Scalable, performant, and resilient large-scale applications of molecular process engineering

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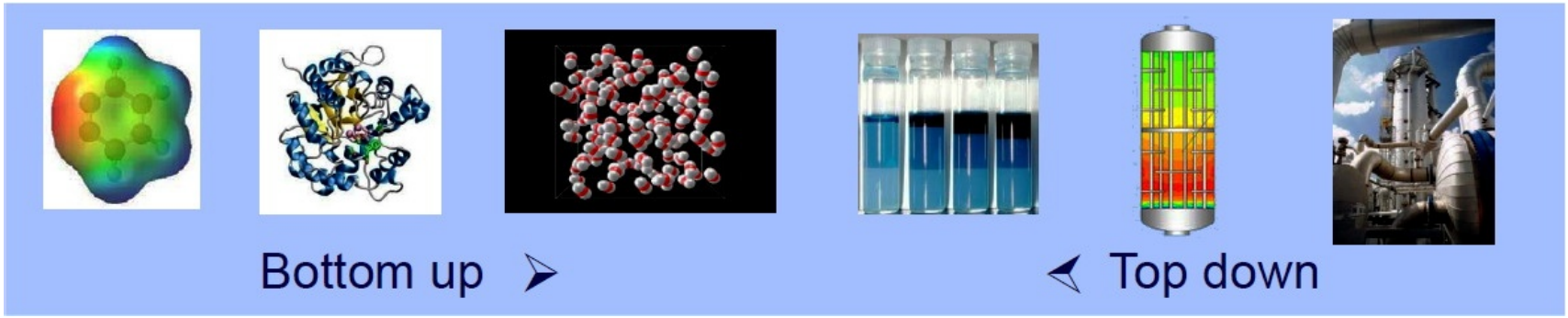
Leibniz Supercomputing Centre, Garching
SuperMUC Status Workshop, 27th April 2016

Molecular Process Engineering



From Physics (qualitative accuracy)

