MD study of Poiseuille/Couette flow and the vapor-liquid interface of methane in nanochannels

Institute for Computational Physics, Stuttgart

Oberseminar “Physik mit Höchstleistungsrechnern“

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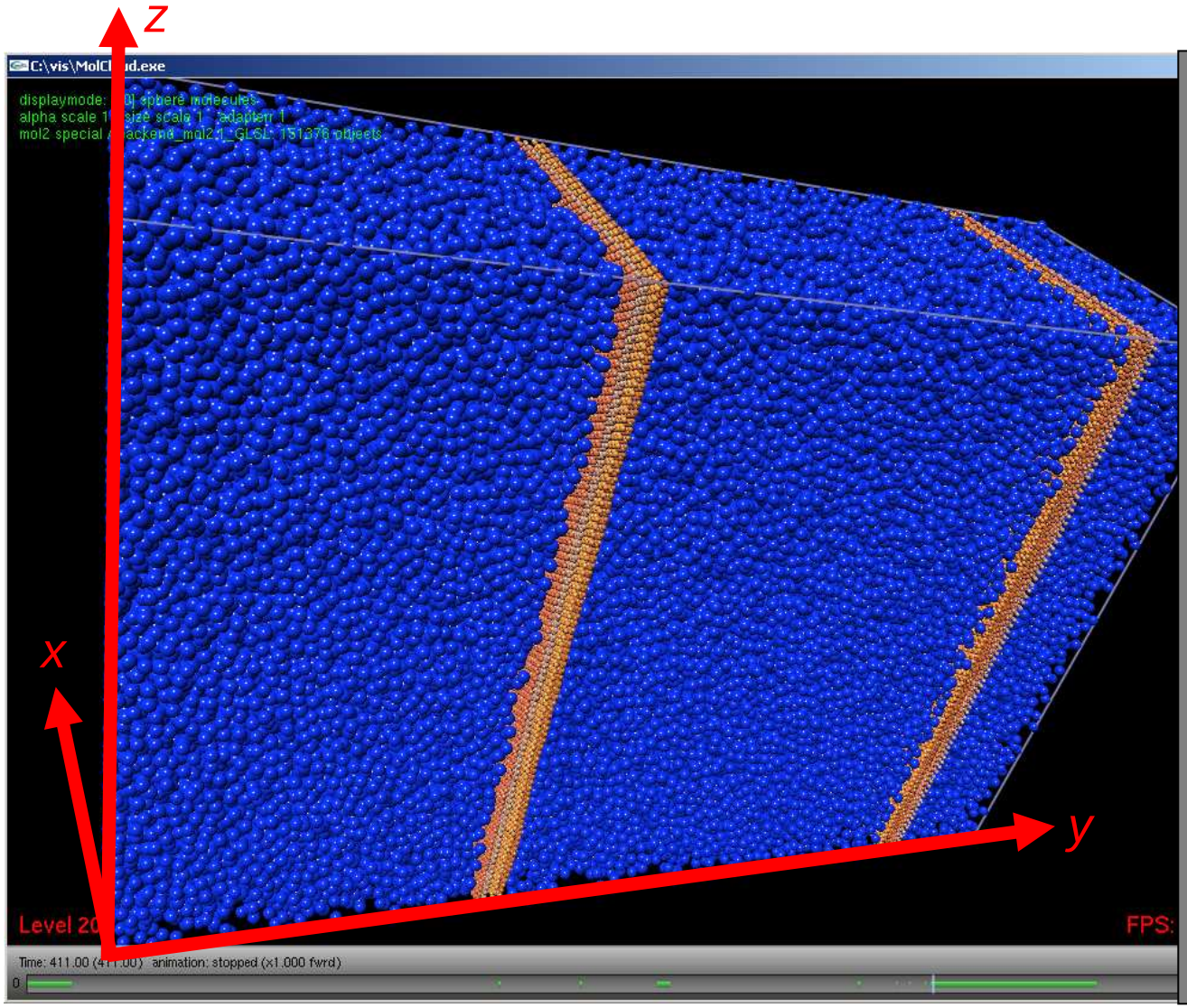
Methane confined in a nanochannel



Poiseuille flow:

The fluid is accelerated in *z* direction

Couette flow:

