



Computational molecular engineering by large-scale molecular dynamics simulation

Martin Thomas Horsch

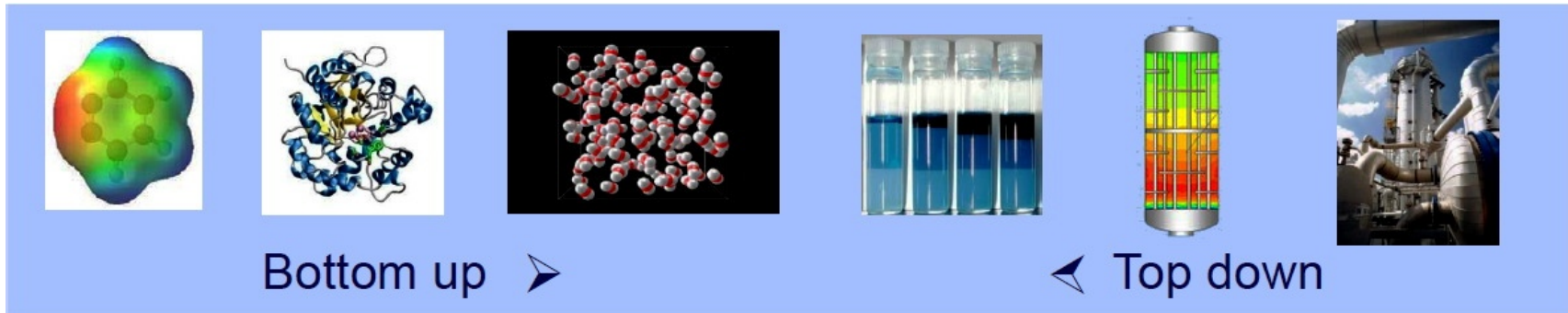
Laboratory of Engineering Thermodynamics,
University of Kaiserslautern, Germany

Agra, India, 22nd February 2015
Indo-German Frontiers of Engineering



**Computational
Molecular Engineering**

Computational Molecular Engineering

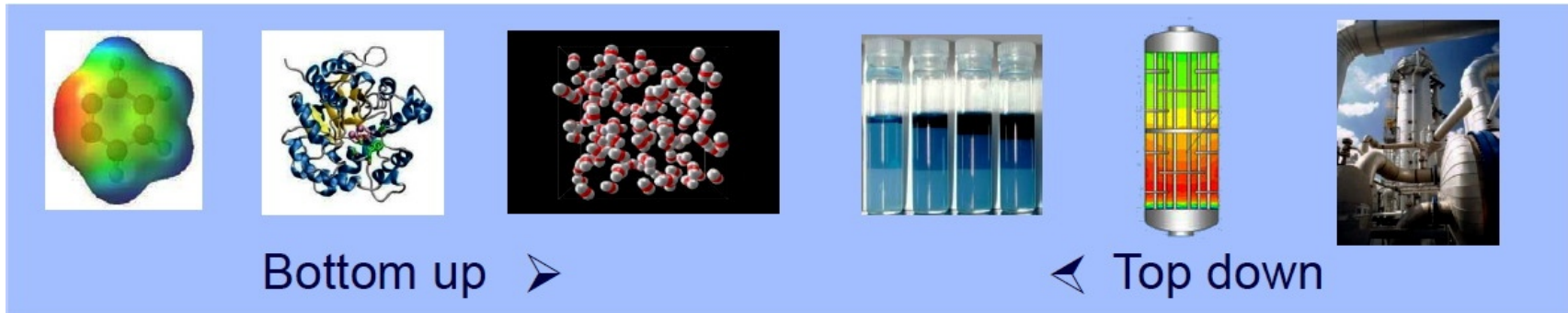


From Physics (qualitative accuracy)

- 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)

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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

