# Turbulence, Heat and Mass Transfer (THMT '09)

## Poiseuille flow of liquid methane in nanoscopic graphite channels by molecular dynamics simulation

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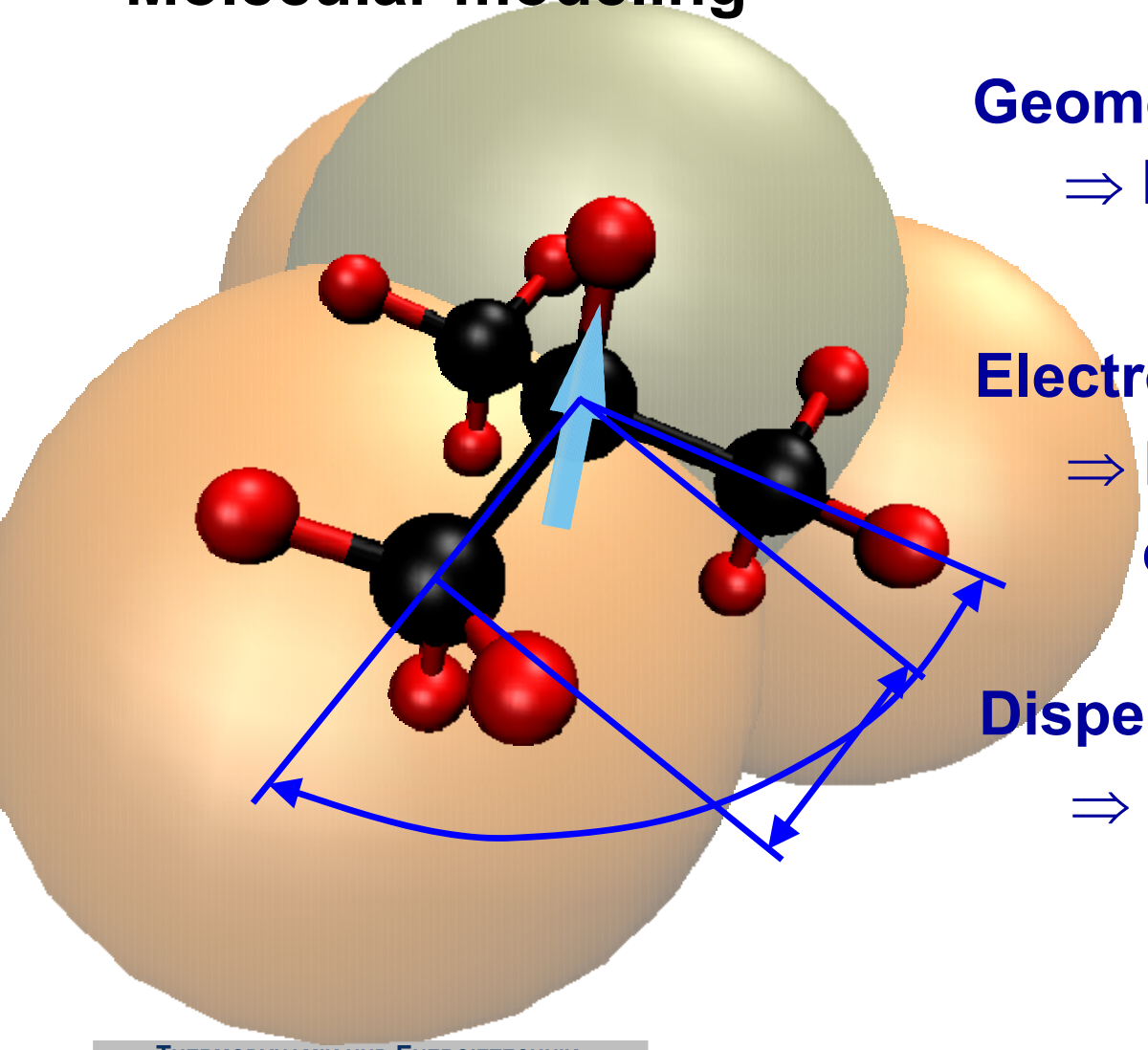
# Molecular modeling