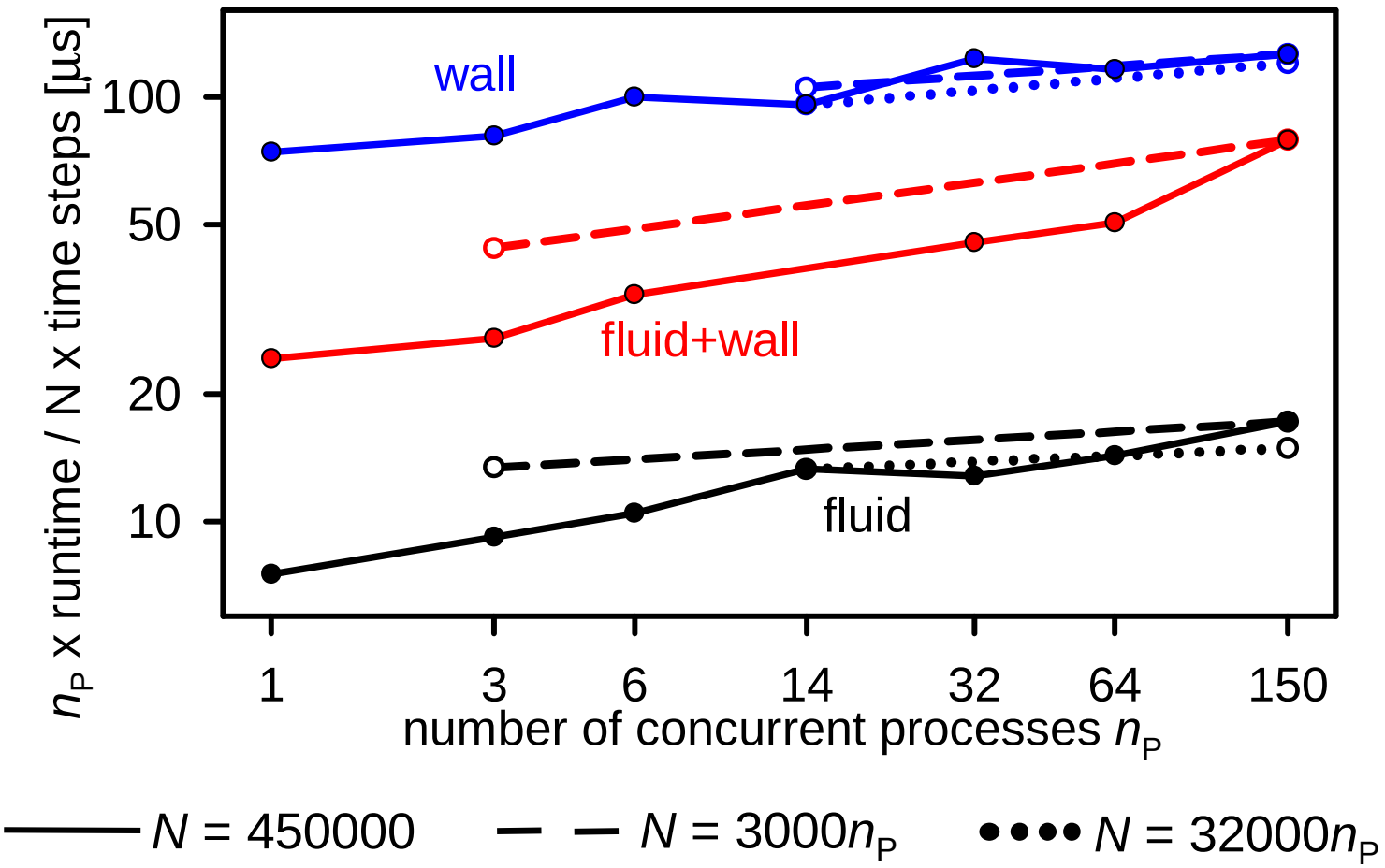
The walls are accelerated in opposite *z* directions

Contact angle:

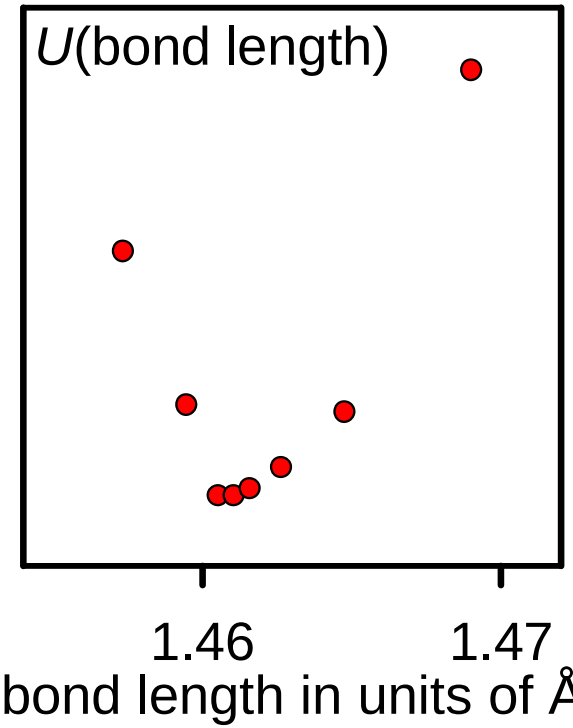
Meniscus perpendicular to the *z* axis

Scaling with isotropic domain decomposition

Molecul**ar dyn**amics code *Mardyn* (developed by the ls1 project):

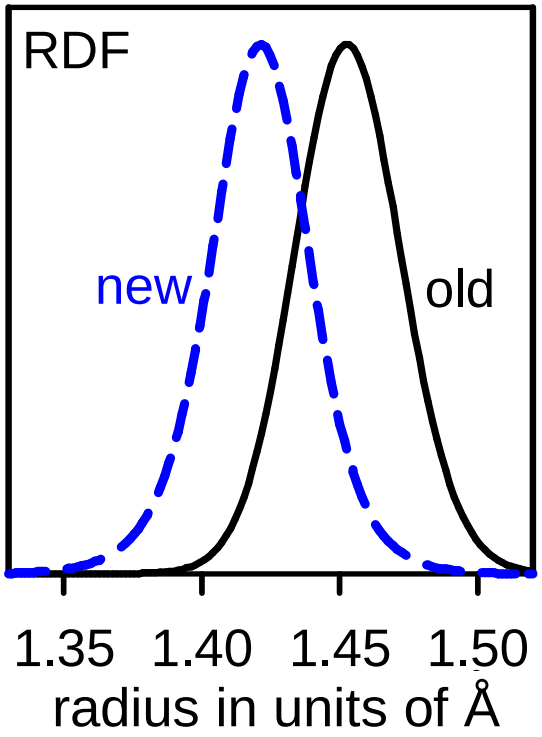


Reparametrization of the Tersoff potential



Bond length:

Tersoff potential: 1.461 Å
Actual graphite: 1.421 Å

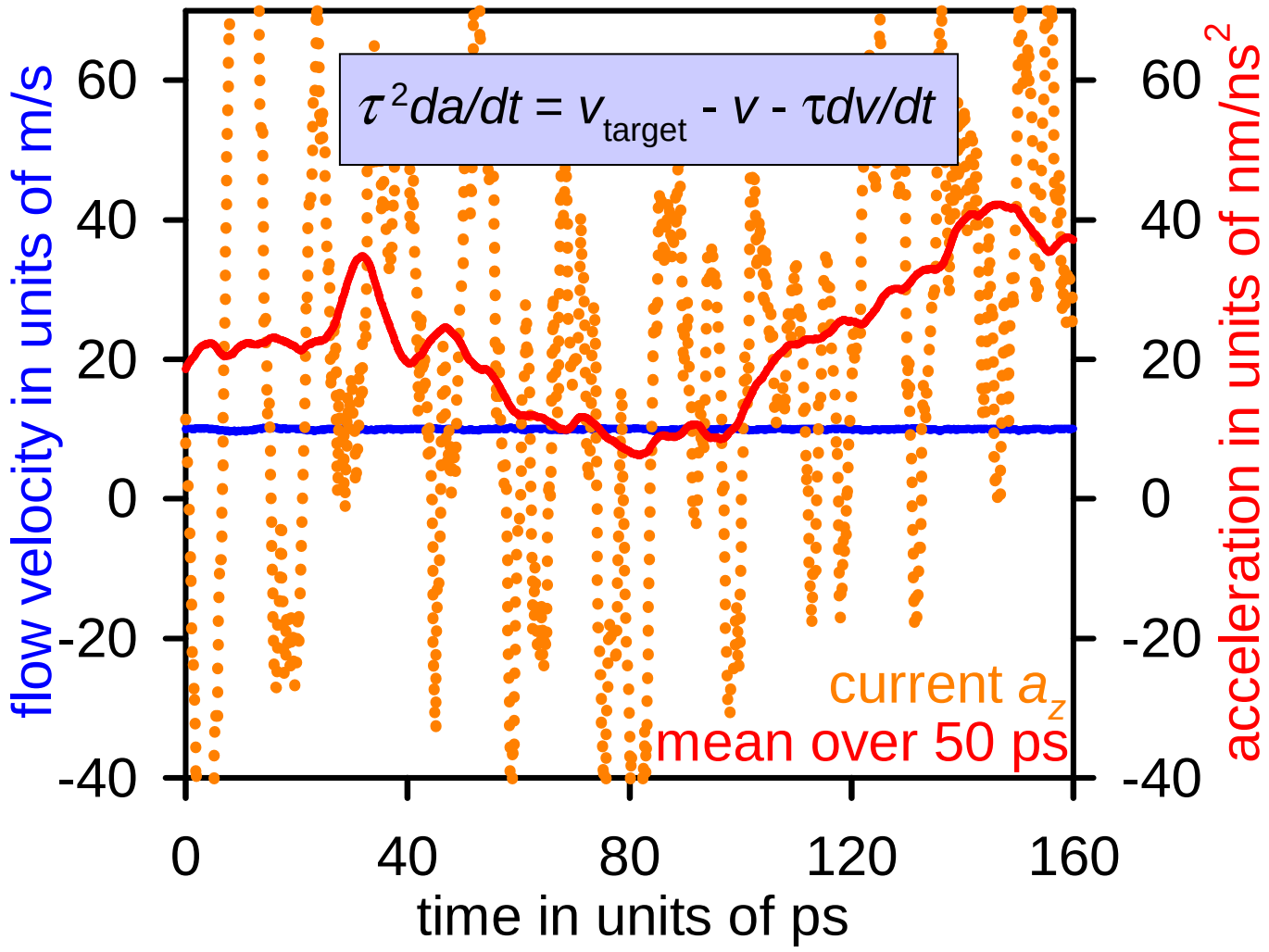


Optimized Tersoff potential parameters for graphite:

Cutoff	Attraction	Repulsion
R = 2.0 Å (1.8 Å)	μ = 2.275 Å^{-1} (2.2119 Å^{-1})	λ = 3.587 Å^{-1} (3.4879 Å^{-1})
S = 2.35 Å (2.1 Å)		

Uniform acceleration (PI controller)

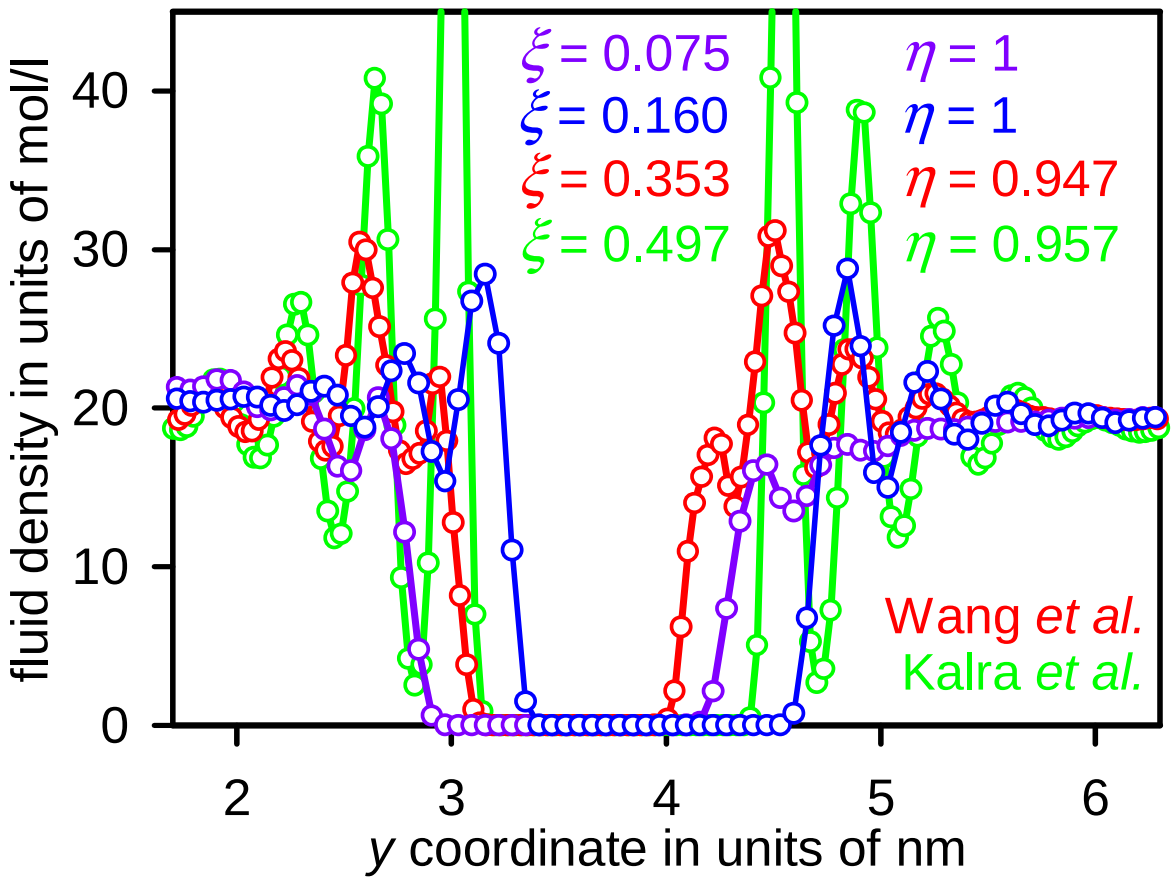
Poiseuille, v_{target} = 10 m/s, τ = 3 ps, L = 15 nm, liquid CH_4 at 166 K