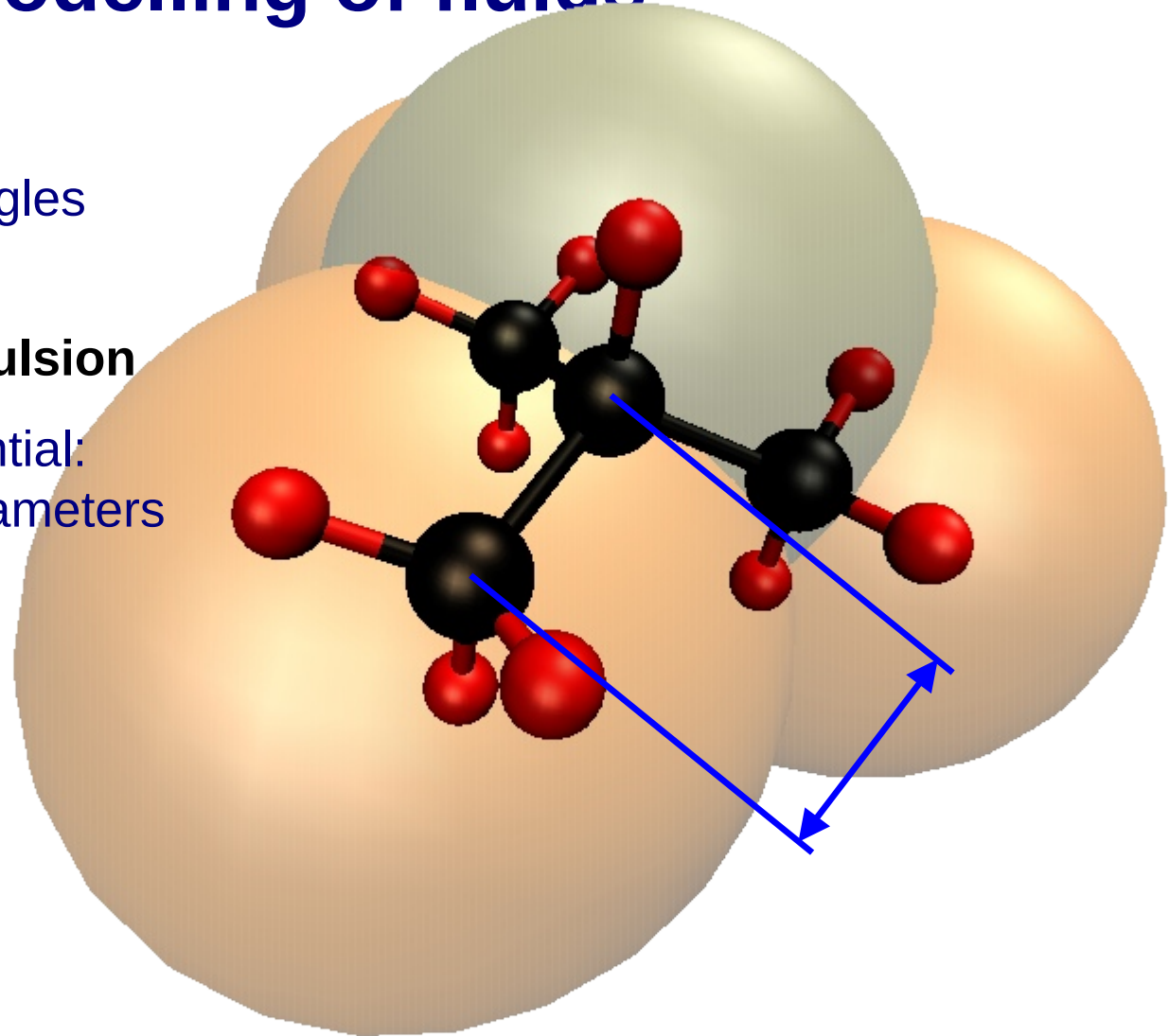
Molecular modelling of fluids

Geometry

Bond lengths and angles

Dispersion and repulsion

Lennard-Jones potential:
Size and energy parameters



Molecular modelling of fluids

Geometry

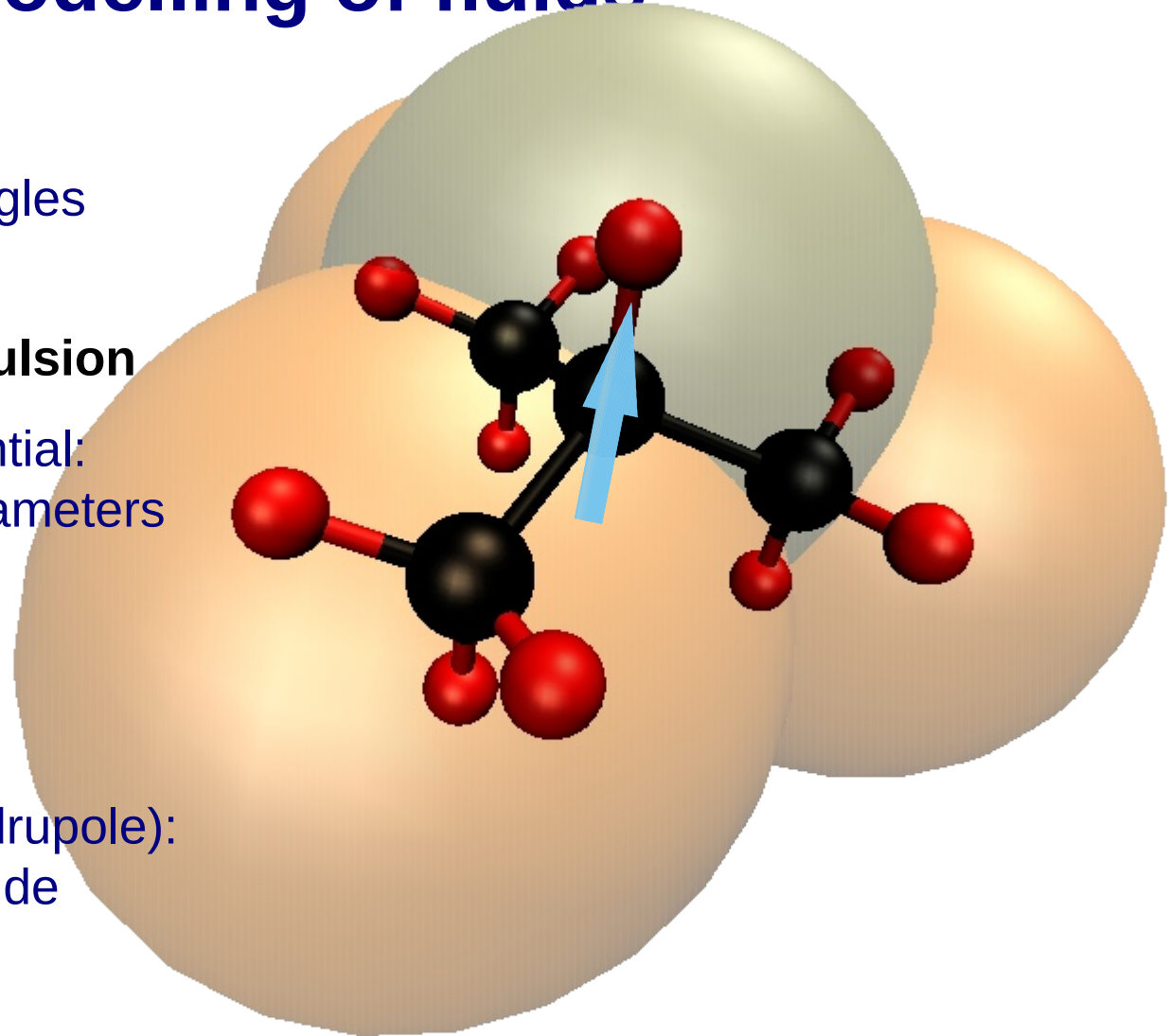
Bond lengths and angles

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Electrostatics

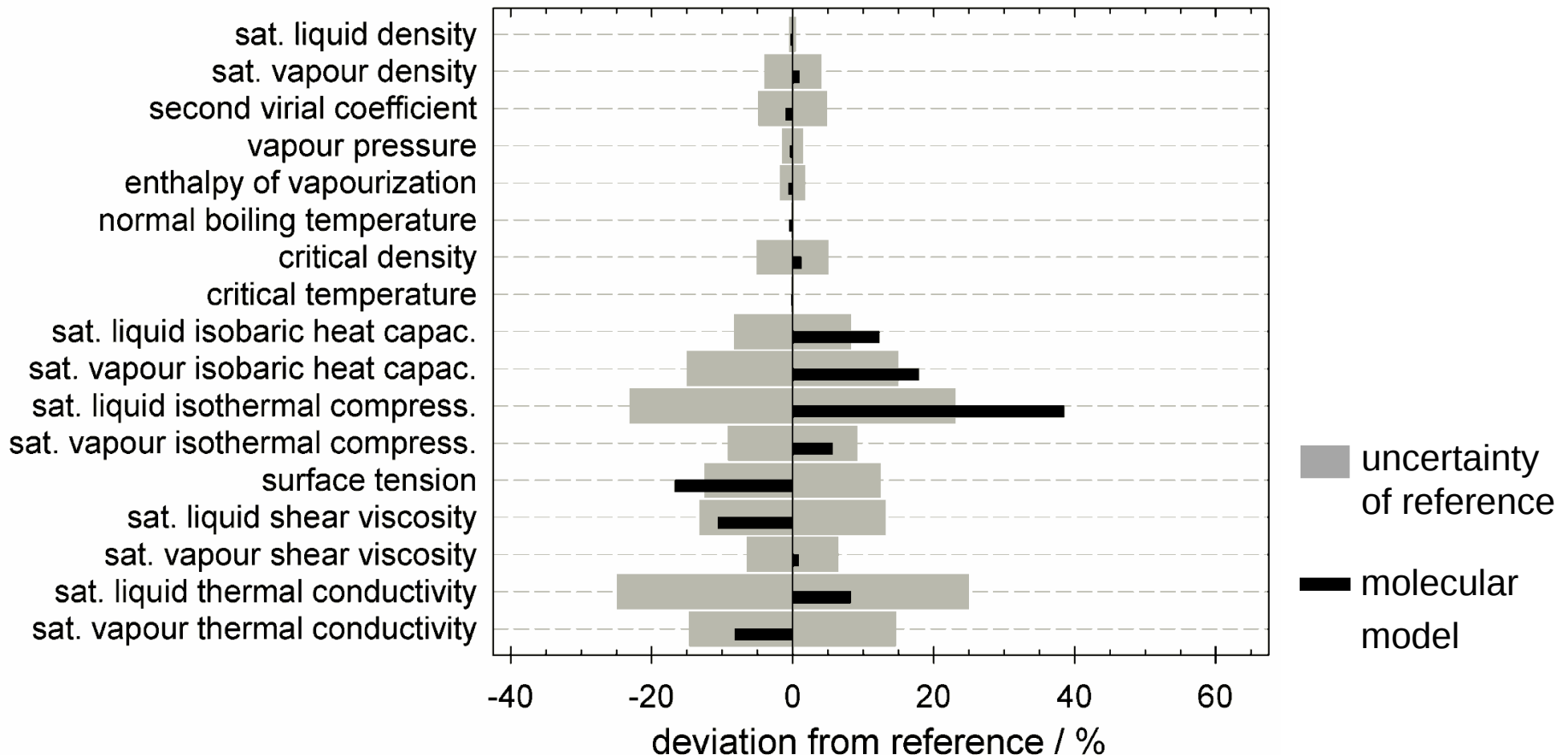
Point polarities
(charge, dipole, quadrupole):
Position and magnitude