**Geometry:**

⇒ Bond lengths and angles

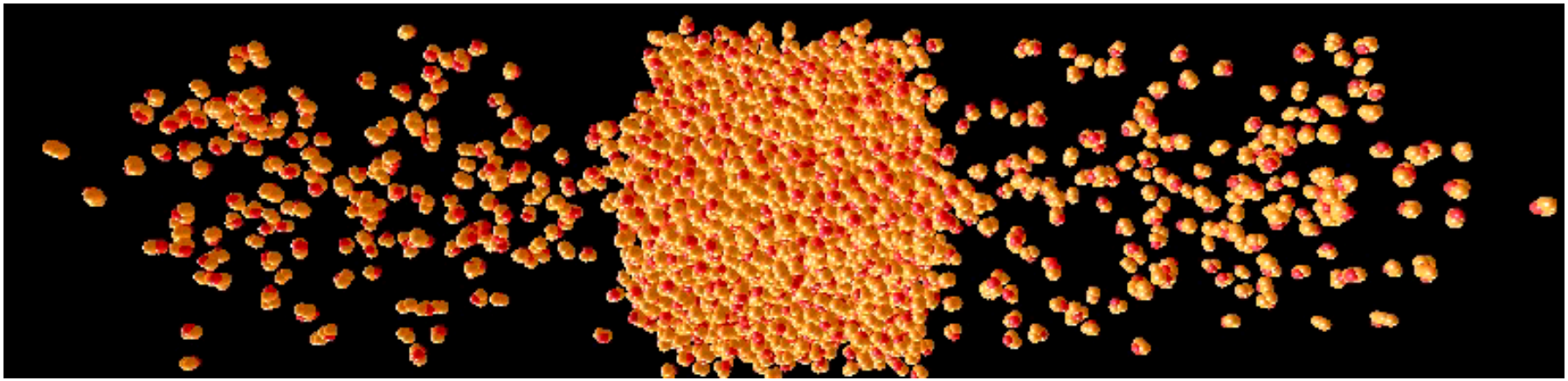
**Electrostatics:**

⇒ Position and magnitude of point polarities

**Dispersion and repulsion:**

⇒ Lennard-Jones potential parameters

# Ethylene oxide: Simulation challenge



Industrial Fluid Properties
Simulation Collective

3M

DUPONT

EXXON

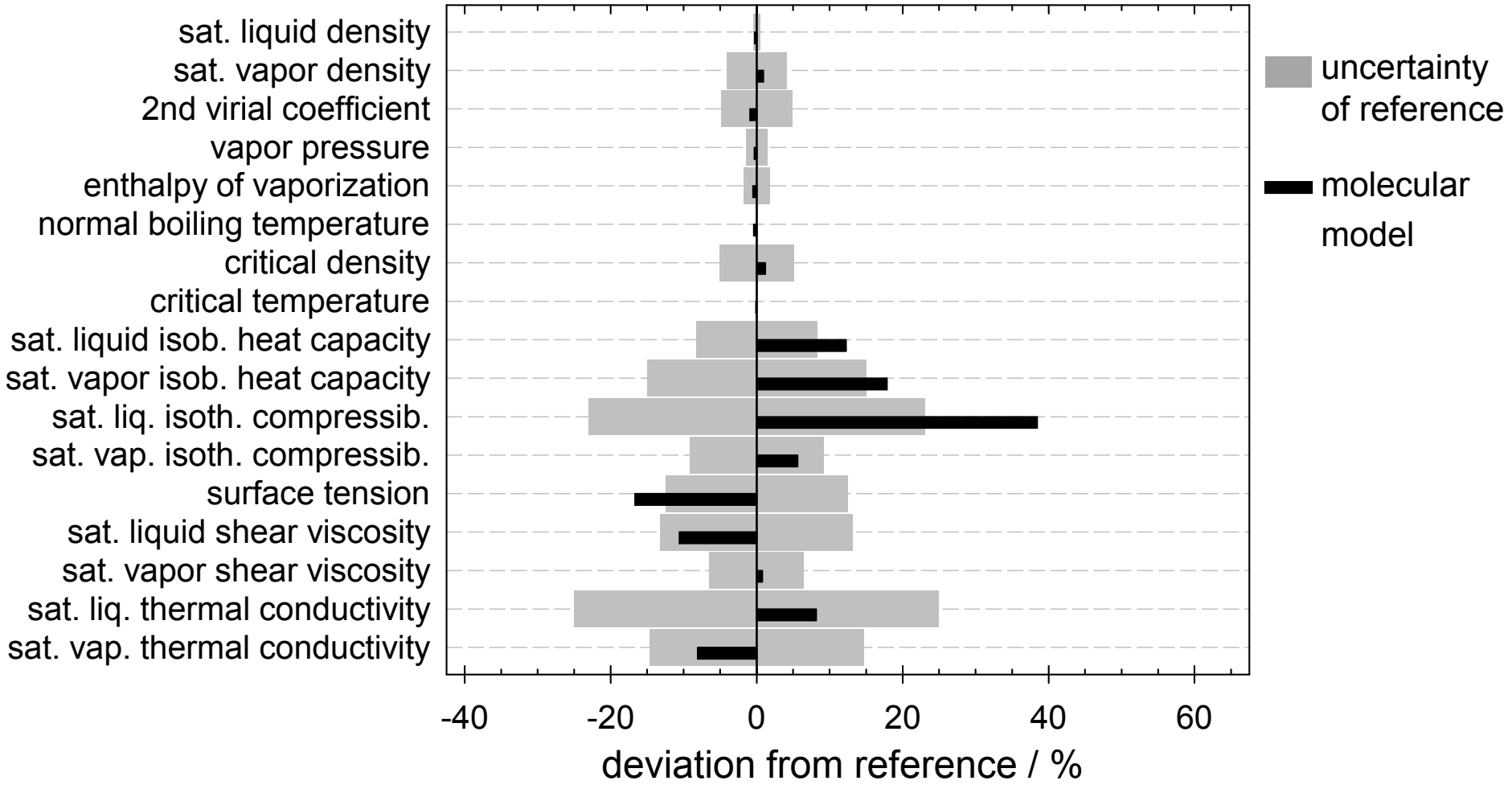
NIST
National Institute of
Standards and Technology

