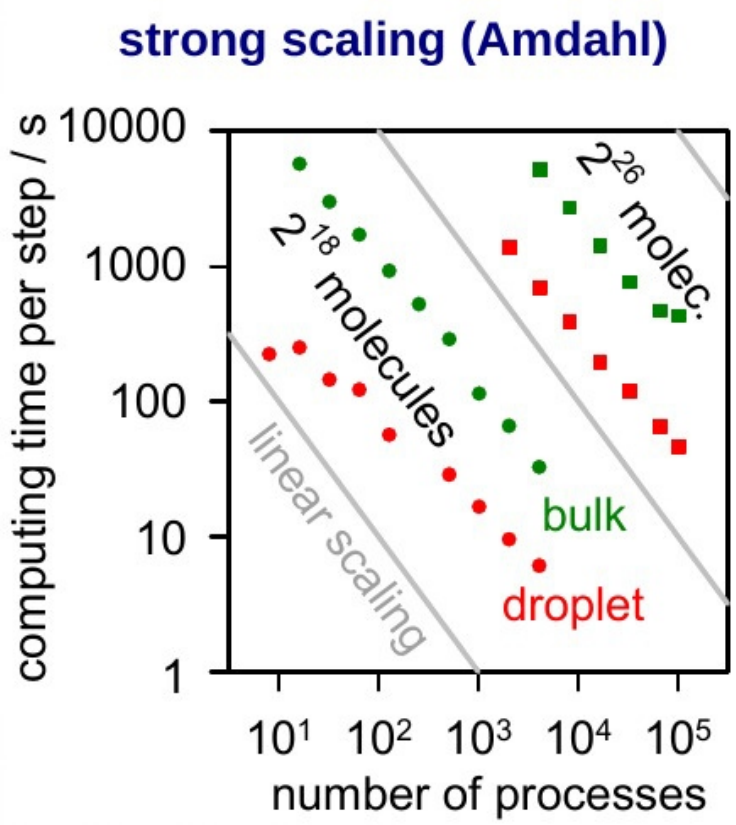
Large systems in molecular dynamics

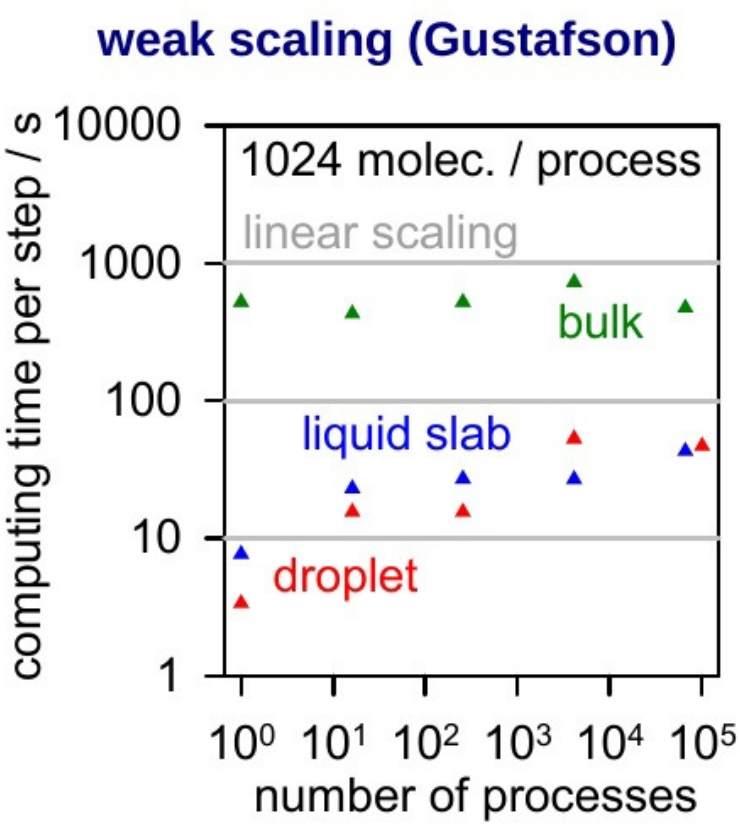


released as free software (BSD license)

Download *ls1 mardyn* on the www.ls1-mardyn.de website.