Fluid-wall interaction

Lennard-Jones energy parameter: $\varepsilon_{FW} = \xi \cdot \varepsilon_{FF}$

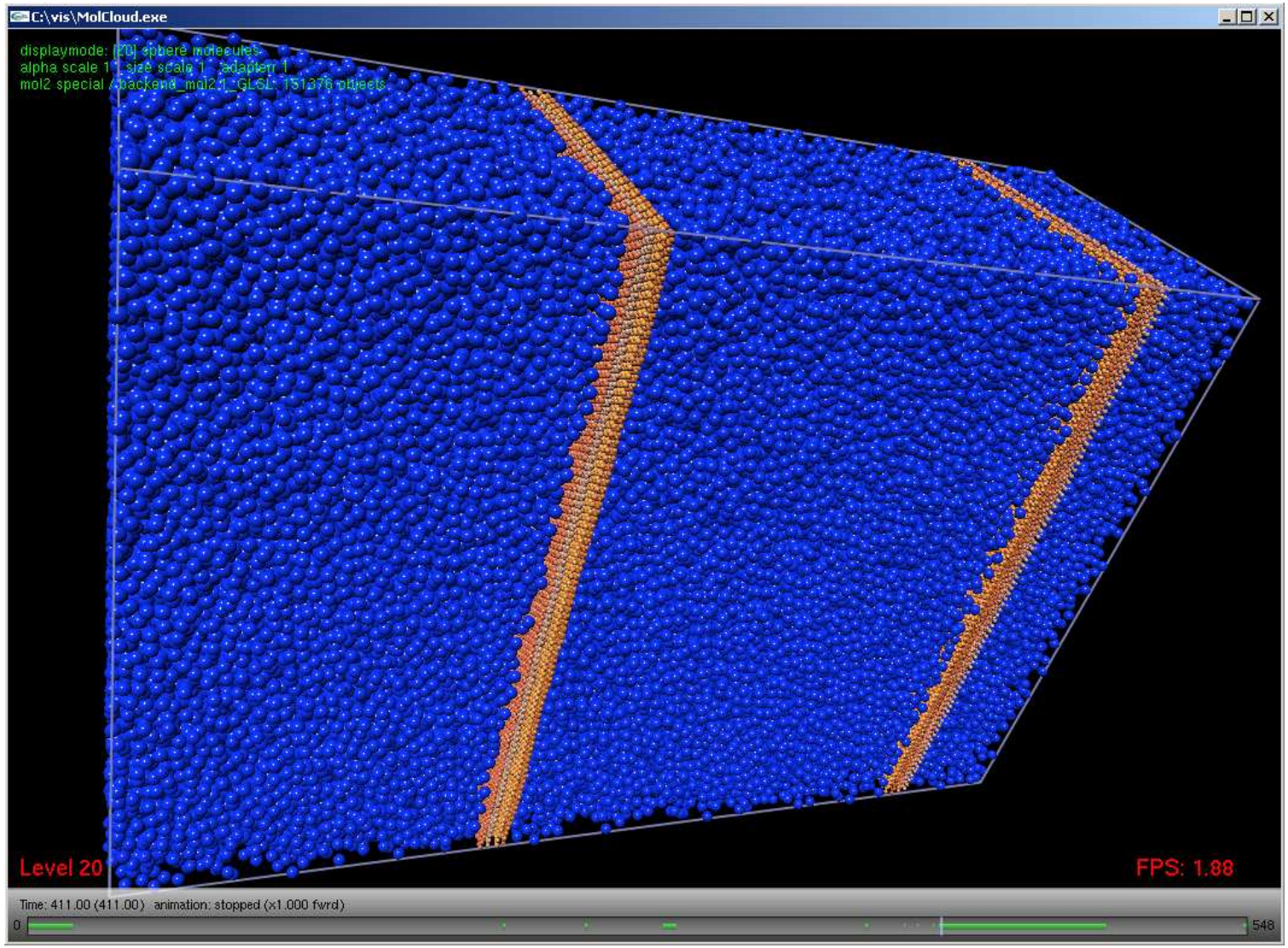
Lennard-Jones size parameter: $\sigma_{FW} = \eta \cdot \sigma_{FF}$