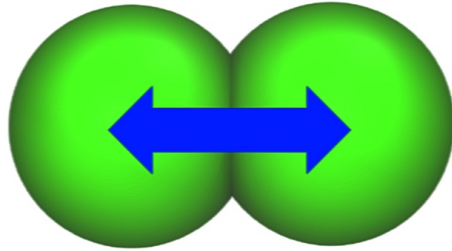


Quantitatively reliable molecular models

ethylene oxide model by Eckl *et al.* (2008)



Molecular models: Parameterization



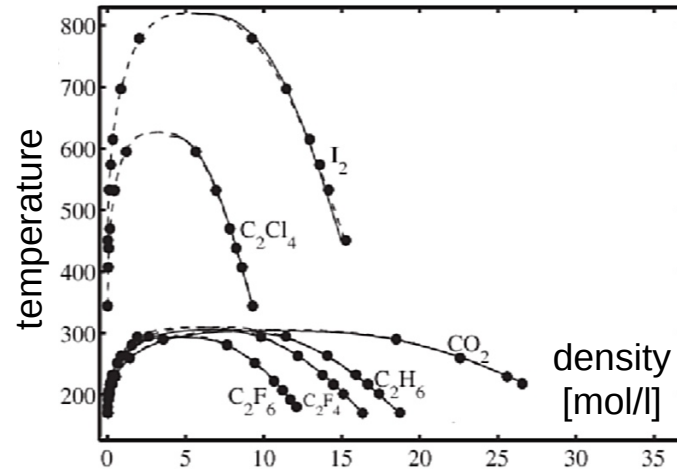
2CLJQ models:

- 2 LJ centres
- Quadrupole

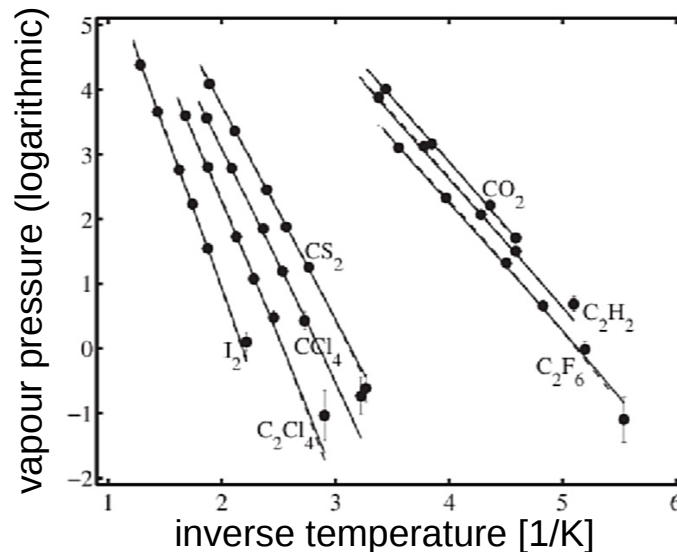
Fit of parameters σ , ϵ , L , Q to VLE data of 29 fluids by Stoll *et al.*

Deviation:

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



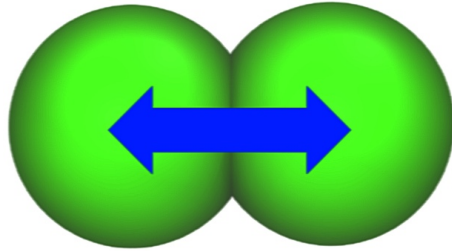
- simulation
- DIPPR correlation



No interfacial properties were considered for the parameterization.