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

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

Pair potentials for low-molecular fluids

Geometry

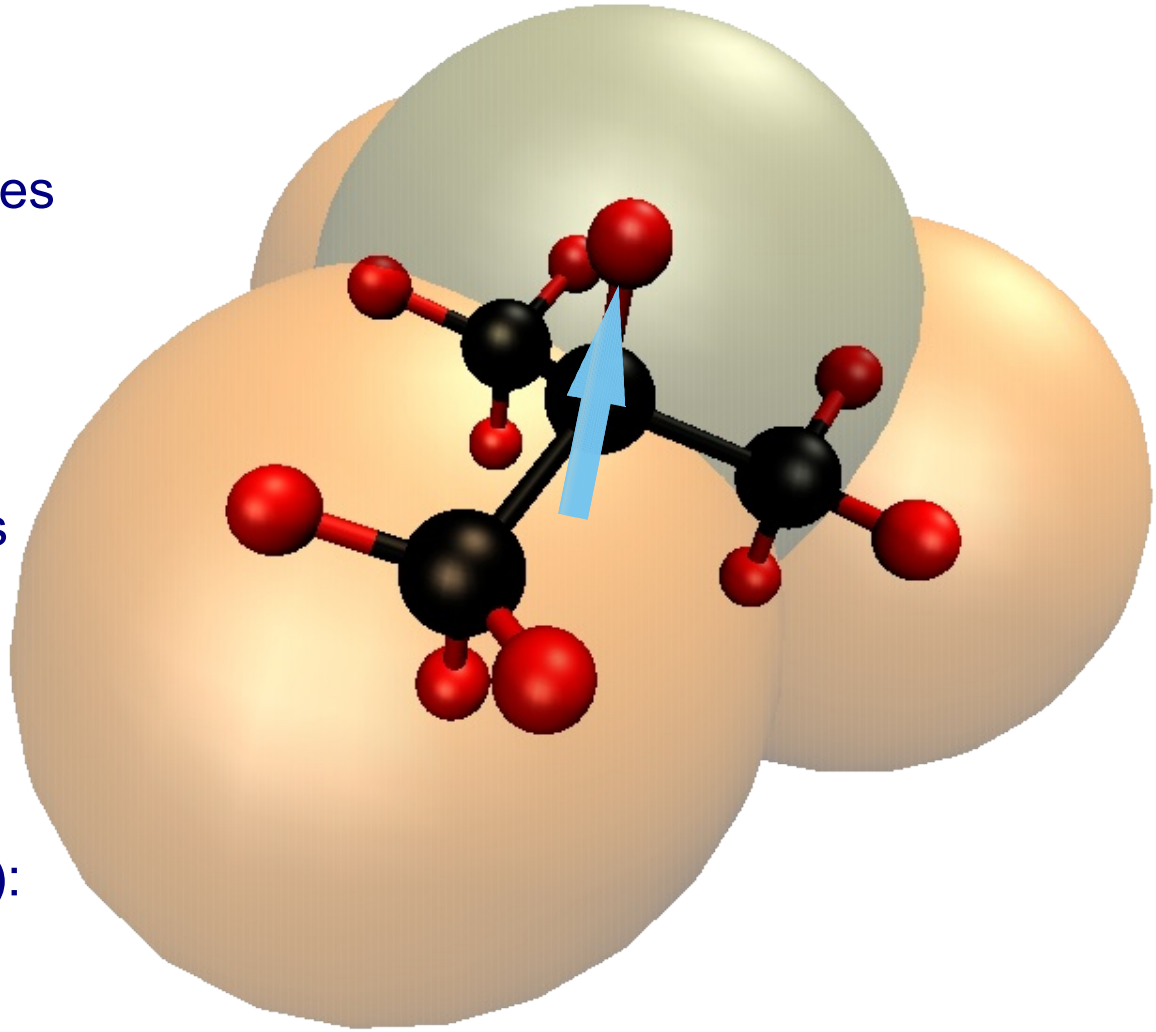
Rigid bond lengths and angles

Dispersion and repulsion

Lennard-Jones potential:
Size and energy parameters

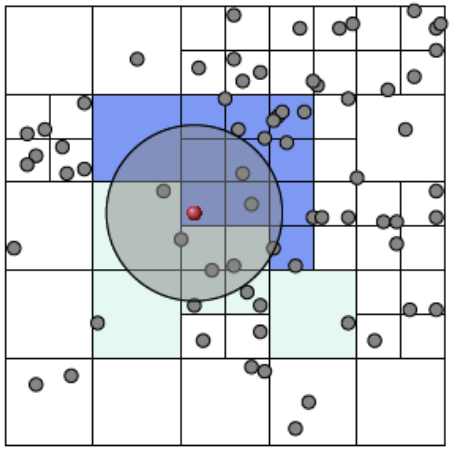
Electrostatics

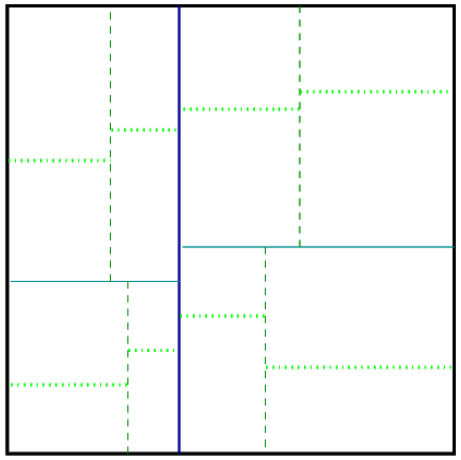
Point polarities
(charge, dipole, quadrupole):
Position and magnitude



Scalable MD simulation: SkaSim

Methods for heterogeneous or fluctuating particle distributions





Bundesministerium für Bildung und Forschung

BASF
The Chemical Company

SkaSim

Lehrstuhl für Thermodynamik
Prof. Dr.-Ing. H. Hasse

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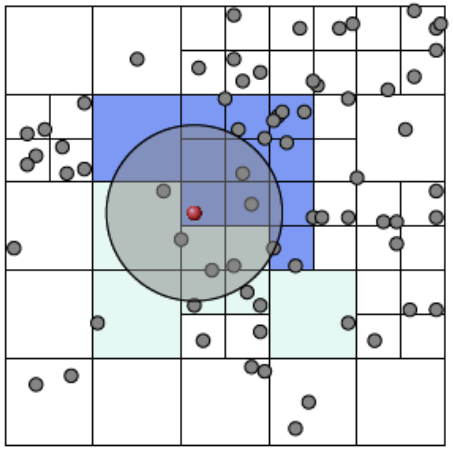
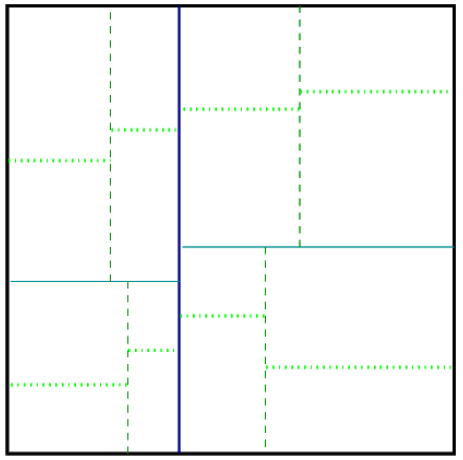
HLRS

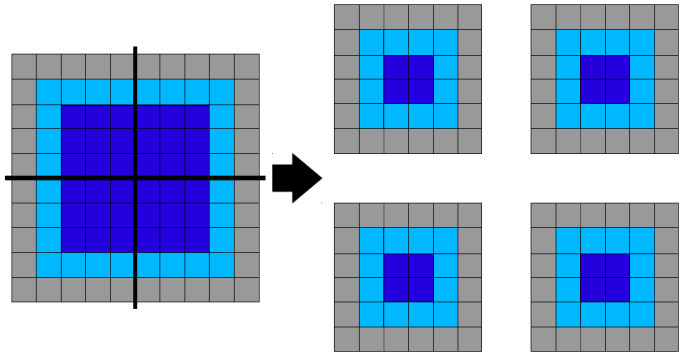
Scalable MD simulation with ls1 mardyn

Methods for heterogeneous or fluctuating particle distributions





Linked-cell data structure suitable for spatial domain decomposition



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

large systems “1”: molecular dynamics

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

Traversal of the linked cells

Cells enter and leave a «sliding window» as they are touched for the first or the last time during each time step:

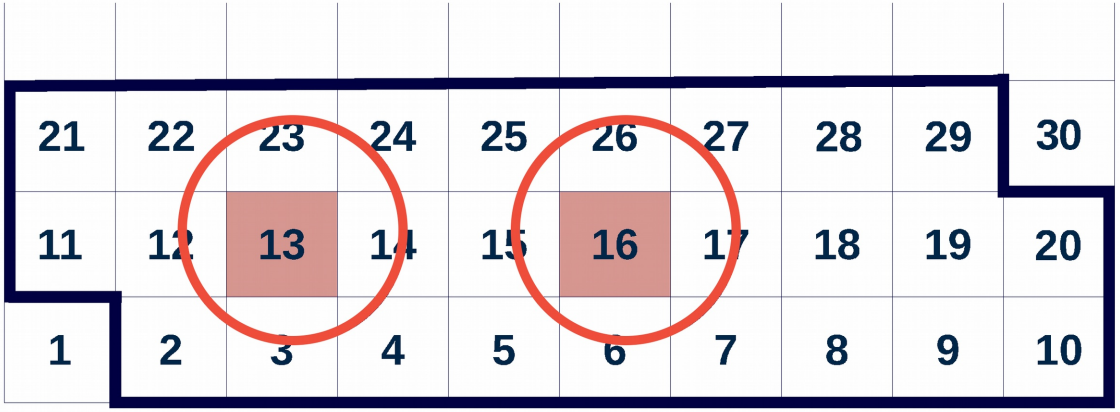
sliding window

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/

Traversal of the linked cells

Hyperthreading and vectorization:



hyperthreaded sliding window

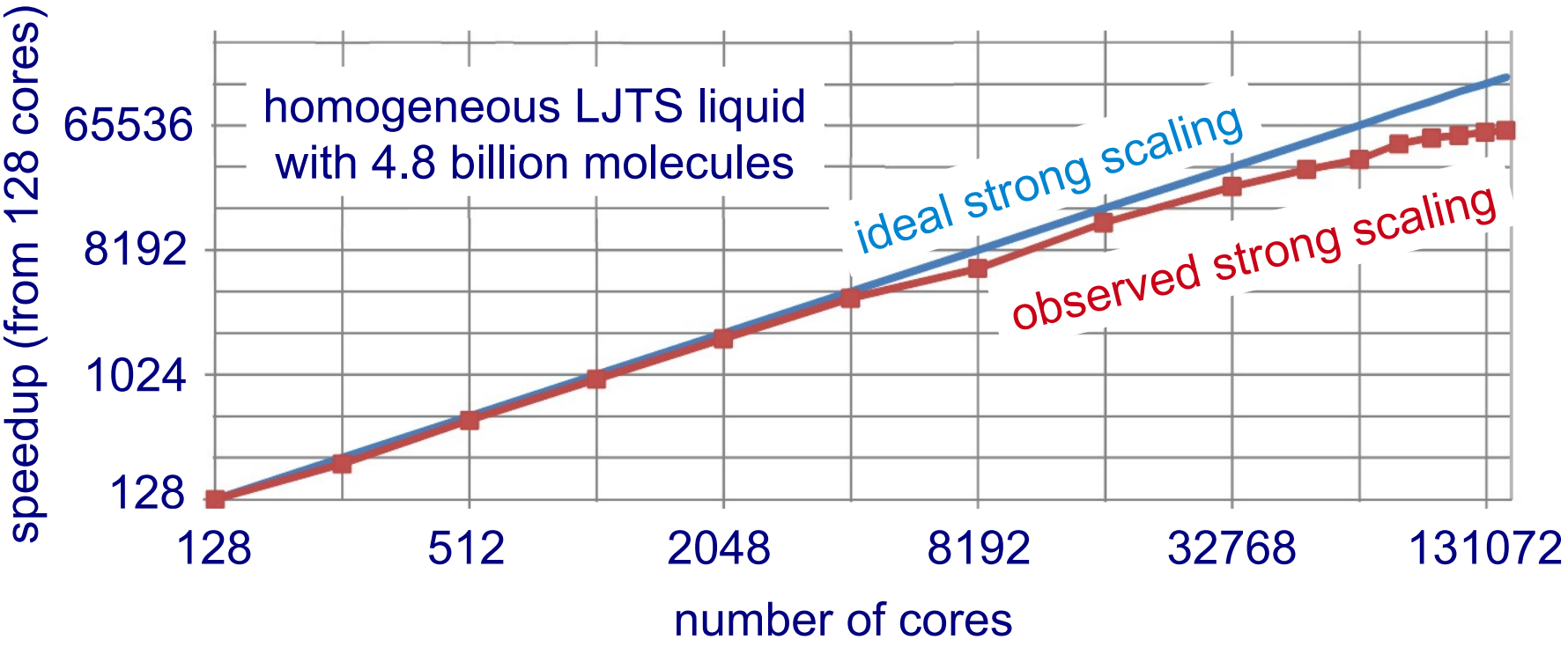
Optionally, forces acting on molecules are only stored until their cell leaves the sliding window.

Efficient vectorization:

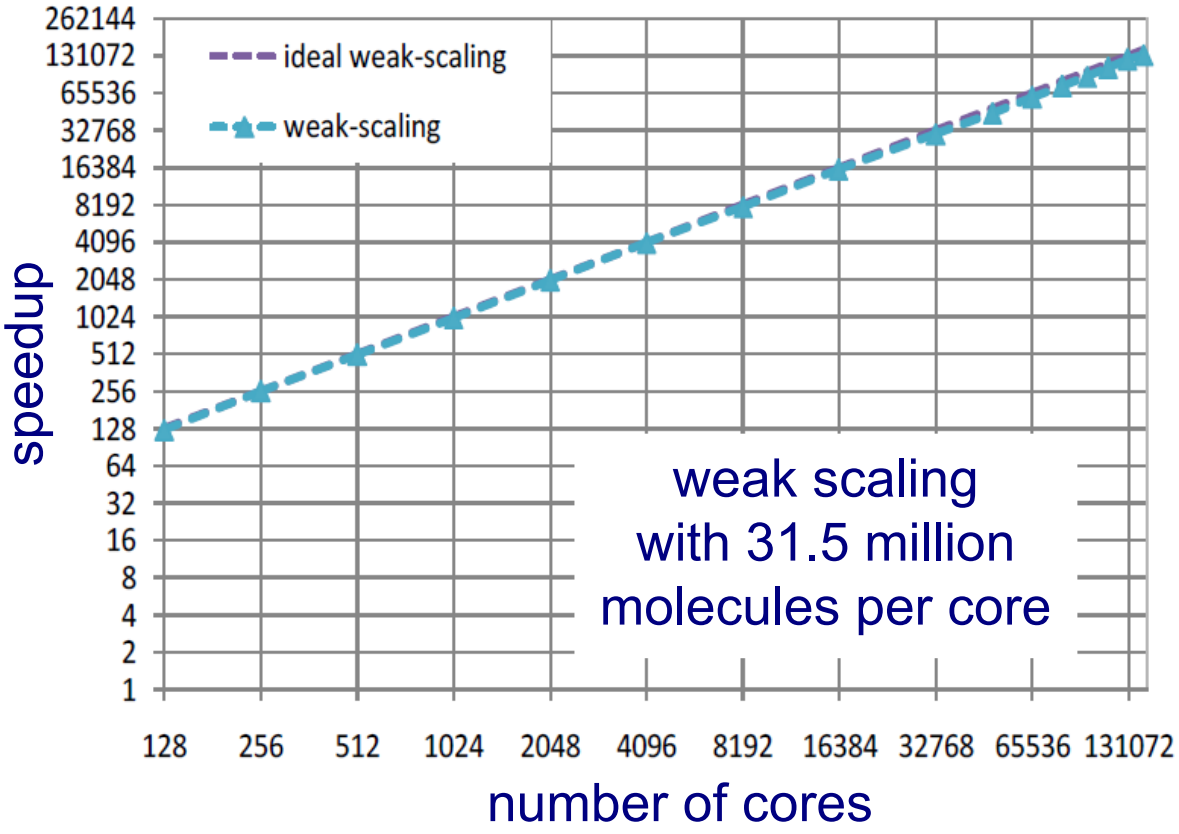
- Optimization by hand, using advanced vector extensions (AVX).
- Conversion from array of structures (AoS) to structure of arrays (SoA).

Strong scaling of ls1 mardyn on SuperMUC

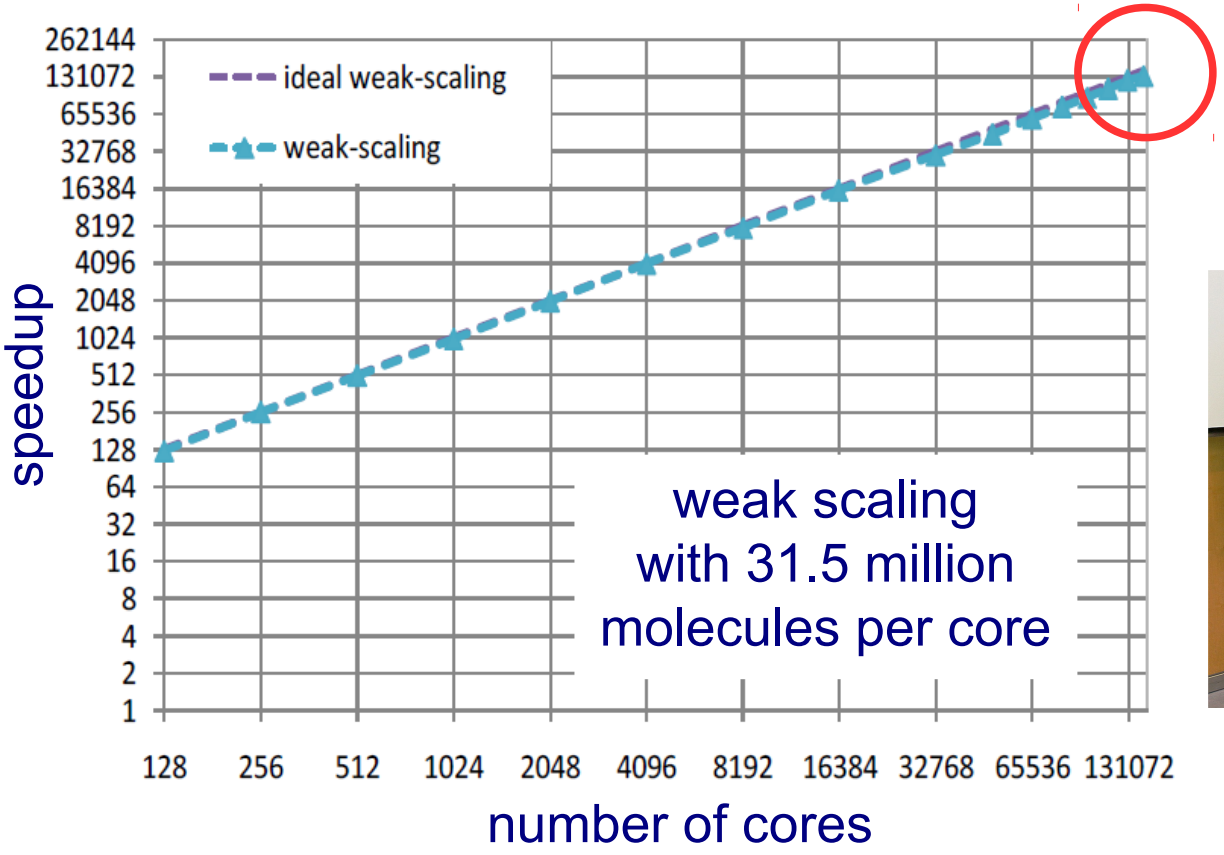
Scaling of *ls1 mardyn* examined on SuperMUC up to 146 016 cores.