bp

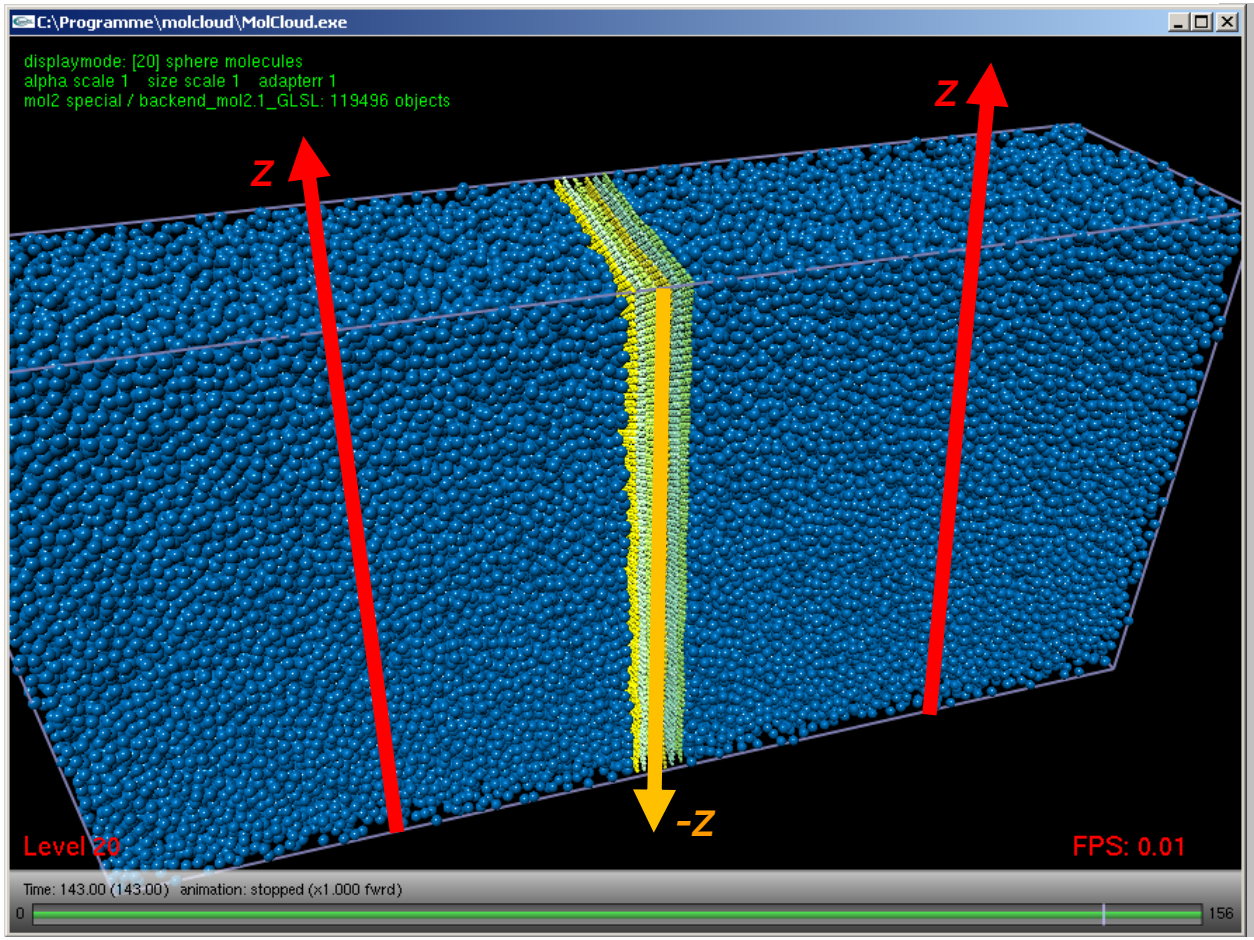
DOW

Ohio Supercomputer Center

# Ethylene oxide: Deviation from experimental data



# Flow induced by an additional force




## Poiseuille flow

⇒ periodic boundary condition

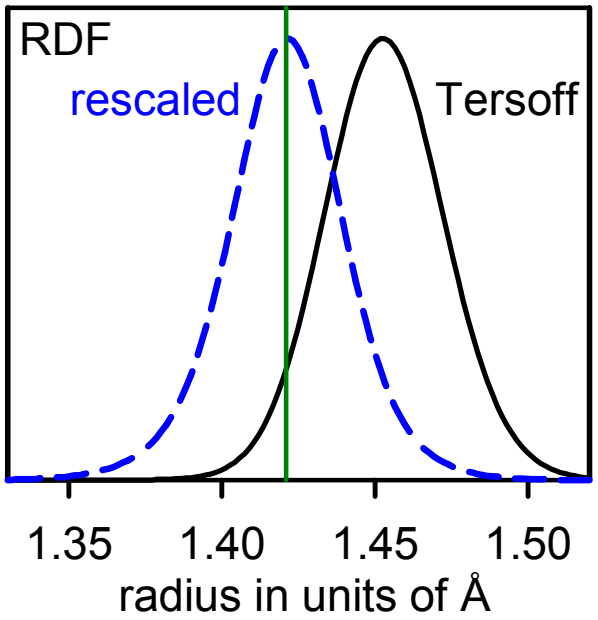
⇒ acceleration $a_z$ of fluid molecules in $z$ direction

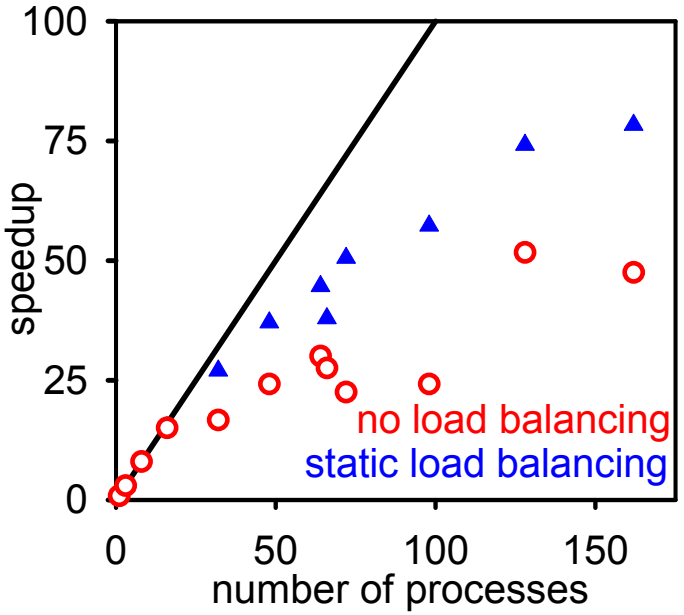
⇒ wall velocity $v_z = 0$ in $z$ direction

Pressure drop:

$$-\frac{dp}{dz} = \frac{F_z}{V} = \rho a_z$$

# Graphite model and implementation

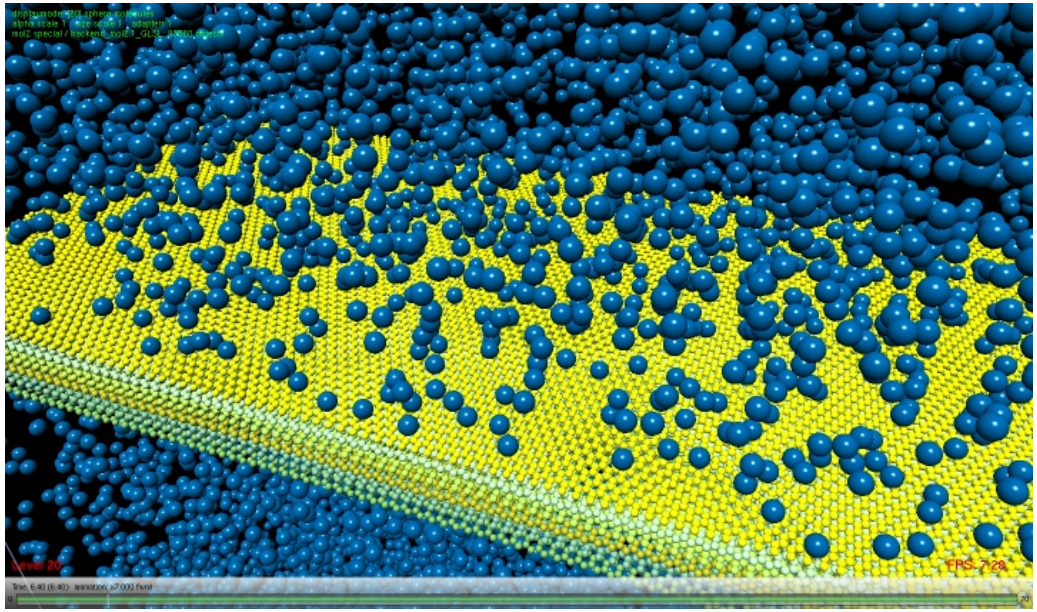


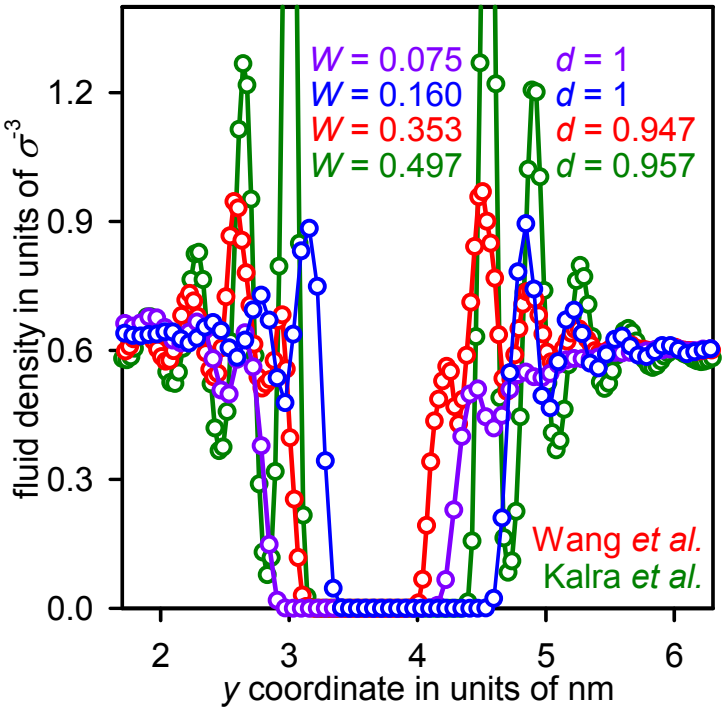




Optimized potential parameters for graphite:

| Cutoff | Attraction | Repulsion |
|---|---|---|
| $R$ = 2.0 Å (1.8 Å)<br>$S$ = 2.35 Å (2.1 Å) | $\mu$ = 2.275 Å$^{-1}$ (2.2119 Å$^{-1}$) | $\lambda$ = 3.587 Å$^{-1}$ (3.4879 Å$^{-1}$) |