Molecular models: Prediction and validation



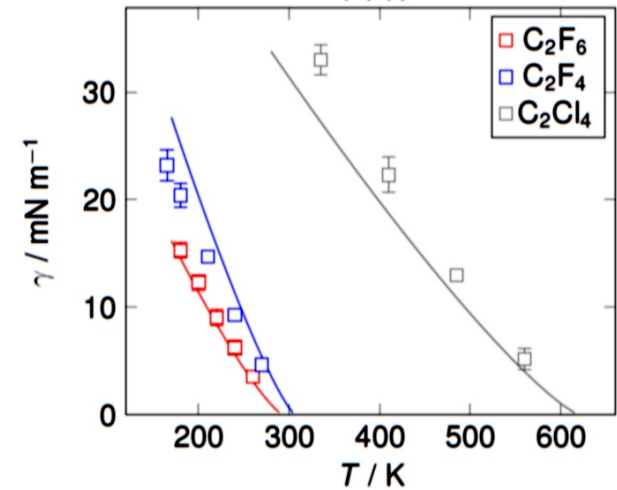
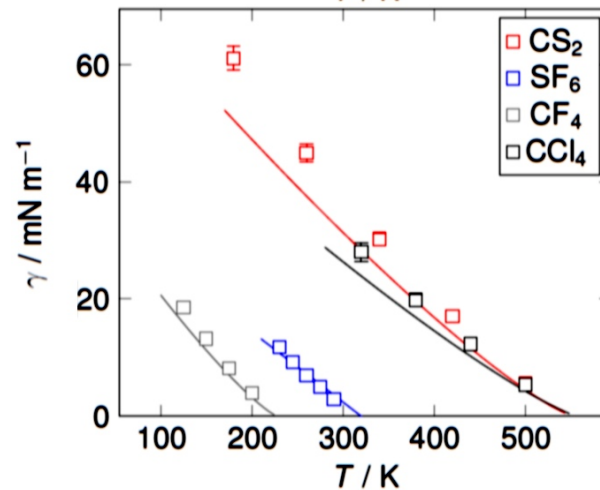
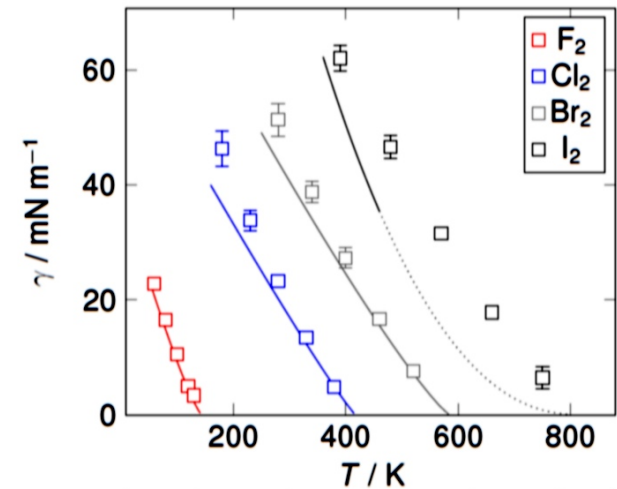
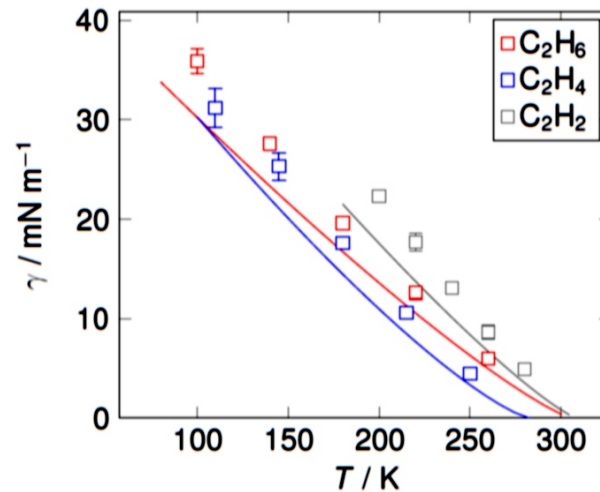
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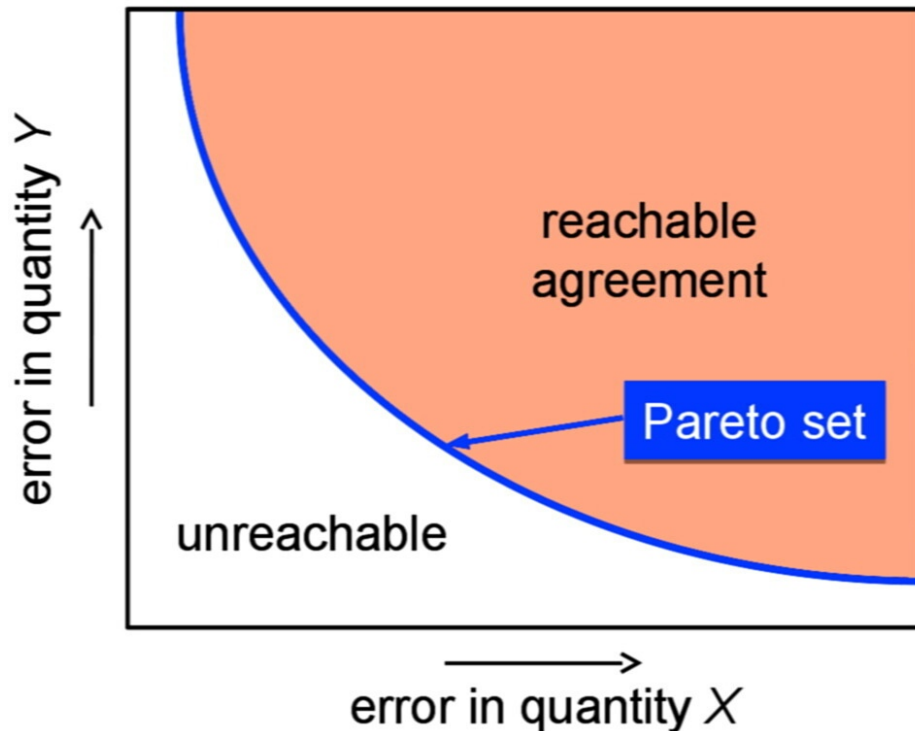
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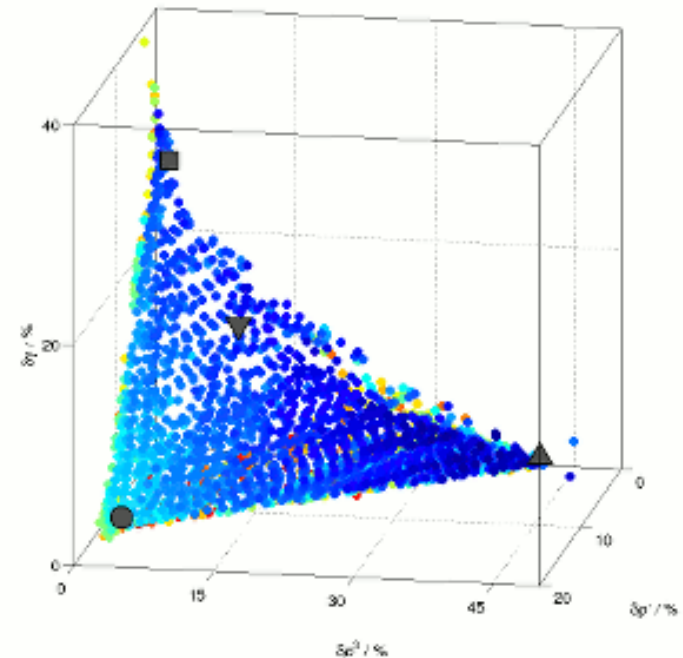


Molecular models: Multicriteria optimization

Pareto optimality criterion



Pareto set for carbon dioxide

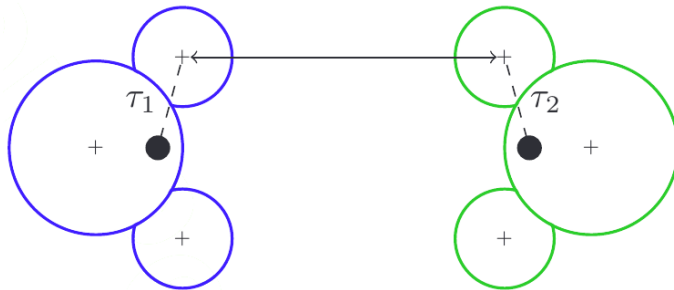


Multicriteria optimization requires massively-parallel molecular modelling.

Separation of length scales for simulation

For planar interfaces:

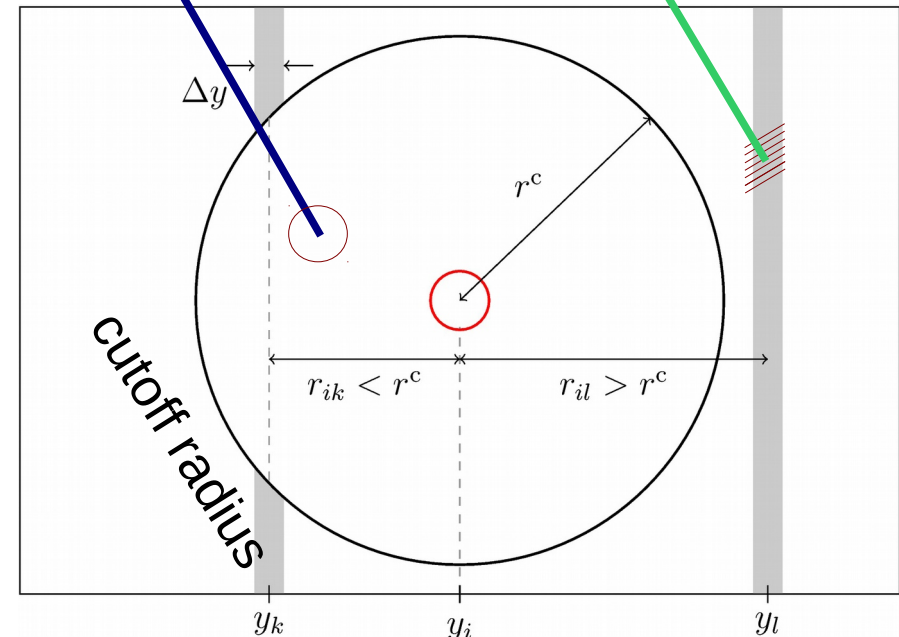
Long-range correction from the density profile, following **Janeček**.



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

short range
(explicit)

long range
(correction)



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

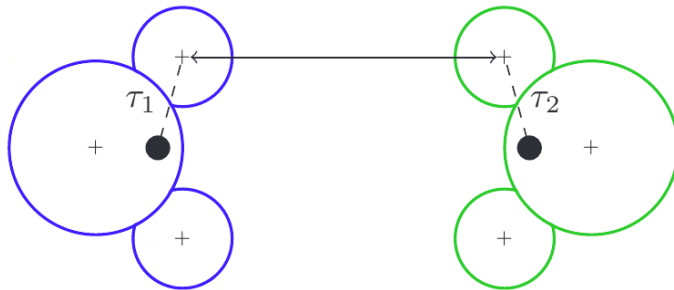
... instead, **short-range interactions** are evaluated for **neighbours**.