Weak scaling of ls1 mardyn on SuperMUC



MD world record simulation on SuperMUC

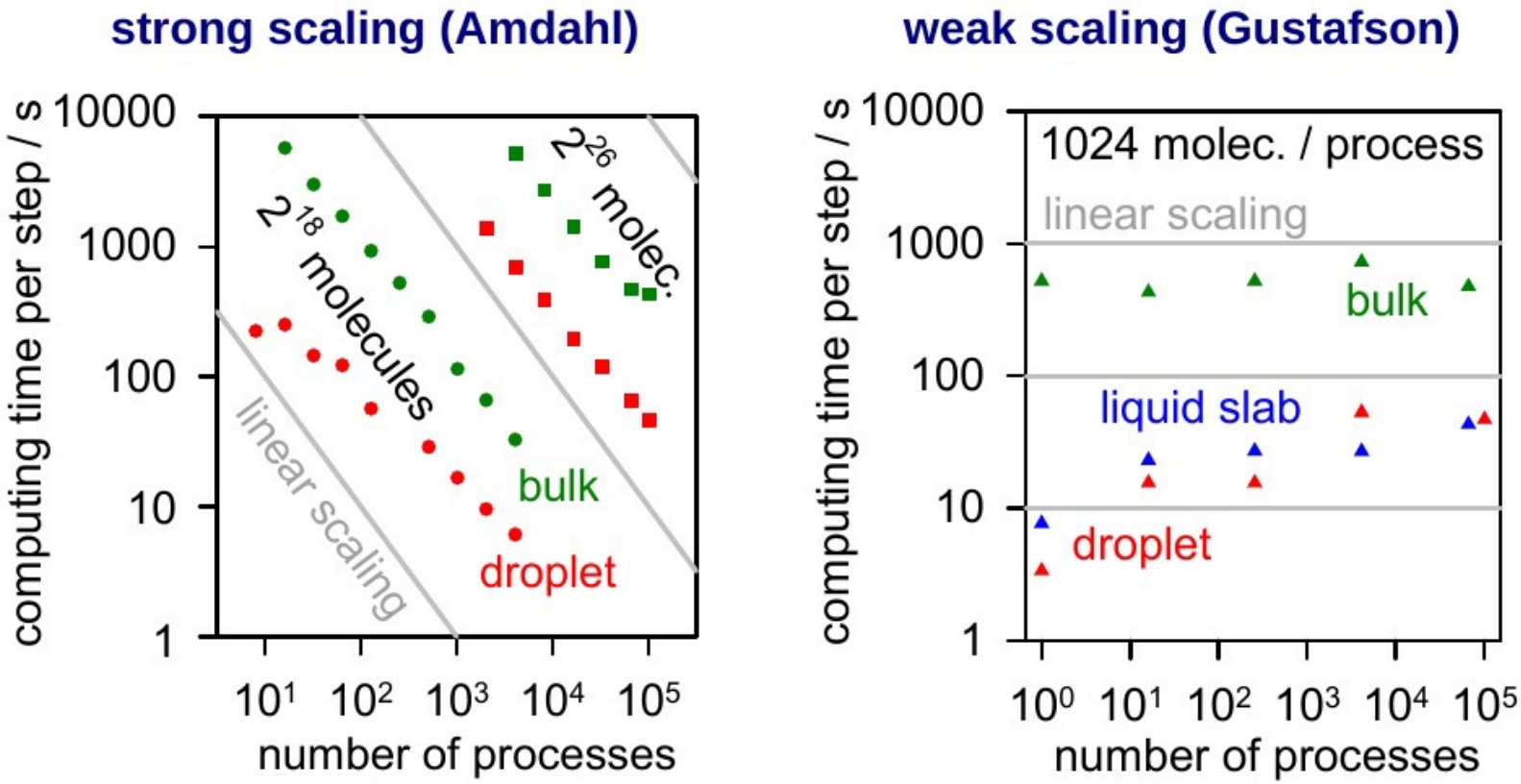


Up to $N = 4 \cdot 10^{12}$ on SuperMUC

PRACE ISC Prize

MD world record achieved from simulations of a homogeneous LJTS liquid.