# Boundary layers and adsorption





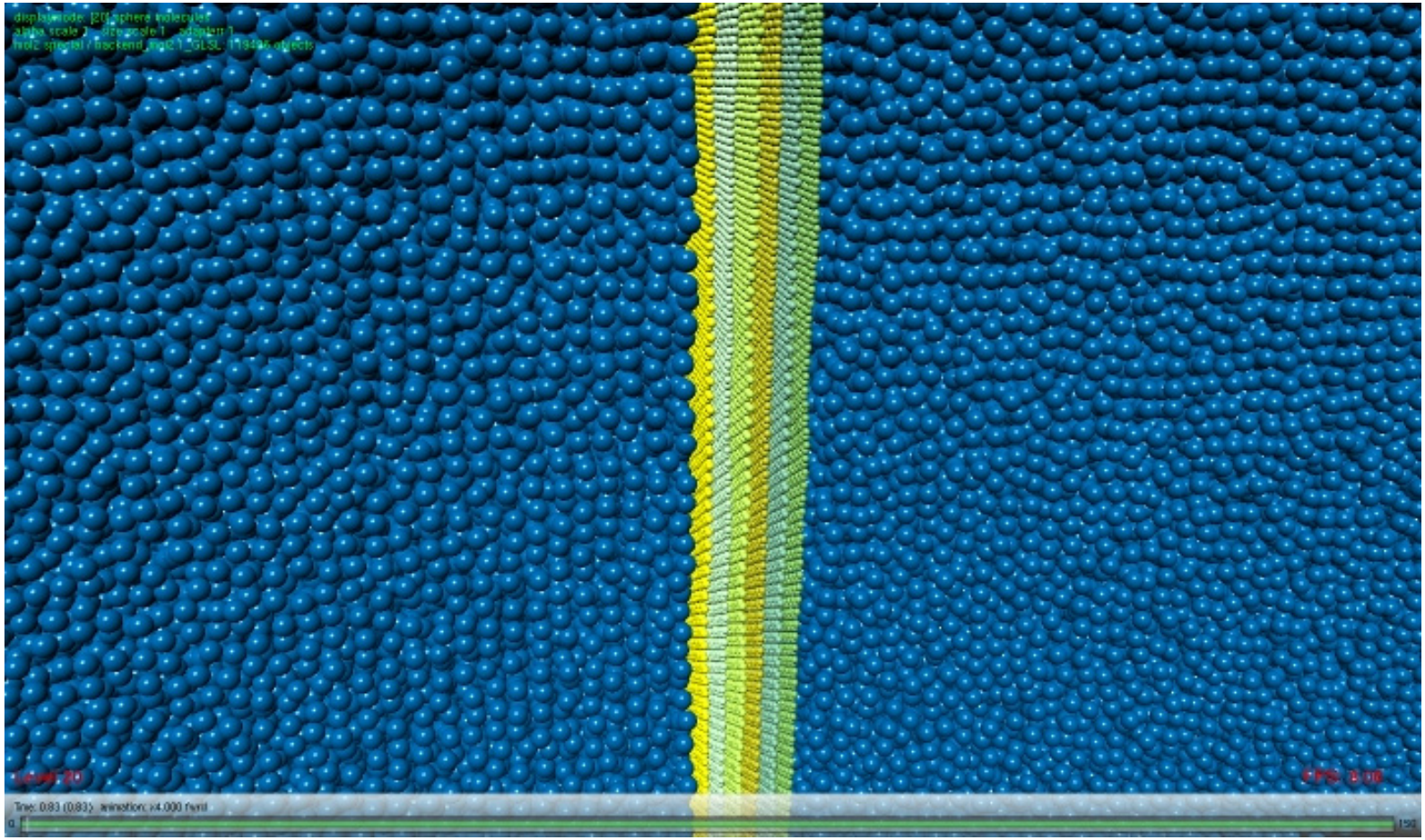

Lennard-Jones energy parameter: $\varepsilon_{FW} = W \cdot \varepsilon$

