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JÜLICH
FORSCHUNGSZENTRUM

# Particle Based Hydrodynamics

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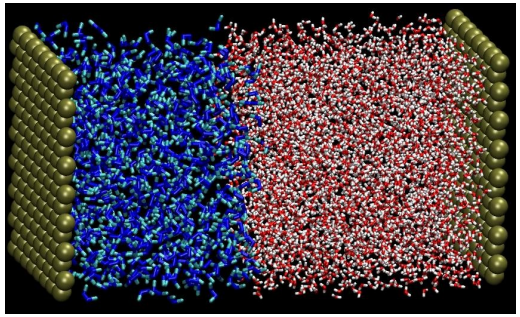
# Simulation Laboratory *Molecular Systems*

## (HPC for Soft Matter and Materials Science)

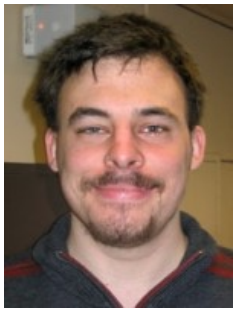
- Research
  - Molecular- / Brownian dynamics
  - Mesoscopic hydrodynamics
  - Ab initio quantum chemistry
  - Long range interactions
  - Parallel algorithms
  - Load balancing
- Activities / Support
  - IBISCO (Univ. Darmstadt)
  - OCCAM (Univ. Salerno)
  - Turbomole
  - Columbus
- Projects
  - ScaFaCoS (BMBF)
  - GASPI (BMBF)
  - 3d-Transport (BMBF)
  - Mont-Blanc (FP7)
  - EESI / EESI-2 (FP7)
  - ESMI (FP7)
- Cooperation
  - Ruhr-University Bochum
  - CECAM
- Teaching
  - University for Applied Sciences Aachen/Jülich



# Simulation Laboratory *Molecular Systems*
## (HPC for Soft Matter and Materials Science)

- Group
  - 3 senior scientists
  - 2 scienific programmer
  - 1 PhD student
  - 3 master students






  - Godehard Sutmann
  - Viorel Chihai
  - Thomas Müller
  - Rene Halver
  - Annika Hagemeier
  - Maya Kletzin
  - Rebecca Swaton
  - Annika Simon

# Simulation Laboratory *Molecular Systems*

(Soft Matter + Quantum Chemistry)

- **Research and Development**

  - Molecular Dynamics, Monte Carlo and stochastic dynamical methods
  - Parallel mesoscopic hydrodynamics (MP2C)
  - Libraries for generic components, e.g. integrators, long range interactions
  - Mathematical methods, e.g. multigrid (wavelets)
  - Load-balancing methods
  - Code development on various architectures (CPU, GPU)
  - Parallel algorithms for specific methods
  - Parallel *ab initio* methods (Turbomole, Columbus)

- **Support in scientific computing**

  - Support for specific problems (methods, algorithms)
  - Provision of parallel programs and single components for simulation and data analysis

- **Administration**

  - Organisation of schools and workshops (CECAM)
  - Third party funding acquisition

# Outline

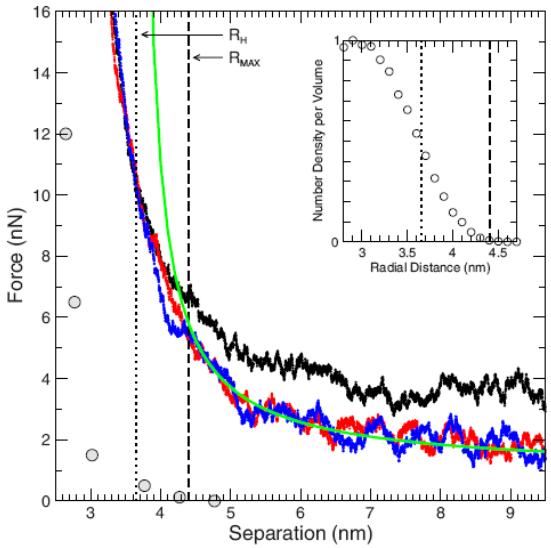
- Introduction
- Multi-Particle Collision Dynamics
- Parallelization
- Some applications