$T = 0.95\ \varepsilon/k$

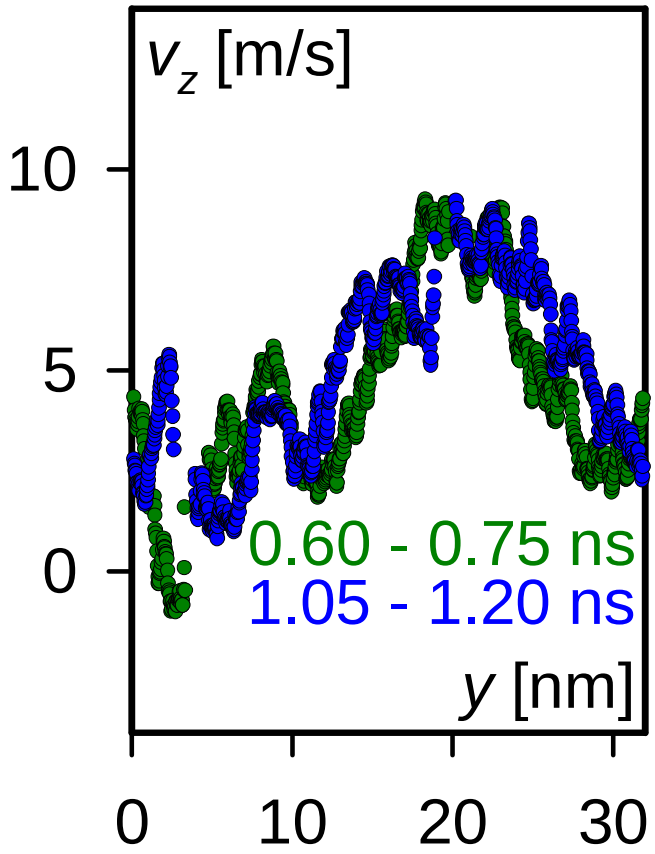
$\rho = 1.005\ \rho'$

MD simulation of Couette flow

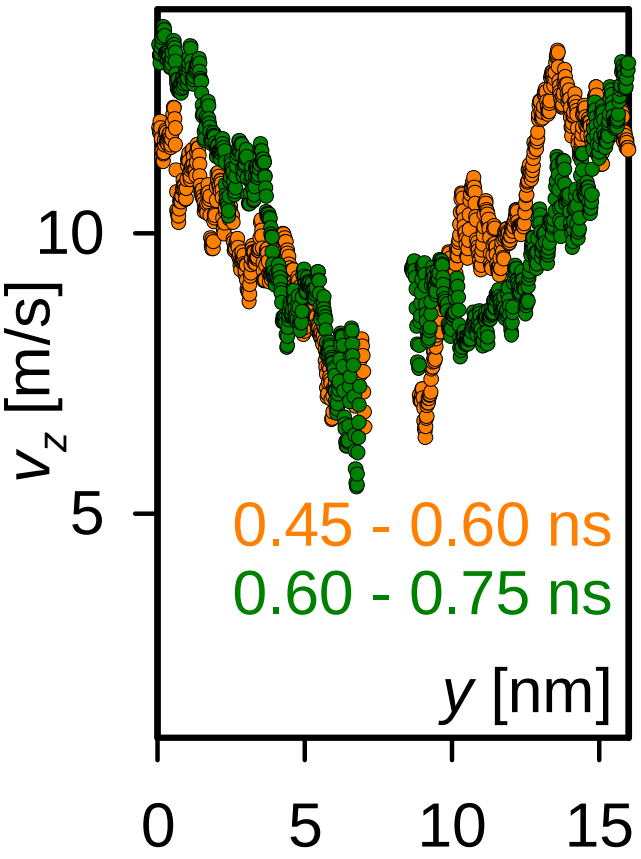


Poiseuille and Couette flow: velocity profile

$T = 0.95\ \varepsilon/k$, $\rho = 1.005\ \rho'$, $v_{target} = 10$ m/s, $\xi = 0.353$, $\eta = 0.9466$ (Wang et al.)