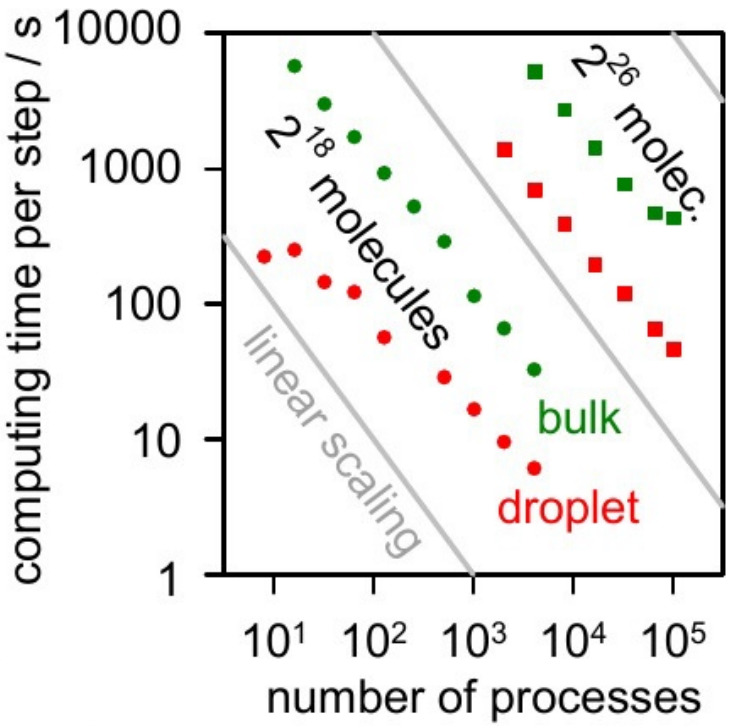
Large-scale production simulations



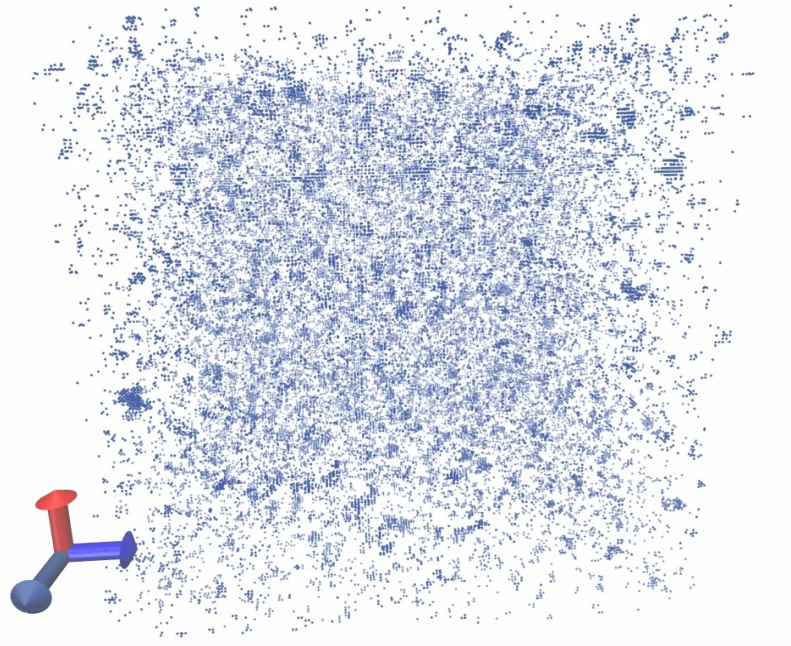
Technically / scientifically relevant simulations of large systems always deal with *heterogeneous* systems (e.g. at vapour-liquid interfaces).

Large-scale production simulations

strong scaling (Amdahl)



homogeneous cavitation

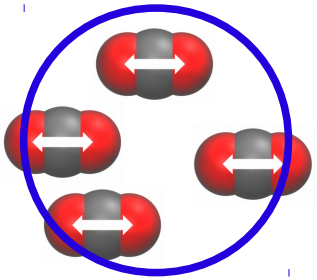


CO_2 (T = 280 K and ρ = 17.2 mol/l), 3CLJQ
100 million interaction sites, 110 592 cores

MD simulation of homogeneous cavitation

Canonical MD simulation of cavitation in carbon dioxide.

Evaluation of local density at 180 x 180 x 180 grid points:

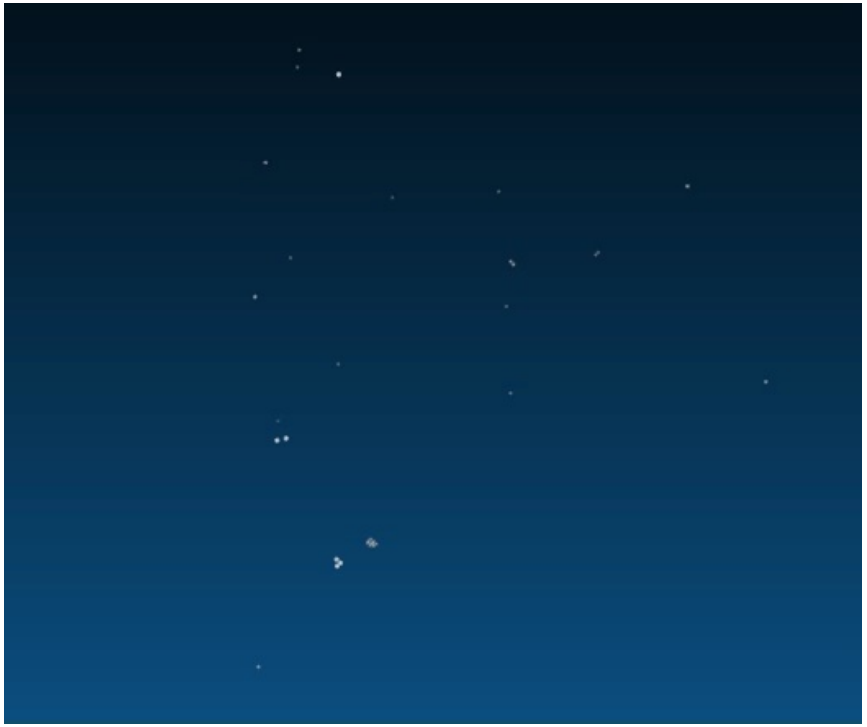


≤ 5 ?