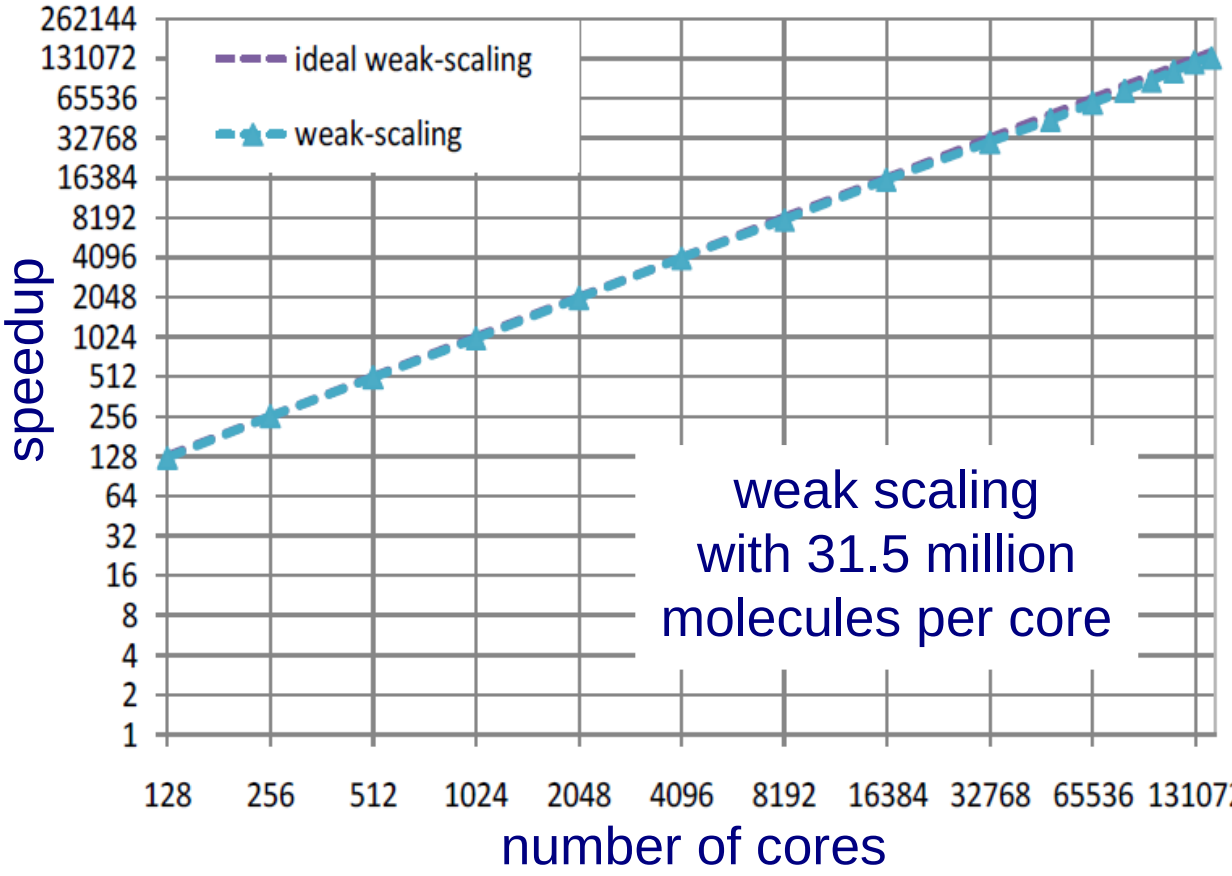
Scaling on *hermit* at HLRS, Stuttgart



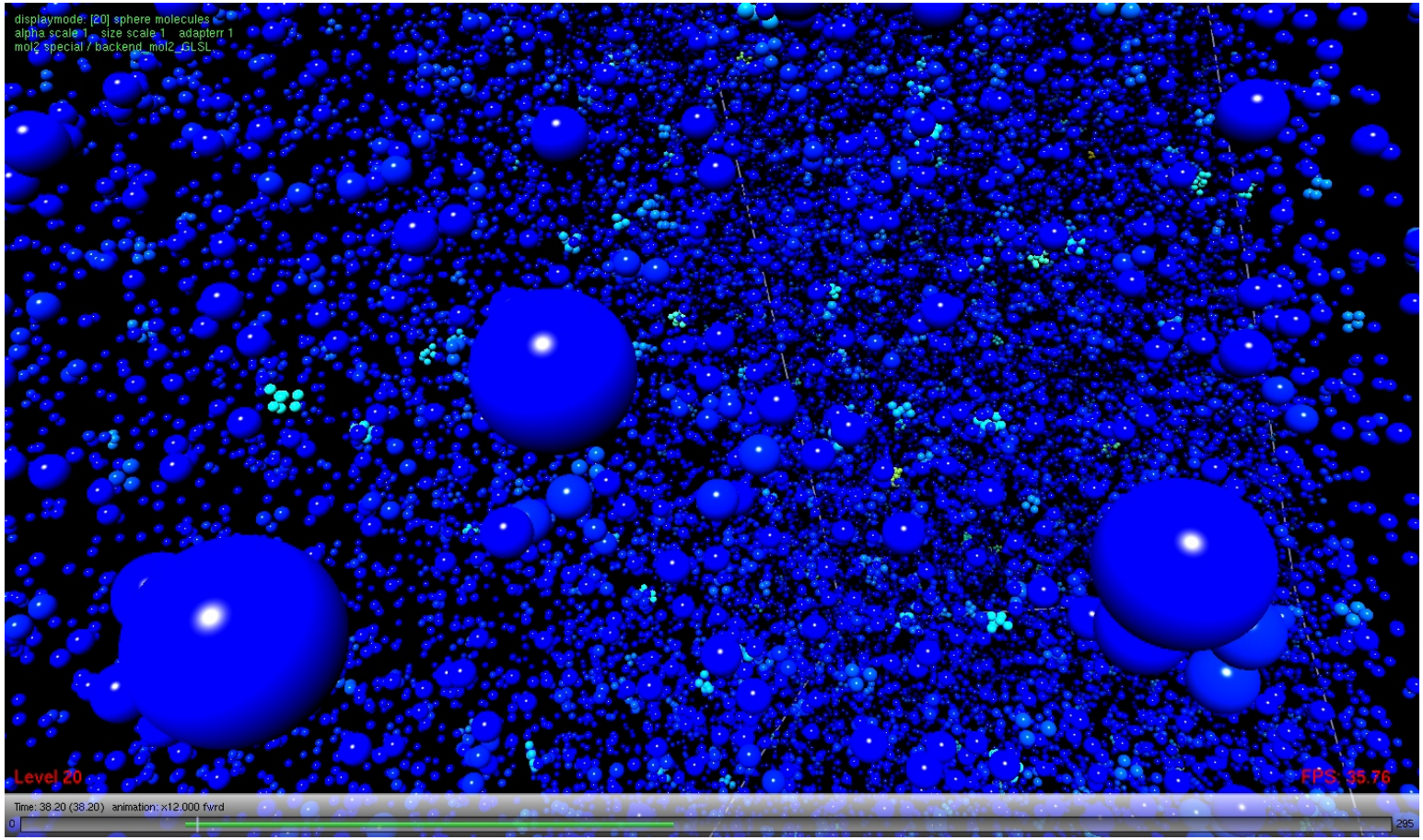


Scaling on *SuperMUC* at LRZ, Garching

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