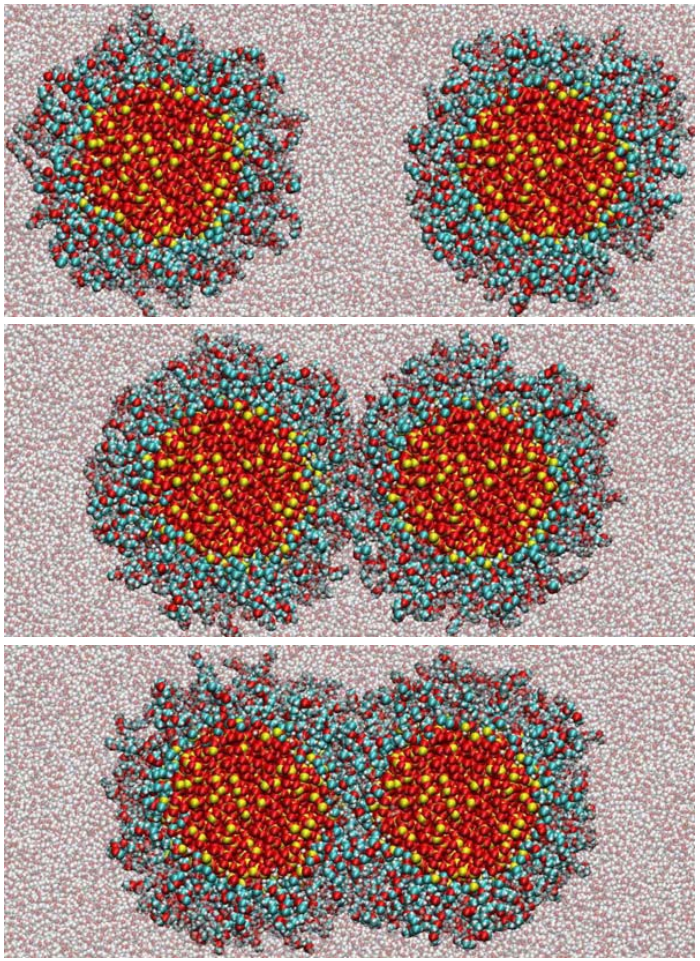
# Acknowledgements

- Gerhard Gompper, Roland Winkler
  Institute for Complex Sysems, FZ Jülich
- Humberto Hijar
  UNAM, Mexico
- Annika Simon, Rene Halver
  Institute for Advanced Simulation, FZ Jülich

# Applications: Interactions of Nanoparticles

Large scale simulation of coated silica nanoparticles
(7 Mio. Atoms, 1 ns ~ 140 h on 1024 procs.



G.Grest et al., PRE 79, 050501 (2009)

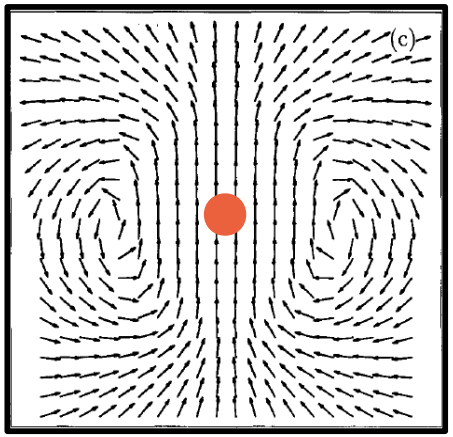
At distances beyond contact, particles behave like Brownian particles, described by Stokes-Einstein in a hydrodynamic medium

Replace explicit waters by effective hydrodynamic media

# Hydrodynamic Interactions

- For small Reynolds numbers (velocities) the NS equations may be linearized

$$\rho\partial_t \mathbf{v} + \nabla p - \eta_{sh}\nabla^2\mathbf{v} = \mathbf{f}$$



- The velocity field is then given by a “response” function to the external perturbation

$$\mathbf{v}(\mathbf{r}) = \int d\mathbf{r}'\, \mathbf{T}(\mathbf{r},\mathbf{r}')\mathbf{f}(\mathbf{r}')$$