(6 mol/l)

Liquid phase detected for more than 5 neighbors within a radius of 6.9 Å around the grid point.

homogeneous cavitation

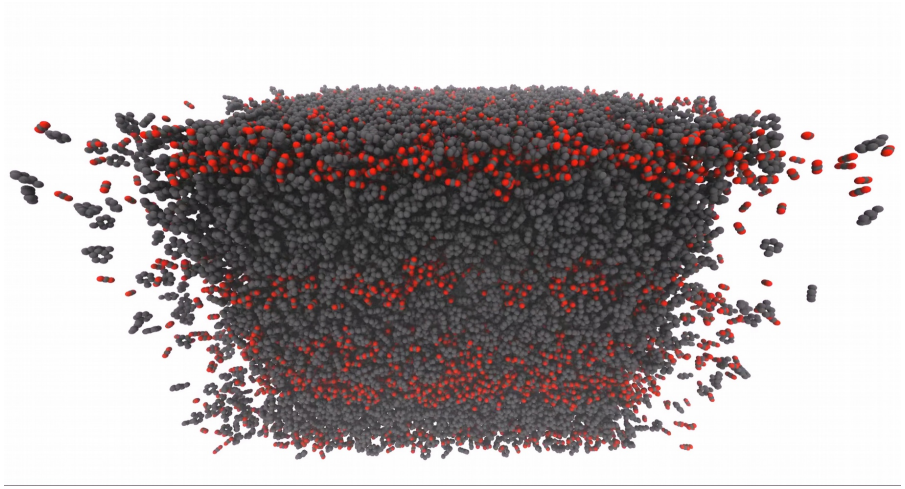


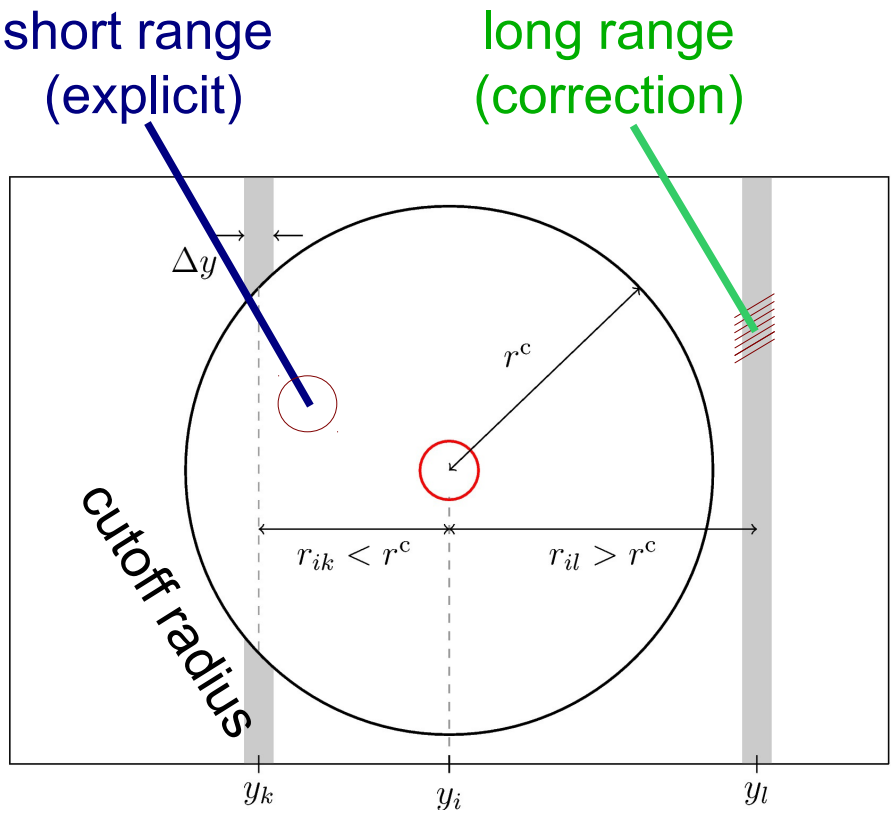
liquid carbon dioxide, 220 K, 23.9 mol/l

Long-range correction for planar interfaces

Example: Vapour-liquid interfaces.

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



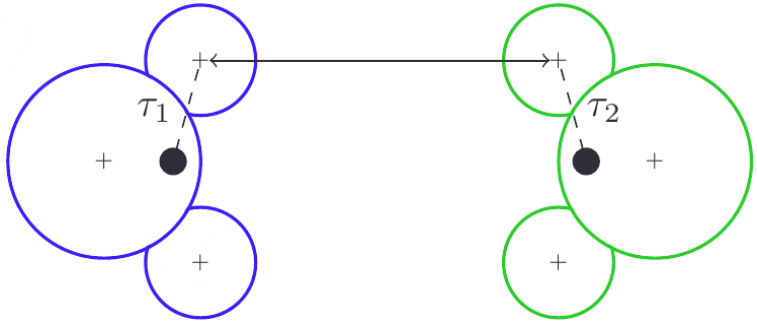


Full evaluation of all pairwise interactions is too expensive ...
... instead, **short-range interactions** are evaluated for **neighbours**.