Lennard-Jones size parameter: $\sigma_{FW} = d \cdot \sigma$

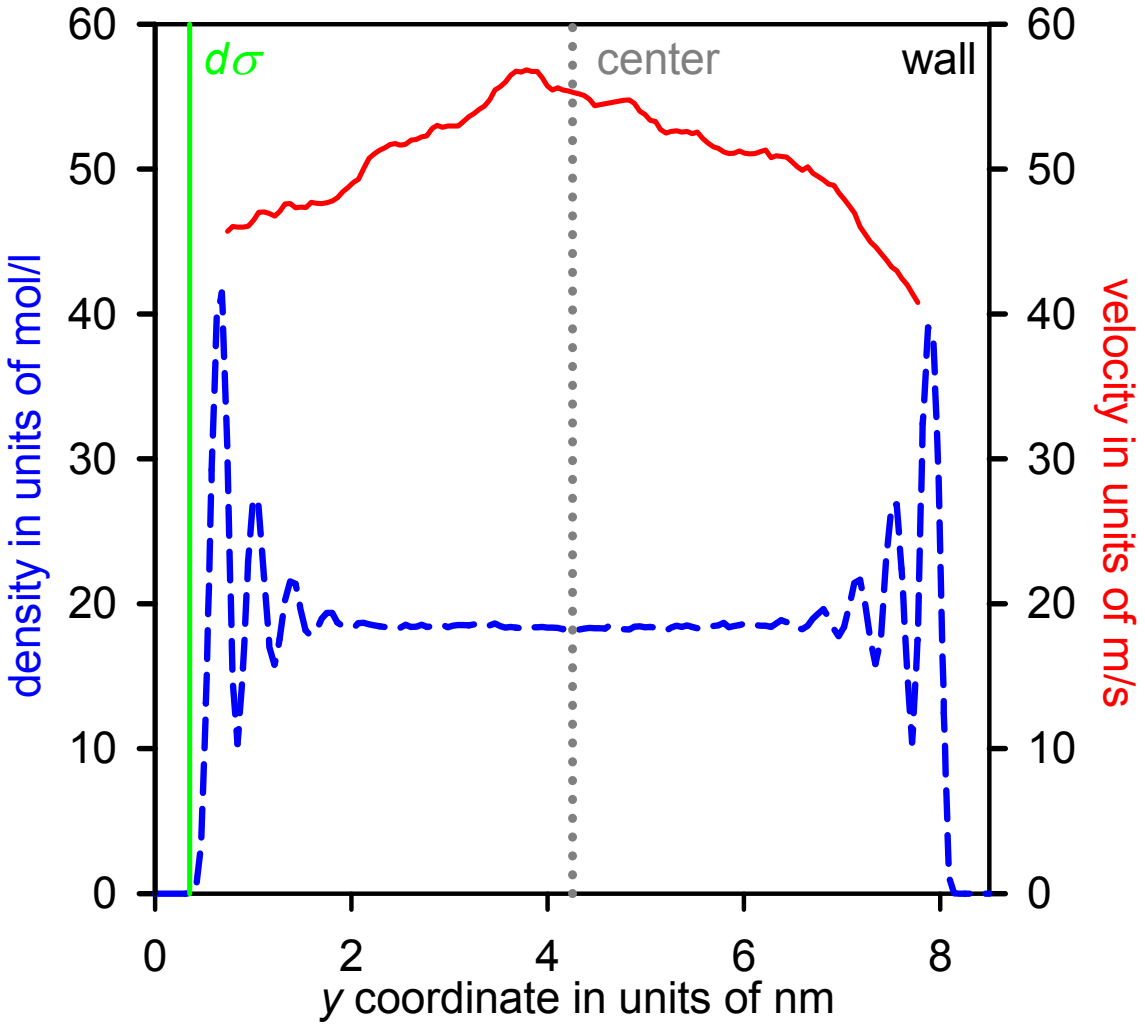