- The Green's function is the Oseen tensor (not positive definite)

$$\mathbf{T}^{(O)}(r) = \frac{1}{8\pi\eta_{sh}r}(\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}})$$

long ranged

- Extension for finite size particles (positive definite)

$$\mathbf{T}^{(RP)}(r) = \frac{1}{6\pi\eta_{sh}r}\left(\frac{3}{4}(\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}) + \frac{1}{2}\frac{a^2}{r^2}(\mathbf{1} - 3\hat{\mathbf{r}}\hat{\mathbf{r}})\right)$$

# Hydrodynamic Interactions

- This description is a simplified view and only valid for dilute solutions
- No thermodynamic fluctuations included
- Hydrodynamic interactions are not pairwise additive
- Leads to involved calculations if one wants to do it correctly
- More rigorous calculations would solve Navier-Stokes equations with solvated particles
  - problem of dynamic boundary conditions at particle positions
  - problem of discretisation of compute domain at particle positions
  - limitation to only a few particles
- Approximate treatment within Stokesian Dynamics

# Discrete schemes for hydrodynamics

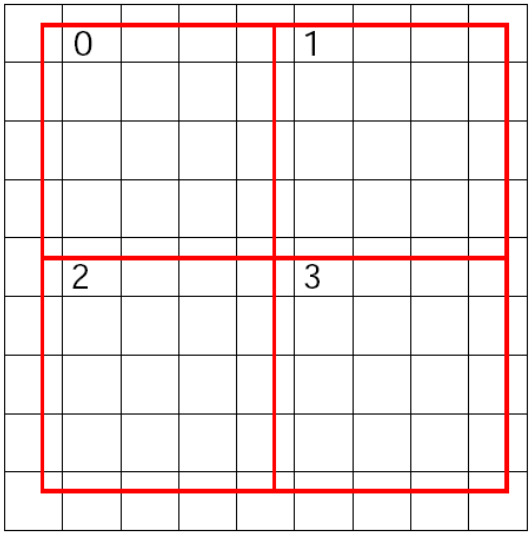
- To facilitate treatment of hydrodynamic interactions, several schemes were developed

  - Lattice-Boltzmann
  - Dissipative Particle Dynamics
  - Smooth Particle Hydrodynamics
  - Direct Simulation Monte Carlo (DSMC)
  - Multi-Particle Collision Dynamics (MPC)
    - Stochastic Rotation Dynamics
    - MPC-variants (Collision rules)
    - thermal fluctuation
    - various boundary conditions

# Multi-Particle Collision Dynamics

- Solvent particles are considered to exchange momentum between solvent and solute particles
  - Momentum exchange occurs after collisions
  - No explicit interactions (no hydrodynamic force field)
  - Microscopic details of solvent collisions are not of interest
  - Therefore modeled by stochastic momentum exchange
- Requirements
  - Conservation of energy
  - conservation of momentum
  - (conservation of angular momentum)

# MPC construction of collision cells

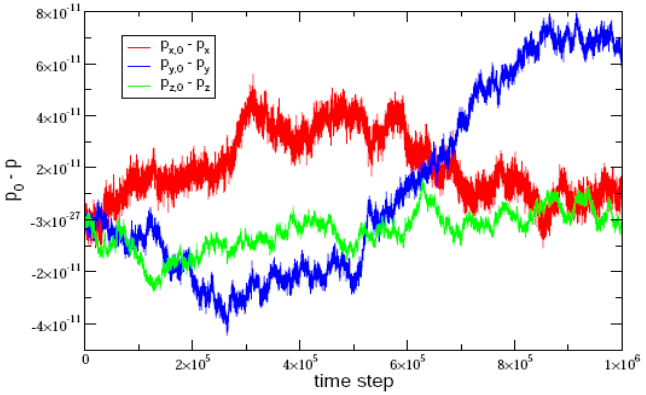



- particles are sorted into collision cells
- to conserve Galilean invariance, cells are shifted by a random offset in every time step

$$\delta L_{c,\alpha} = \xi_\alpha L_{c,\alpha} \qquad \xi_\alpha \mapsto \mathrm{U}[0,1]$$