Non-equilibrium molecular dynamics

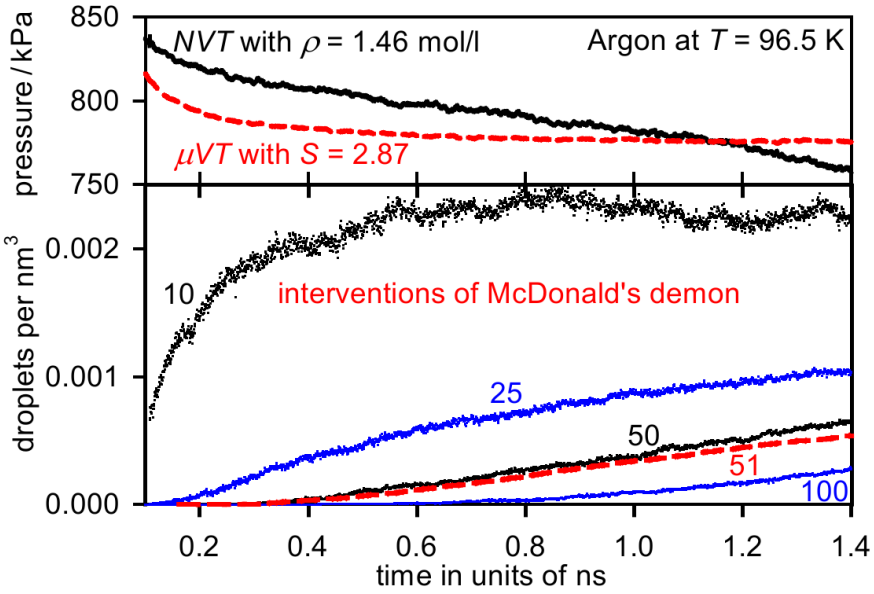


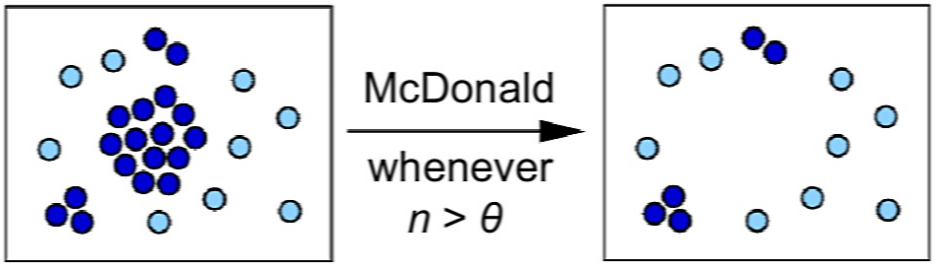
Non-equilibrium molecular dynamics

Non-equilibrium MD (NEMD): Process