Long-range correction for planar interfaces

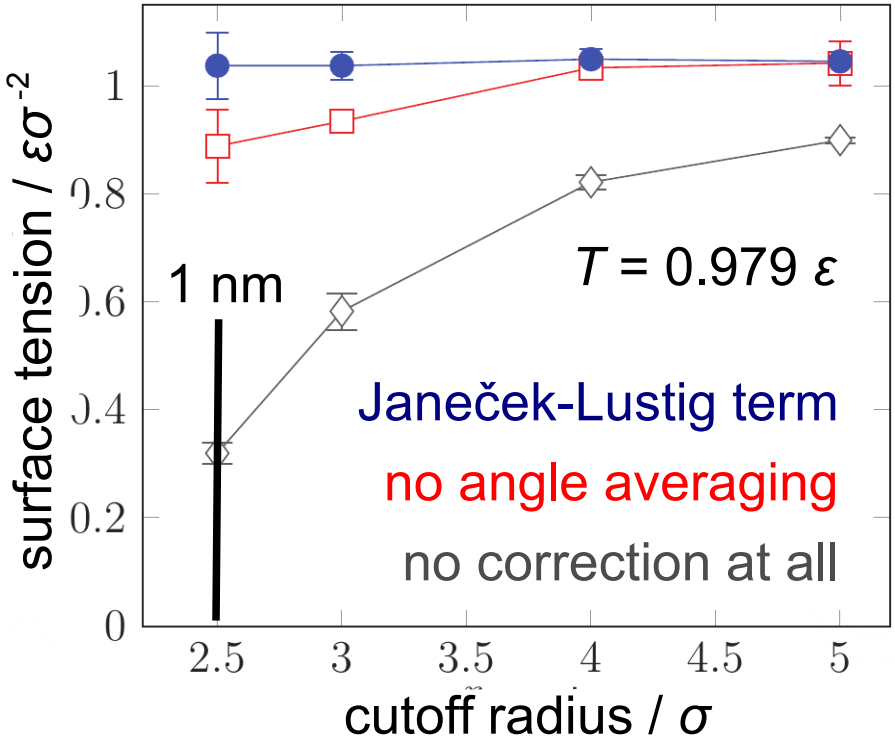
Example: Vapour-liquid interfaces.

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



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

Two-centre LJ fluid (2CLJ)



Computationally efficient correction scheme for **polarity** and **dispersion**.

Computing project pr83ri (2013 – 2015)

Simulation of capillary waves and fluctuations of liquid droplets

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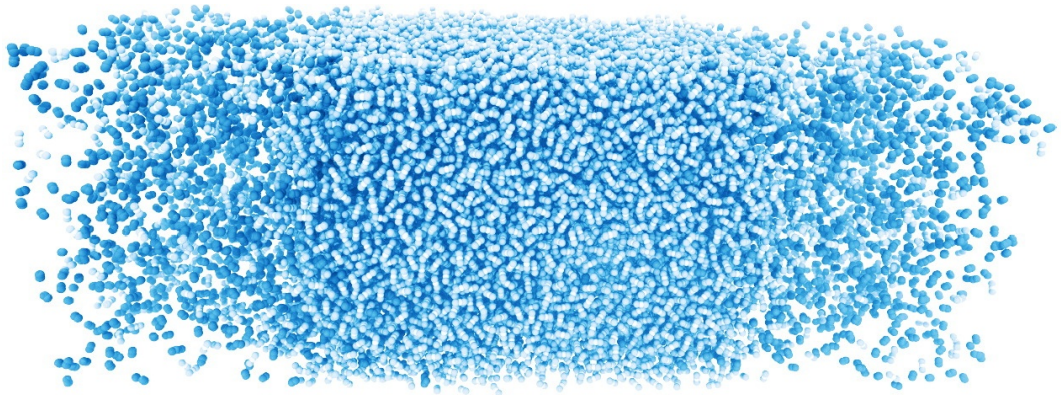

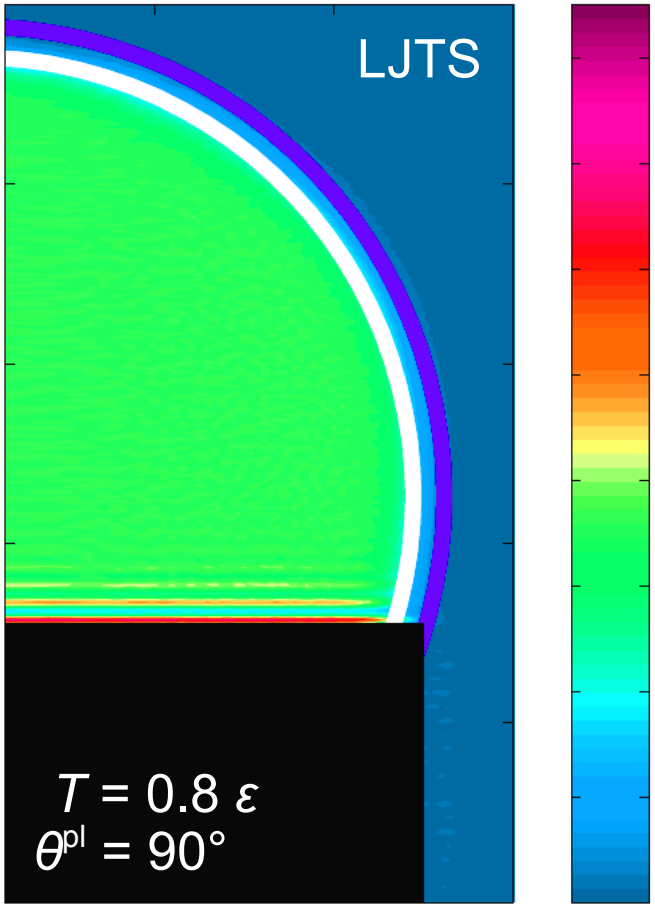

Computing project pr48te (2016 – 2018)

Scalable, performant, and resilient large-scale applications of molecular process engineering (Sparlampe)

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Approved in March 2016

Increased resiliency by data reduction and reconstruction from local radial distribution functions

Efficient long-range corrections for spherical and arbitrary geometries