- Equivalent to shift ALL particles by random offset
  - Shift ALL particles by random offset
  - Sort into FIXED cells
  - Perform collisions
  - Shift back ALL particles

In parallel implementation would induce large Data transfer across processors




$$K' \quad = \quad \frac{1}{2}\sum m_i(\mathbf{v}_{cm} + R\{\delta\mathbf{v}_i\})^2 \quad = \quad K$$

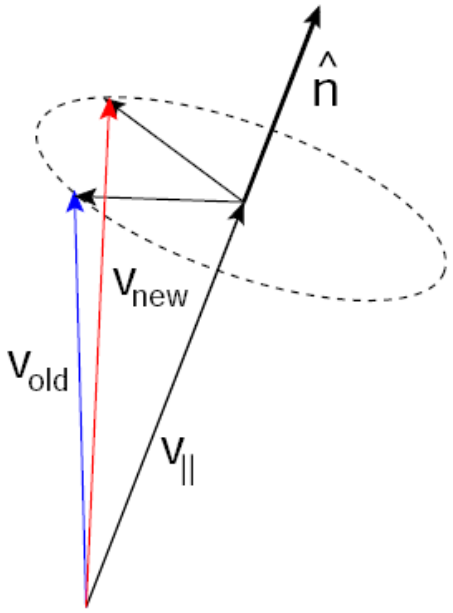
$$\mathbf{P}' = \sum_{i\in\Omega} m_i(\mathbf{v}_{cm} + \delta\mathbf{v}_i) = \sum_{i\in\Omega} m_i(\mathbf{v}_{cm} + R\{\delta\mathbf{v}_i\}) = \mathbf{P}$$

# MPC collision: random rotation

- Perform a random rotation of relative velocities by

$$\tilde{\mathbf{v}}_i \mapsto \tilde{\mathbf{v}}_{i,\parallel} + R(\tilde{\mathbf{v}}_{i,\perp}; \alpha)$$

with $$R(\mathbf{v}; \alpha) = \mathbf{v}\, \cos 2\pi\alpha + (\mathbf{v} \times \hat{\mathbf{n}})\, \sin 2\pi\alpha$$




- for every collision cell calculate a random rotation axis

$$\hat{n}_x = \sqrt{1-(2\xi_1-1)^2}\cos 2\pi\xi_2 \qquad \hat{n}_y = \sqrt{1-(2\xi_1-1)^2}\sin 2\pi\xi_2$$

$$\hat{n}_z = 2\xi_1 - 1$$

- add com velocity of the cell to rotated relative velocities to get new particle velocities *after* a collision

$$\mathbf{v}_i \mapsto \tilde{\mathbf{v}}_i + \mathbf{v}_{c,cm}$$

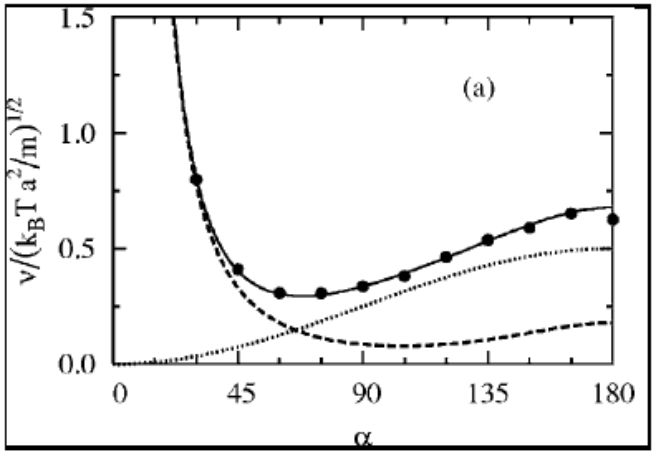
# MPC: theoretical background

- it may be shown that MPC represents a discretised description of linearized Navier-Stokes equations
- theoretical expressions for transport coefficients
  - viscosity of the fluid $\eta = \eta_{kin} + \eta_{col}$

$$\eta_{coll} = (\gamma - 1 + e^{-\gamma}) \frac{m\,[1 - \cos\alpha]}{12 a \delta t}$$

$$\eta_{kin} = \rho k_B T \delta t \left( \frac{1}{1-w} - \frac{1}{2} \right)$$

$$w = 1 - \left( \frac{\gamma - 1 + e^{-\gamma}}{5\gamma} \right) [4 - 2\cos\alpha - 2\cos 2\alpha]$$




| | |
|---|---|
| $\gamma$ | numb. part./cell |
| $m$ | particle mass |
| $\alpha$ | rotation angle |
| $a$ | coll. cell size |
| $\delta t$ | time step |