is simulated in a steady state.

Requires the intervention of a regulatory mechanism (dæmon)

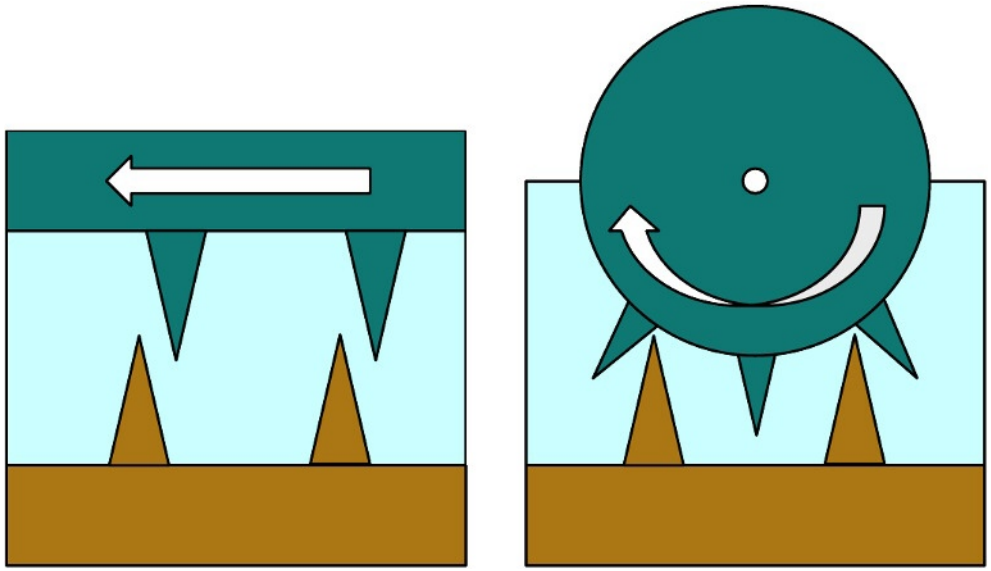
Example: Grand canonical MD simulation with McDonald's dæmon