Couette flow



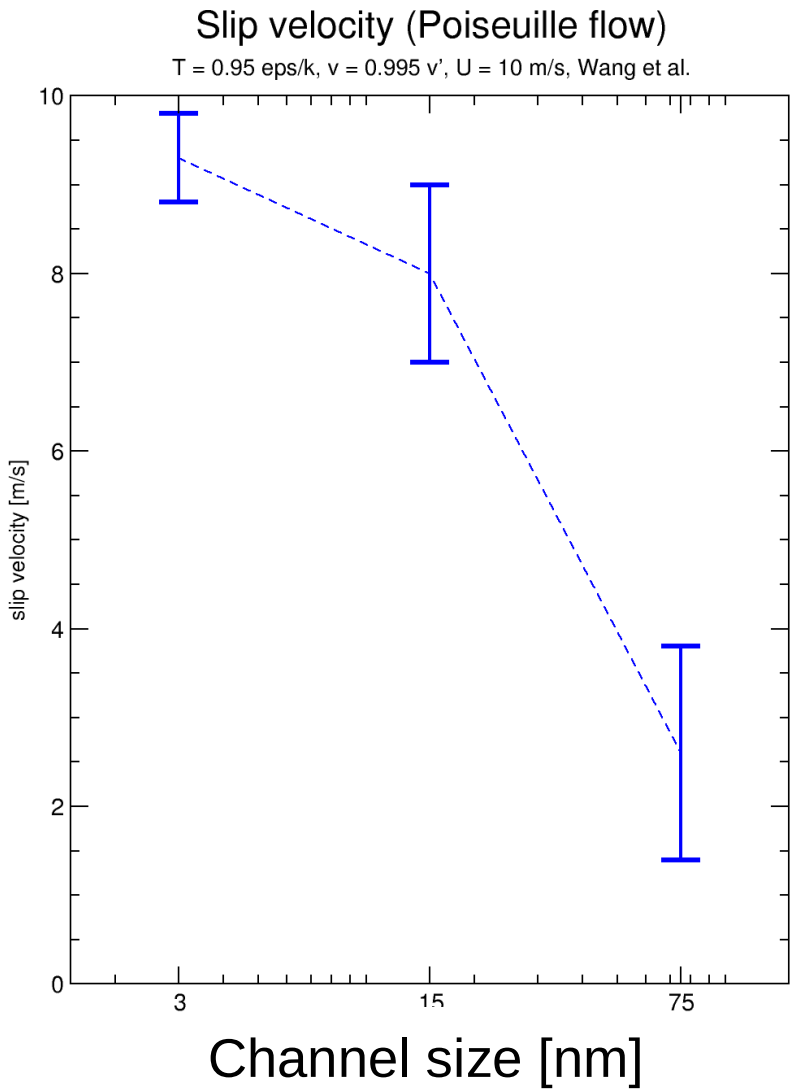
Poiseuille flow

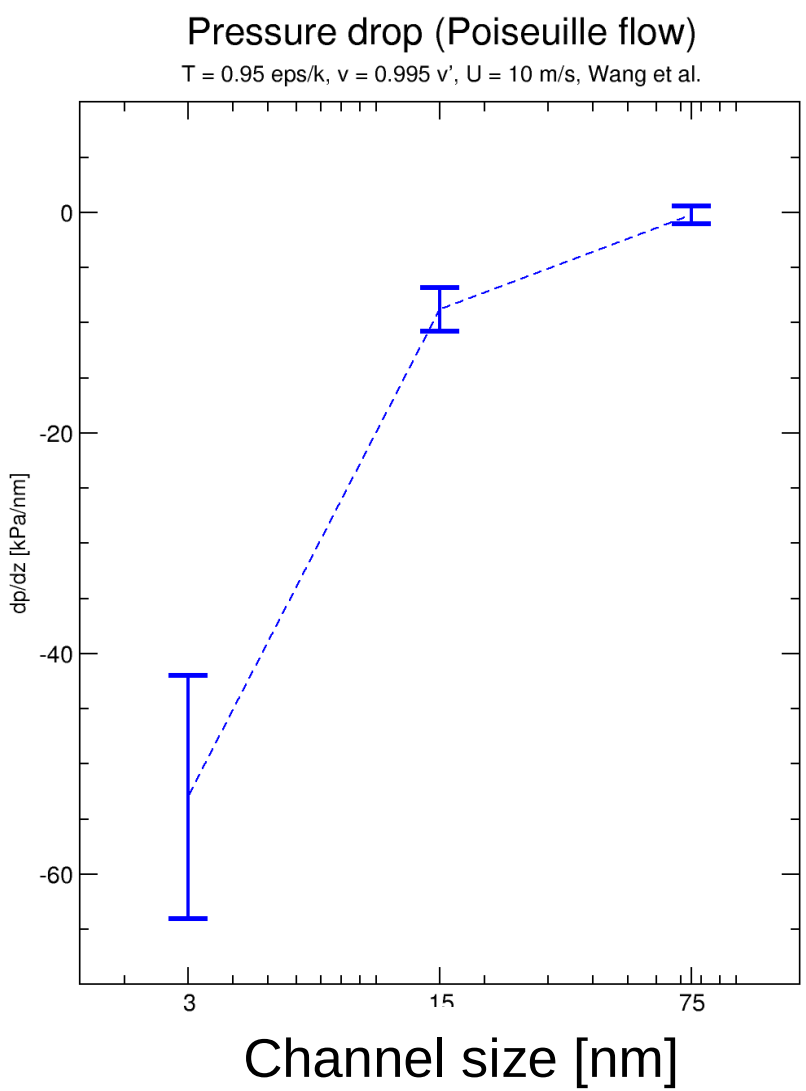
Poiseuille and Couette flow: viscosity

$T = 0.95\ \varepsilon/k$, $\rho = 1.005\ \rho_c$, $v_{target} = 10$ m/s, $\xi = 0.353$, $\eta = 0.9466$ (Wang et al.)

Couette flow	**Poiseuille flow**
Slip velocity $v_s = 2$ m/s	Slip velocity $v_s = 8$ m/s
Shear stress $\tau = 200$ kPa	Pressure drop $dp/dz = -9$ kPa/nm
Kinematic viscosity $\nu = 1 \cdot 10^{-6}$ m^2/s	Kinematic viscosity $\nu = 2 \cdot 10^{-7}$ m^2/s
Reynolds number $0.08 < Re < 0.6$	Reynolds number $0.6 < Re < 1.0$