Separation of length scales for simulation

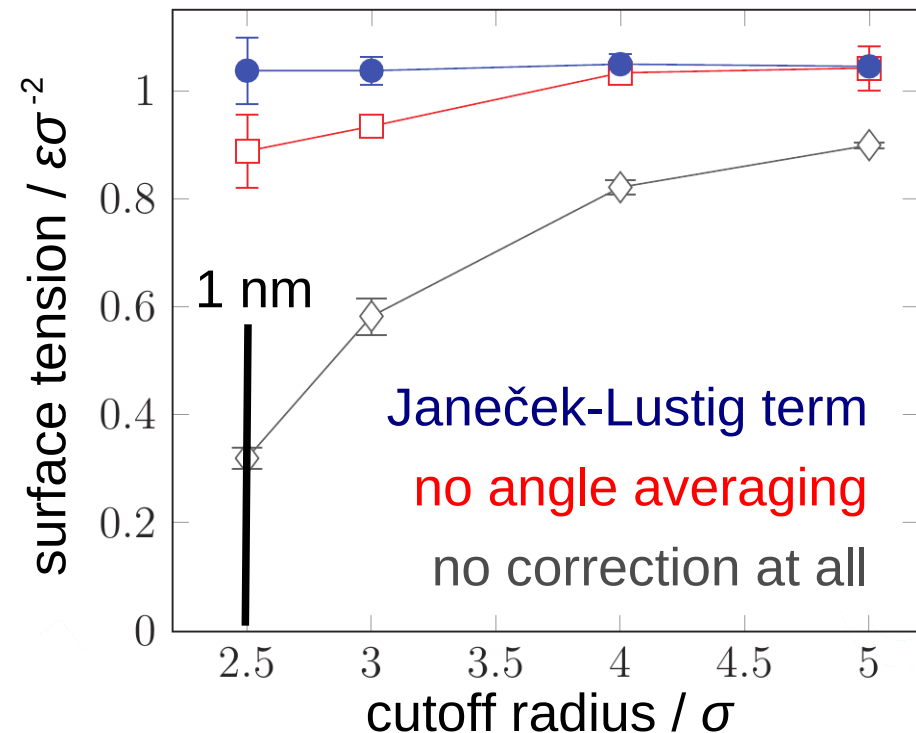
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Two-centre LJ fluid (2CLJ)

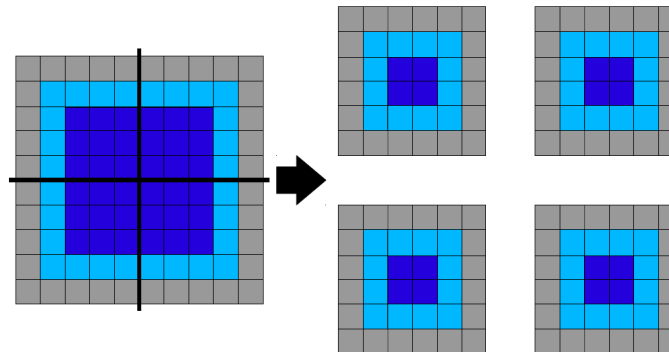


For arbitrary geometries, e.g. the fast multipole method can be employed.



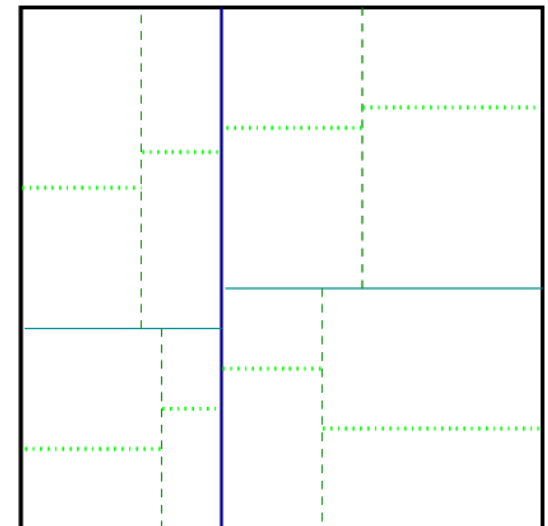
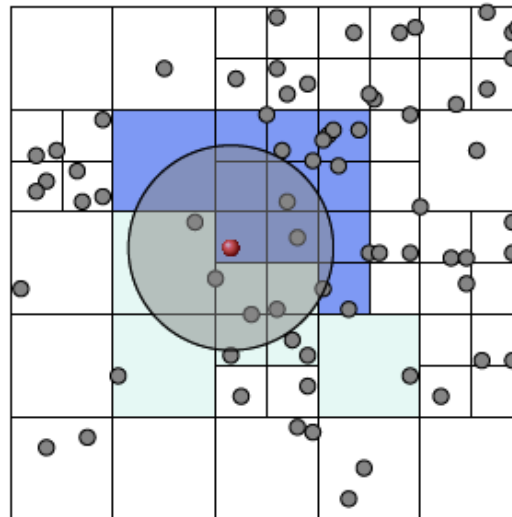
Scalable data structures for large systems

Linked-cell data structure suitable for spatial domain decomposition:

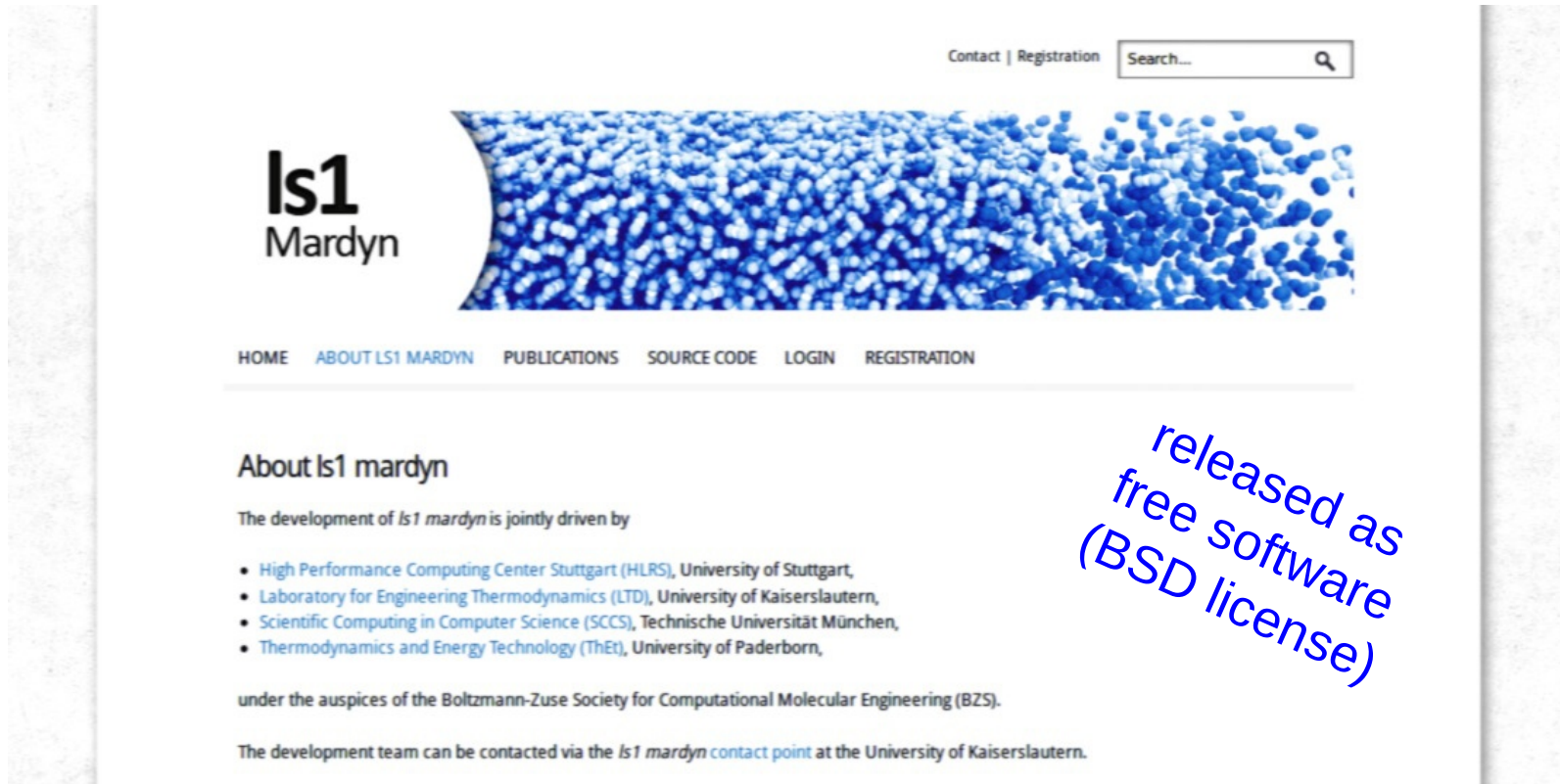


(non-blocking, overlapping MPI send/receive operations)

Methods for heterogeneous or fluctuating particle distributions:



Large systems in molecular dynamics



The screenshot shows the homepage of the Is1 Mardyn website. At the top right, there are links for 'Contact' and 'Registration', and a search bar. The main header features the 'Is1 Mardyn' logo on the left and a large image of blue particles on the right. Below the header is a navigation menu with links for 'HOME', 'ABOUT LS1 MARDYN', 'PUBLICATIONS', 'SOURCE CODE', 'LOGIN', and 'REGISTRATION'. The main content area is titled 'About Is1 mardyn' and contains the following text:

The development of *Is1 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).

The development team can be contacted via the *Is1 mardyn* [contact point](#) at the University of Kaiserslautern.

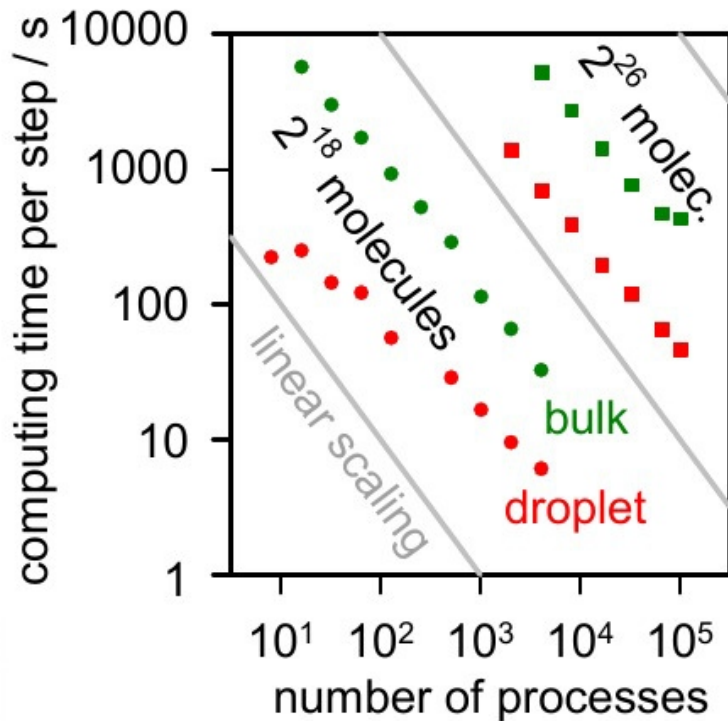
A blue diagonal stamp is overlaid on the right side of the screenshot, reading: 'released as free software (BSD license)'.

Download *Is1 mardyn* on the www.ls1-mardyn.de website.

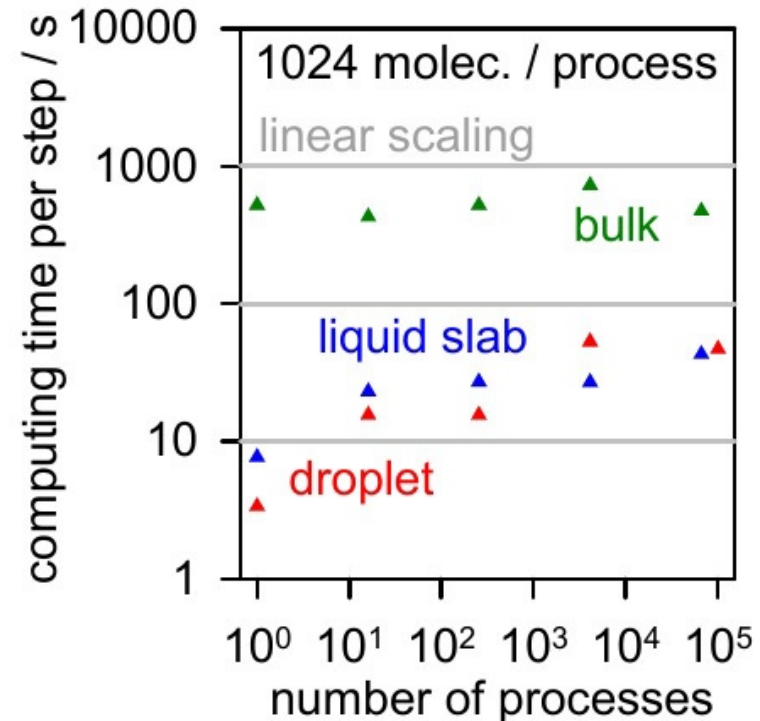


Scaling on *hermit* at HLRS, Stuttgart

strong scaling (Amdahl)