Challenge: Realistic fluid-solid contact

- Adsorption and wetting
- Contact angle and line pinning
- Lubrication and heat transfer
- Modelling of cutting liquids
- Tribological effects



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UNIVERSITY OF CALIFORNIA

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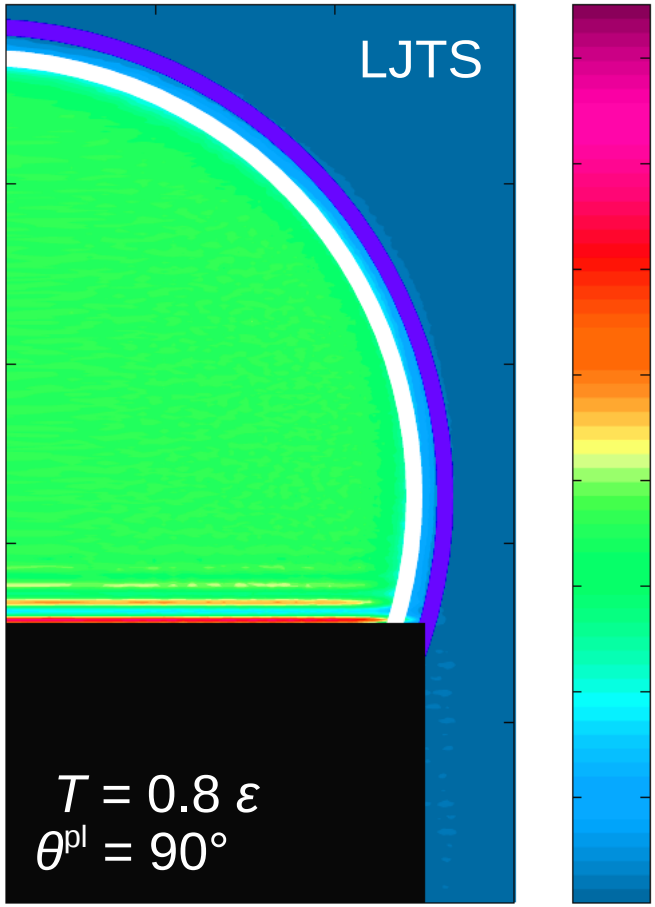
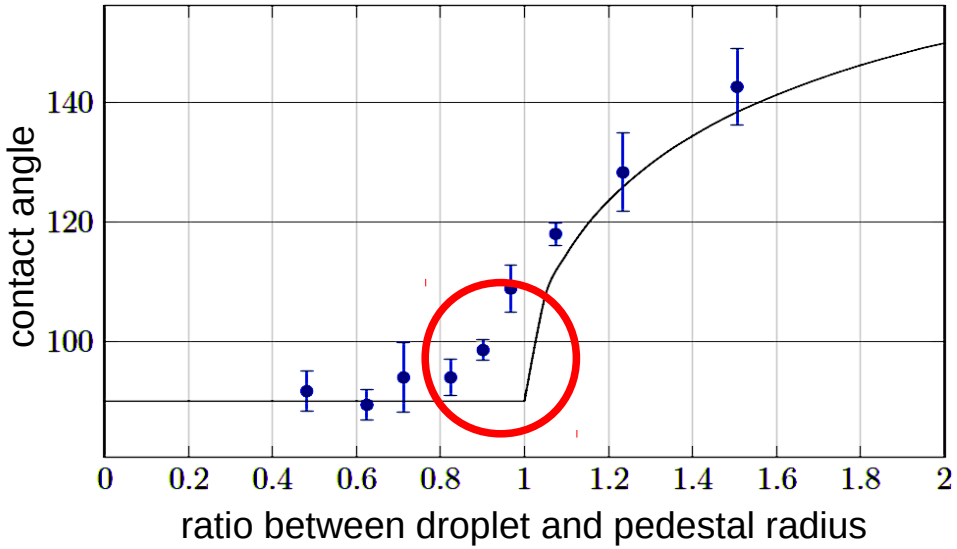
Challenge: Realistic fluid-solid contact

Wetting and contact line pinning





CRC 926 MICOS
Component Surfaces

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