Dependence of flow properties on the channel size

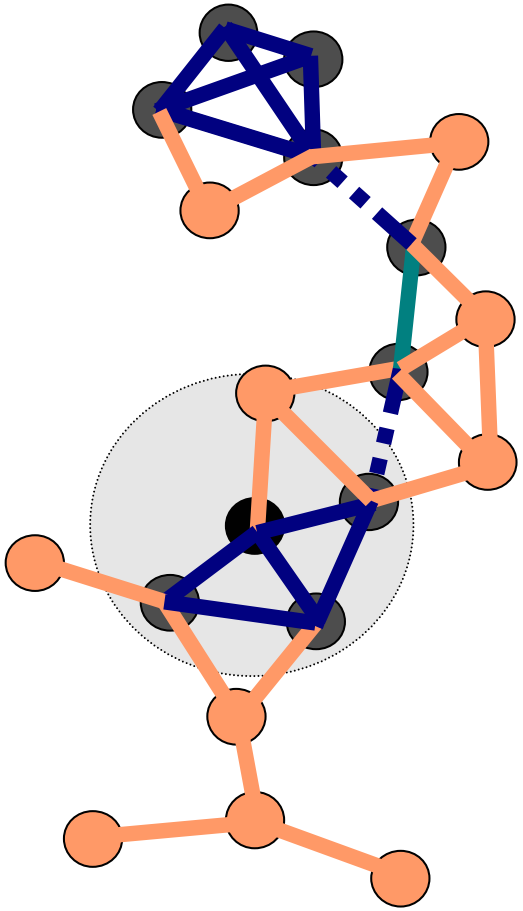




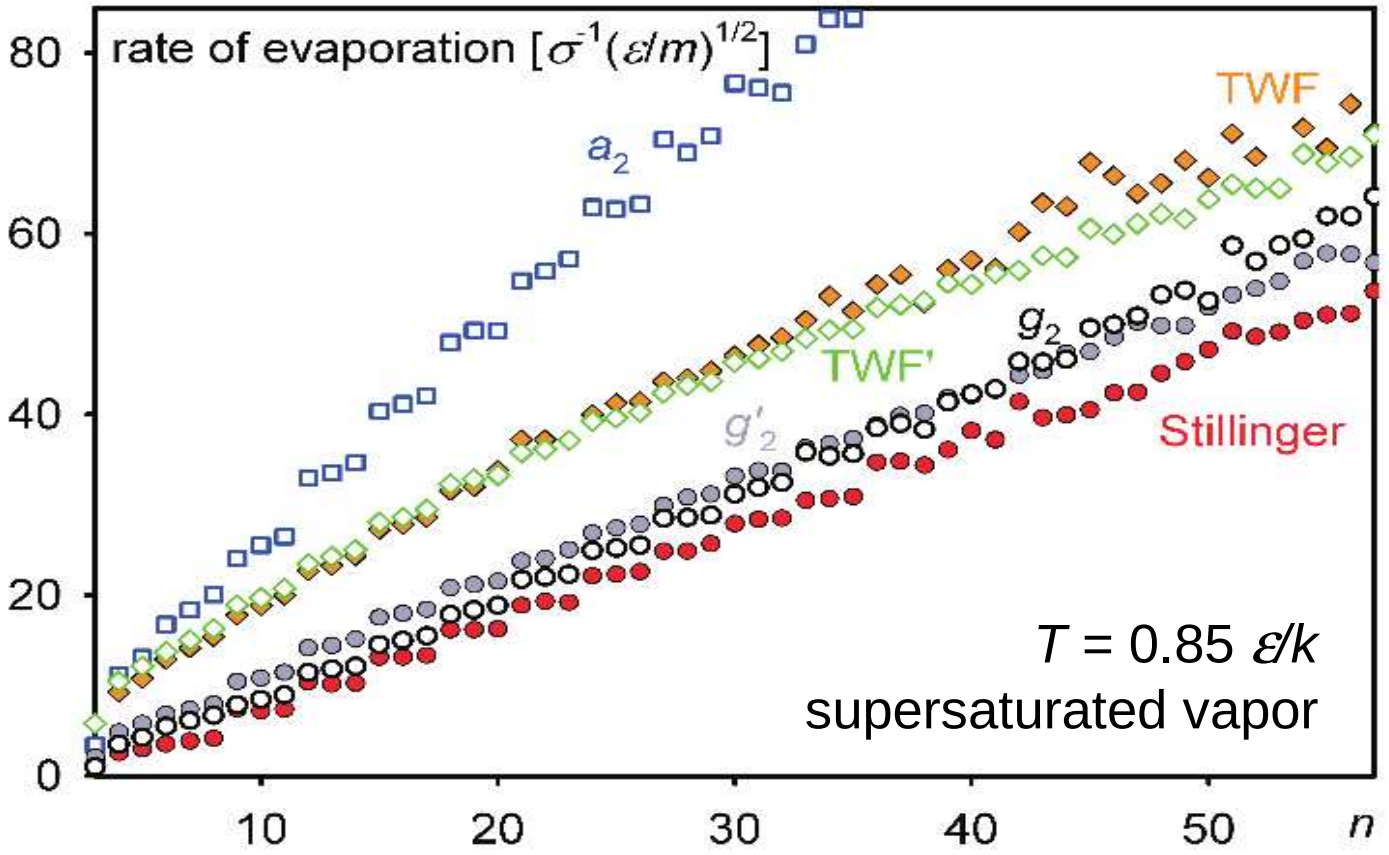
Disperse systems: cluster criteria

Stillinger: molecules with a distance of 1.5σ or less are liquid.
Ten Wolde and Frenkel (TWF): molecules with at least four neighbors within a distance of 1.5σ are liquid.
Arithmetic mean, *n* neighbors (a_n): a molecule is liquid if the density in the sphere containing its *n* nearest neighbors exceeds $(\rho'+\rho'')/2$.
Geometric mean, *n* neighbors (g_n): analogous, the required density is $(\rho'\rho'')^{1/2}$.

Nuclei can also be determined as **biconnected** (instead of connected) components, such that no nucleus can be separated by removing a single molecule (TWF' and g'_2 criteria).