$T = 0.95\ \varepsilon/k$

$\rho = 1.005\ \rho'$

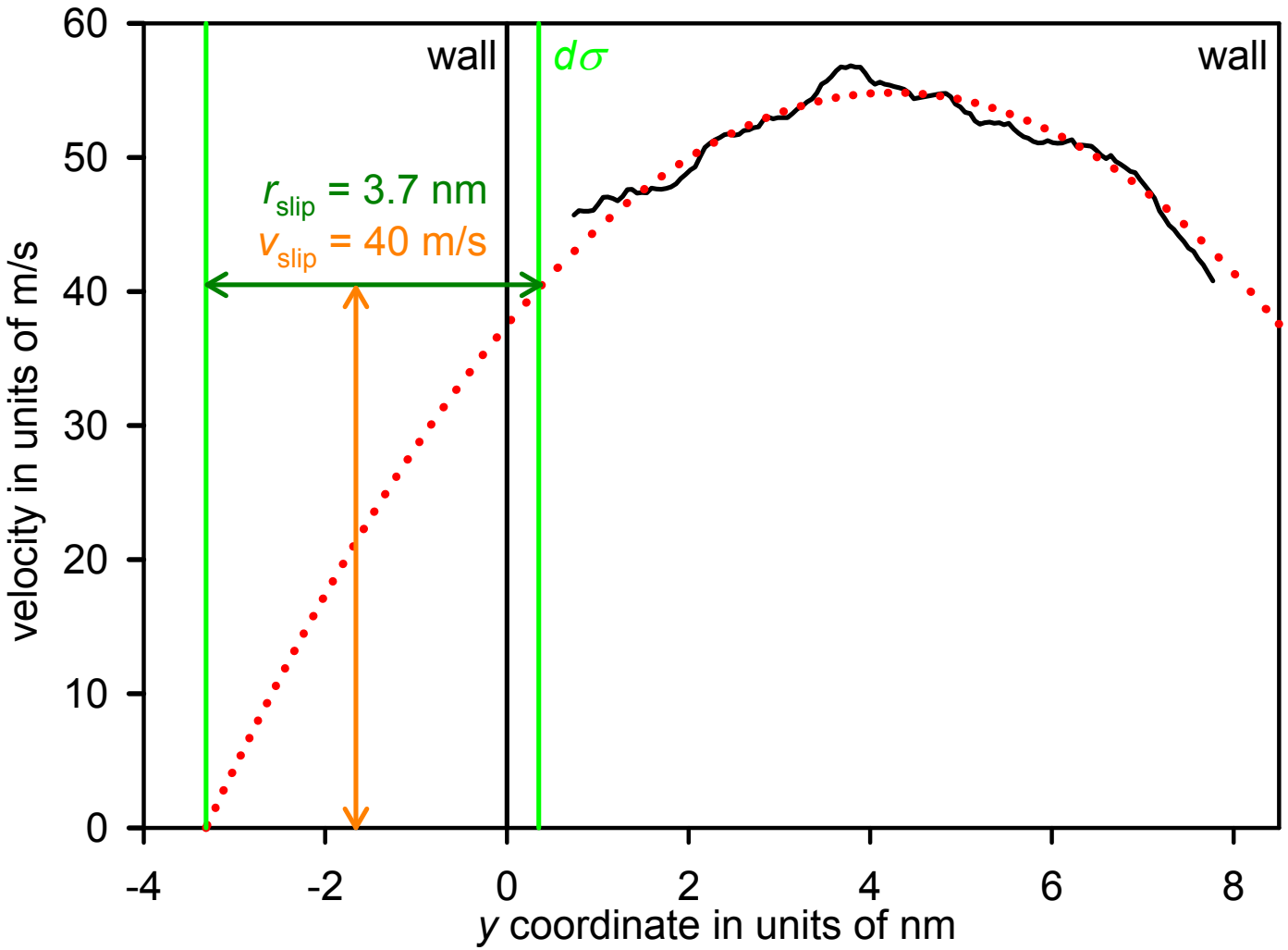
# Poiseuille flow of methane in a graphite channel