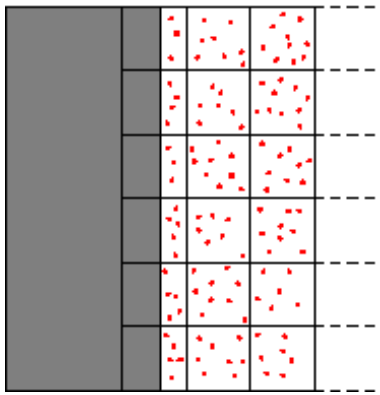
A.Malevanets and R.Kapral, J.Chem.Phys. **110**, 8605-8613 (1999)

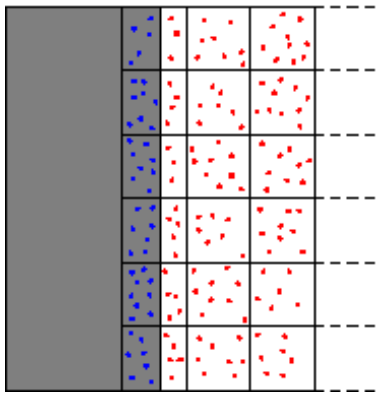
# MPC: boundary conditions

- Boundary conditions for flow problems
  ( often surfaces with no-slip), e.g.
  - shear conditions between plates
  - Poiseuille flow
  - embedded obstacles

- overlapping cells might show wrong statistics / dynamics
  - e.g. one particle would have no collision
  - com never on the surface

- introduce virtual particles inside wall
  - takes into account momentum transfer to the wall