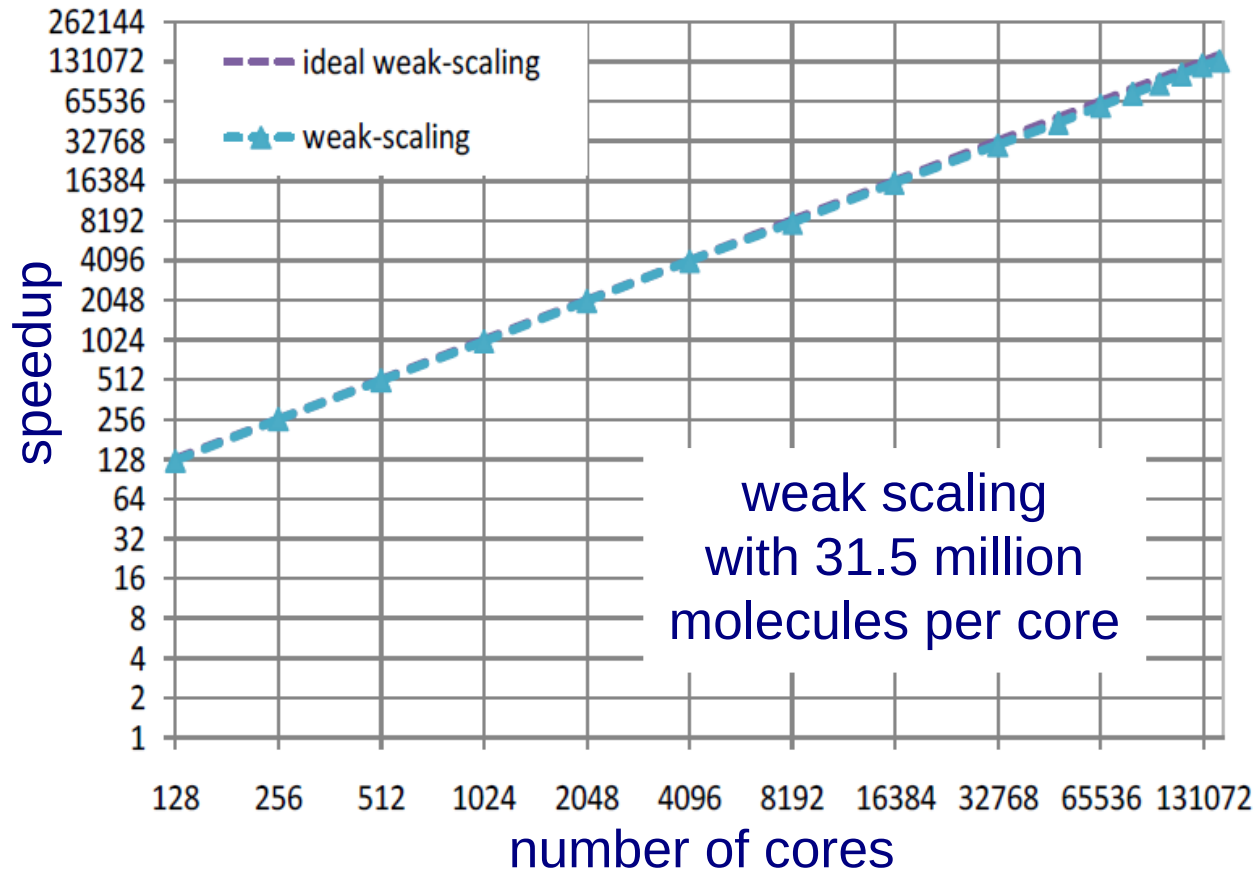
weak scaling (Gustafson)