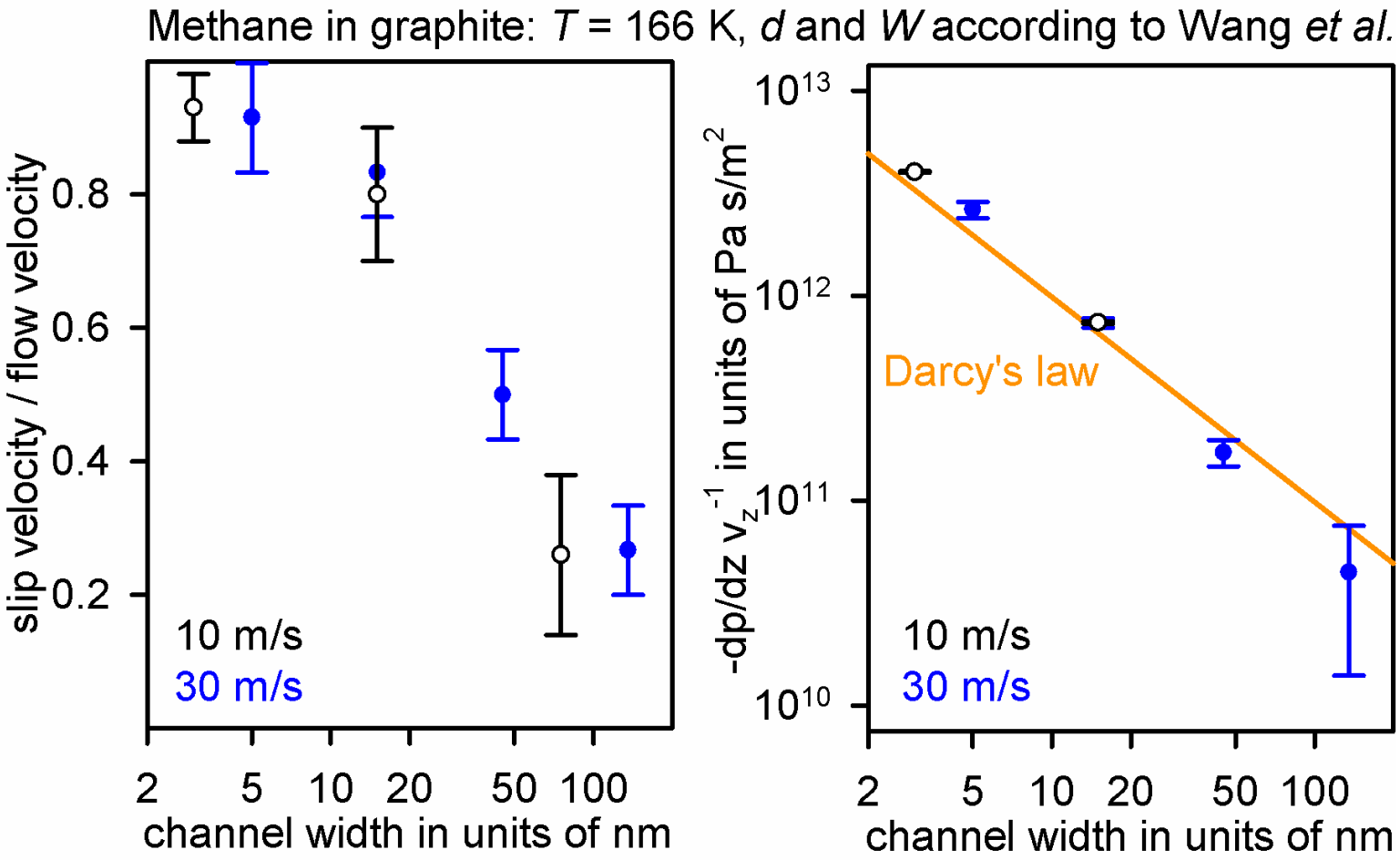
# Fluid velocity profile



# Fluid velocity profile



# Properties of nanoscopic Poiseuille flow



# Conclusion

Molecular simulation …

- … is of increasing relevance for chemical engineering
- … can be applied to nanoscopic flow, heat and mass transfer
- … can analyze systems up to the µm scale as a HPC application

⇒ Fluid flow in nanoscopic channels can be simulated by imposing an additional uniform acceleration on fluid molecules

⇒ Highly accurate effective potentials for many fluids and solids are available, facilitating the simulation of real surface effects