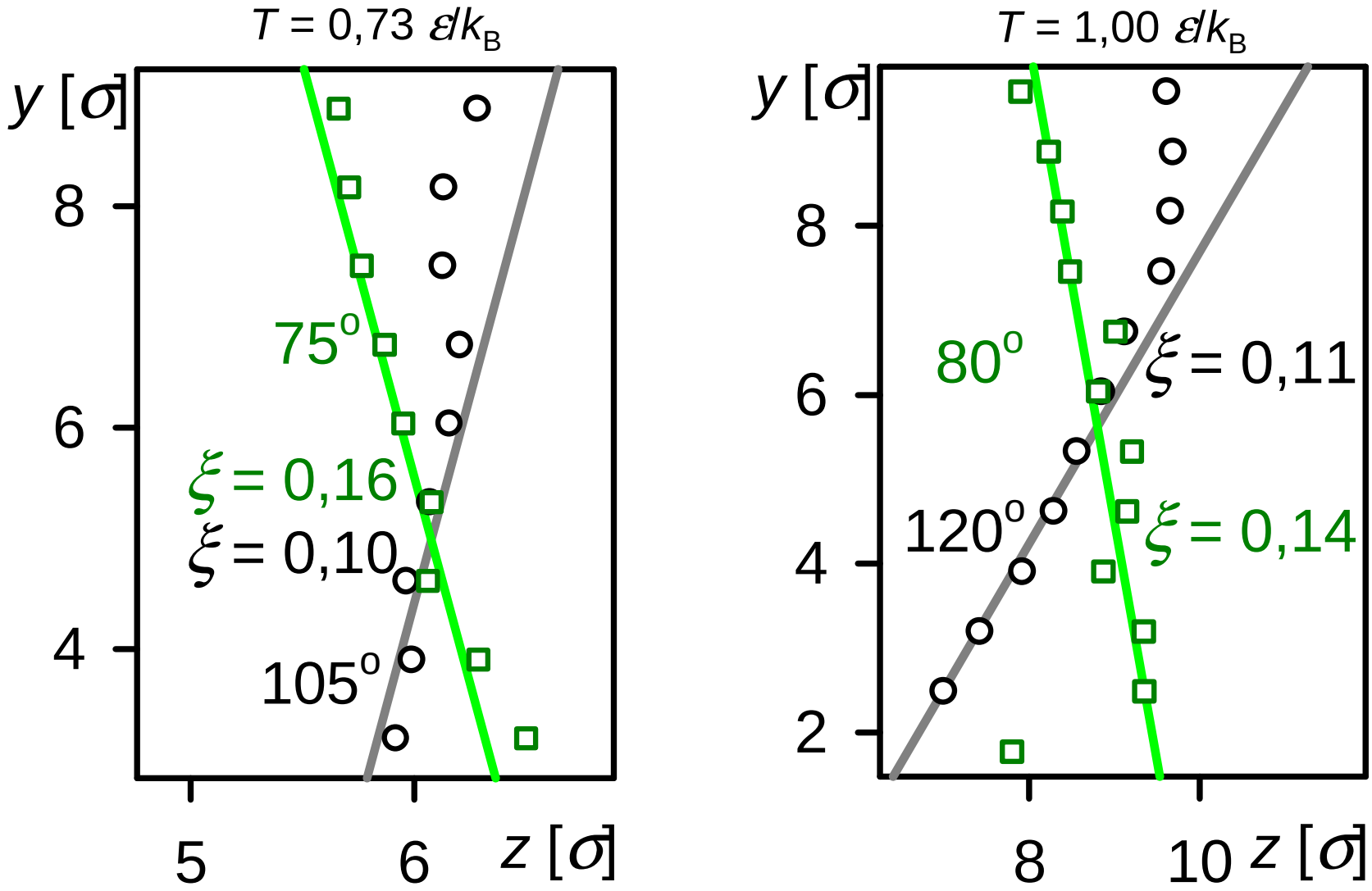


Comparison of cluster criteria

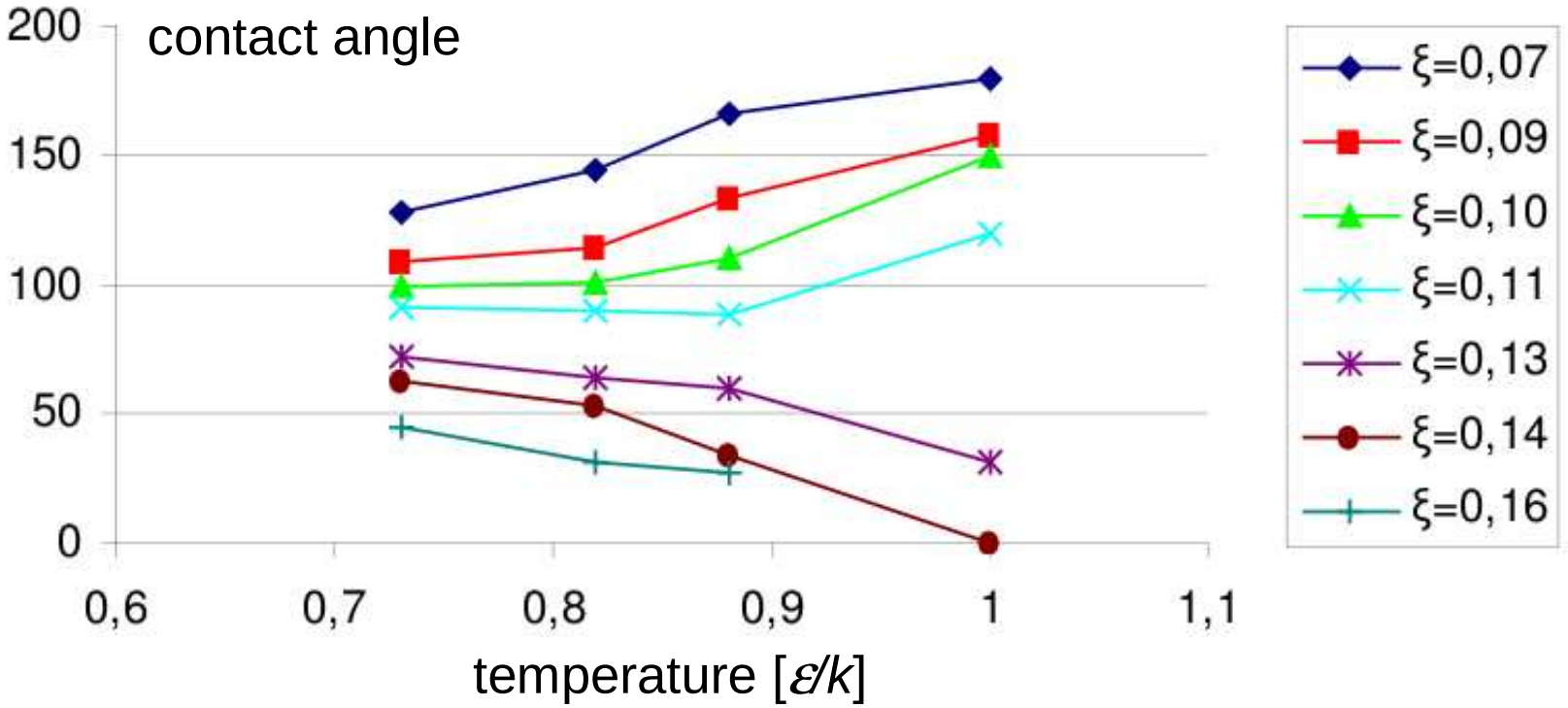


Fluctuation in equilibrium: $7.0 \cdot 10^{-4}$ (Stillinger), $7.4 \cdot 10^{-4}$ (g_2), $3.6 \cdot 10^{-4}$ (g'_2)

Dependence of the contact angle on ξ



Dependence of the contact angle on T and ξ



Simulation results for the LJTS fluid can be correlated as

$$\cos\theta(T^*, \xi) = \tanh[\exp(6.25T^*)(0.156\xi - 0.0170)].$$

Conclusion

System size: acceptable scaling of *Mardyn*, *L* up to 75 nm easily possible

the system geometry requires (static) load balancing

Flow simulations: were carried out in the canonical ensemble

unknown interaction parameters ξ and η

Vapor-liquid interface: dependence of the contact angle on ξ and T

suitable criterion for the interface: $\rho = (\rho' \rho'')^{1/2}$