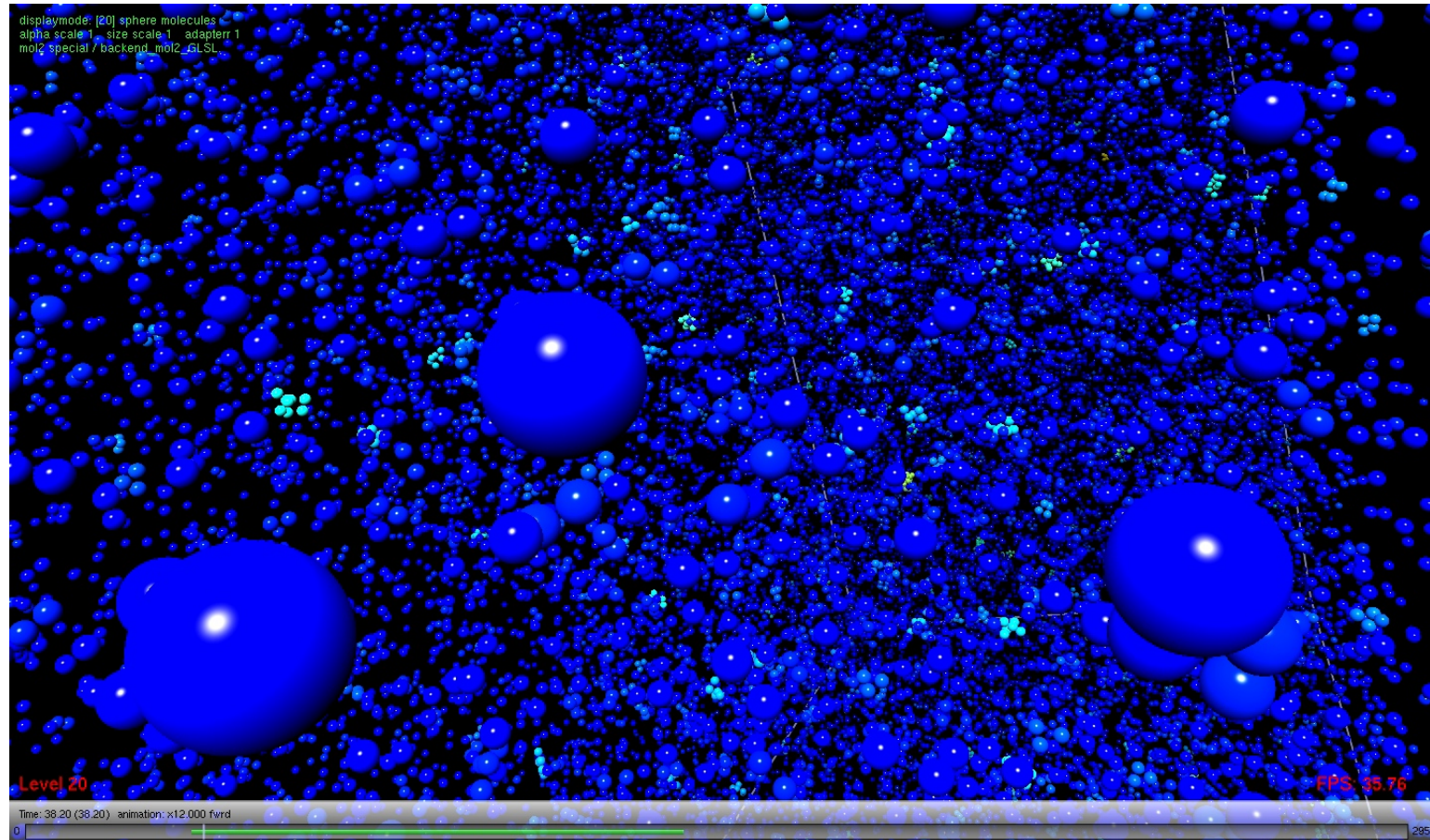


Scaling on *SuperMUC* at LRZ, Garching

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



Non-equilibrium molecular dynamics

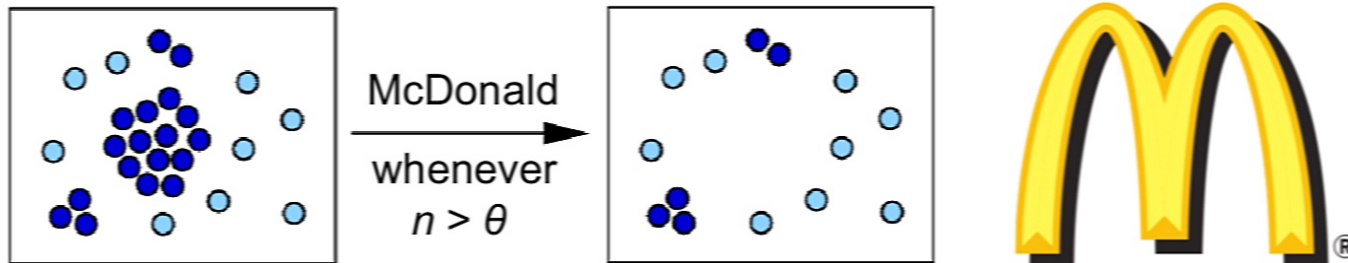
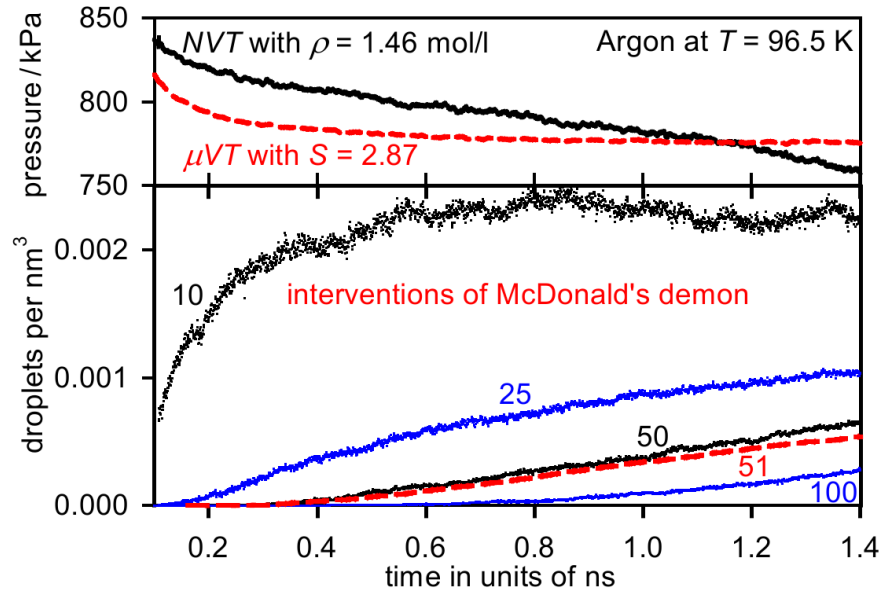


Non-equilibrium molecular dynamics

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

Requires the intervention of a regulatory mechanism (dæmon)

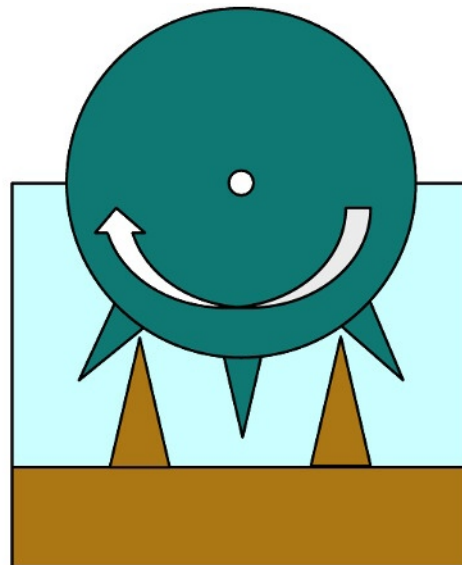
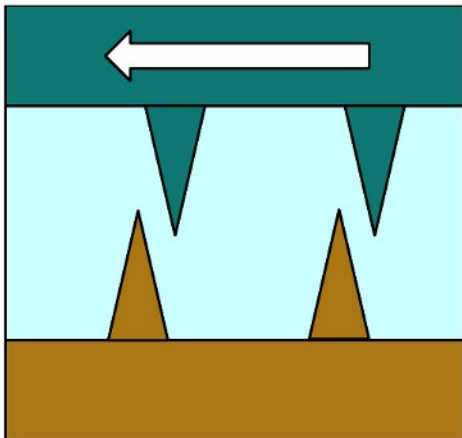
Example: Grand canonical MD simulation with McDonald's dæmon





Challenge: Realistic fluid-solid contact

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



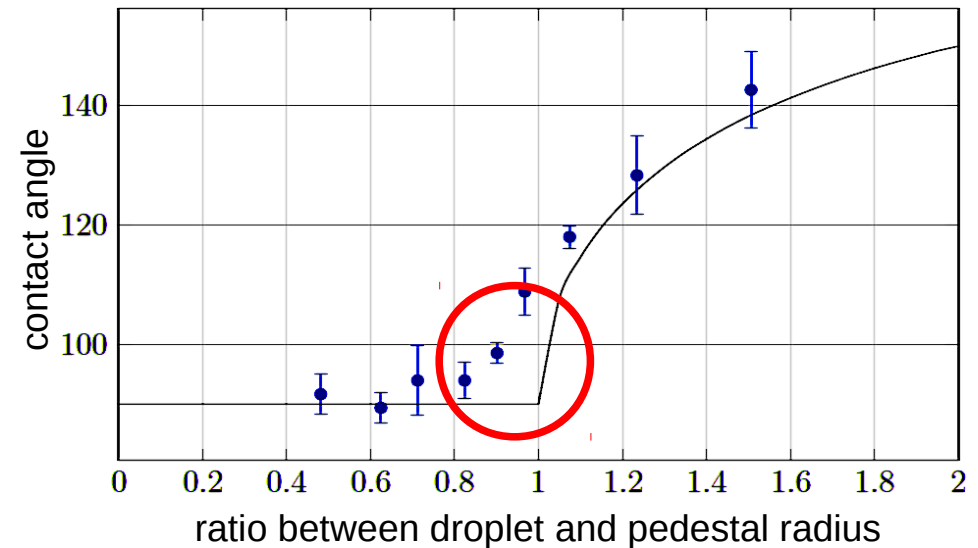
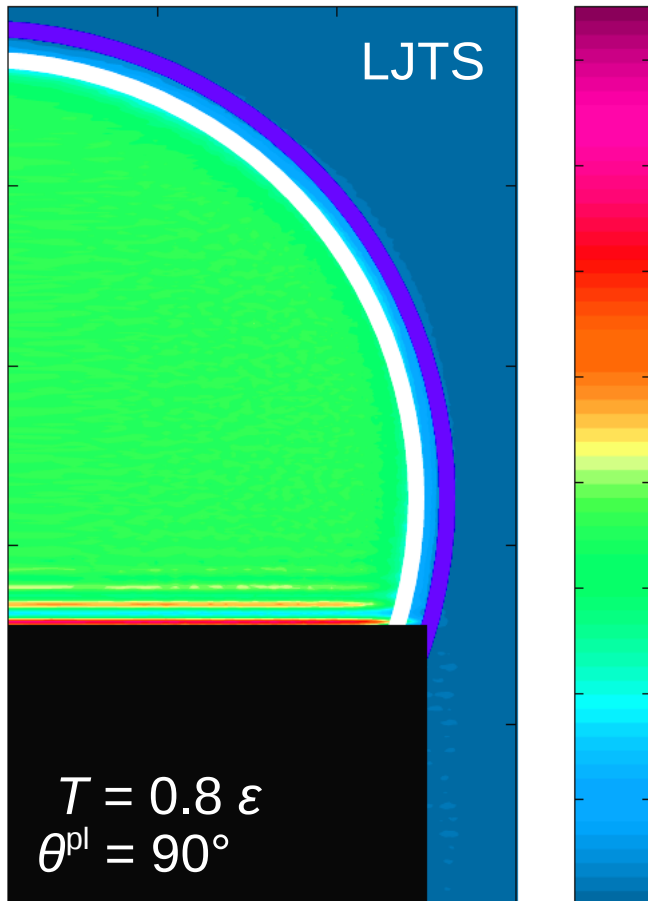
Berkeley
UNIVERSITY OF CALIFORNIA

UC DAVIS
UNIVERSITY OF CALIFORNIA



Challenge: Realistic fluid-solid contact

Wetting and contact line pinning





Computational Molecular Engineering