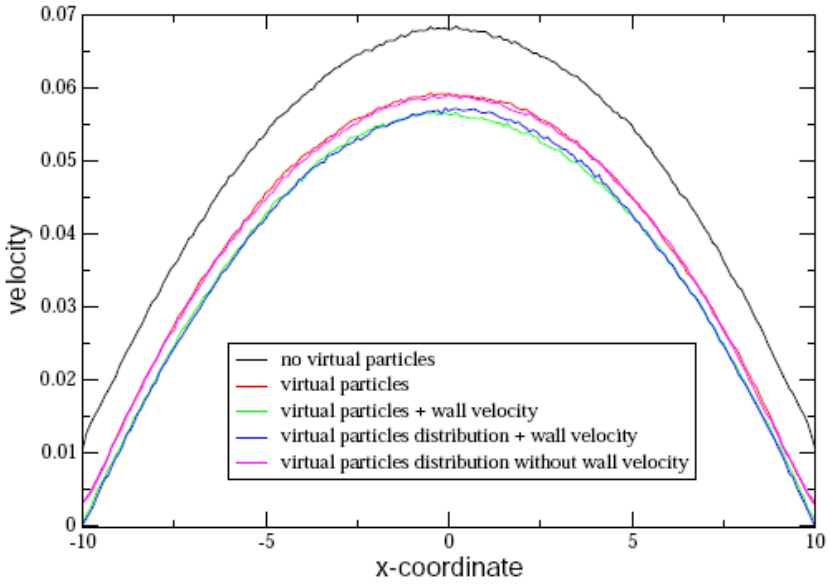


$$v_\xi = \sqrt{n_{virt}\frac{k_B T}{m}}$$

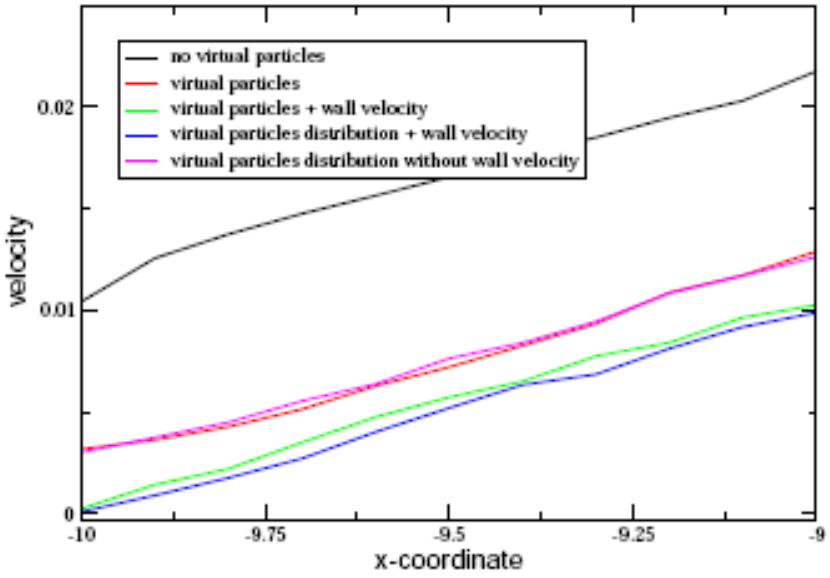
# MPC: boundary conditions

- Example Poiseuille flow
  - boundary conditions: no-slip

Velocity profile




Velocity close to the surface



# MPC: boundary conditions

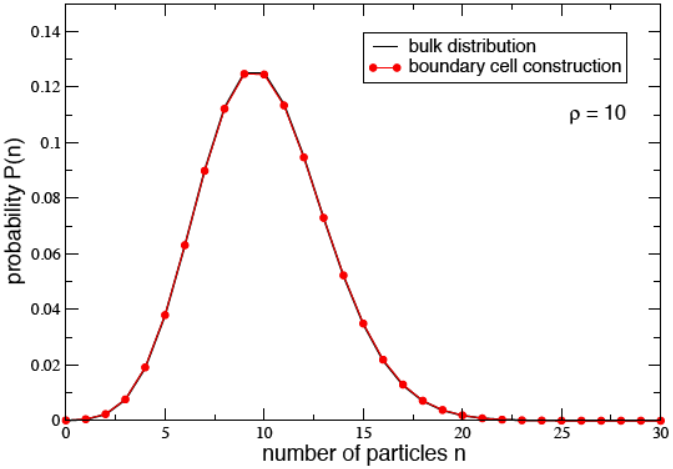
- Statistics for particle distribution
  - particles are Poisson distributed in cells with given average number according to density

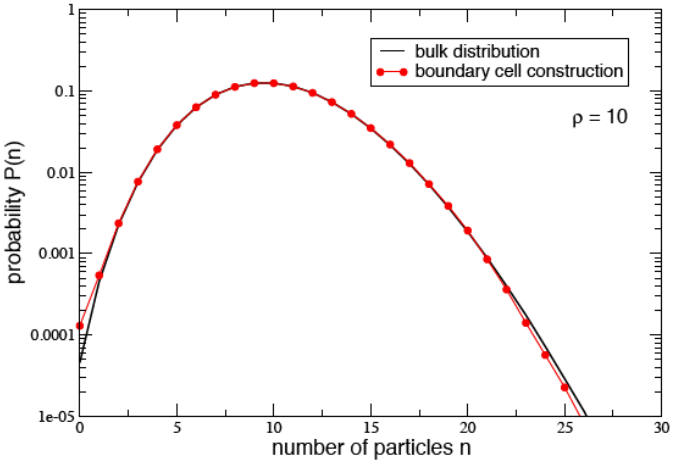
$$p_{\langle x \rangle_{k\delta x}}(m) = \frac{\langle n \rangle_{k\delta x}^{m}}{m!} e^{-\langle n \rangle_{k\delta x}}$$

$$\mu = \mu_1 + \mu_2$$

$$\sigma^2 = \sigma_1^2 + \sigma_2^2$$

- Fill overlapping volume of cells with proper no. of virtual particles to get correct density fluctuations
  - consider real partial cell as realization of random draw
  - add virtual particles according to average no. in overlap volume



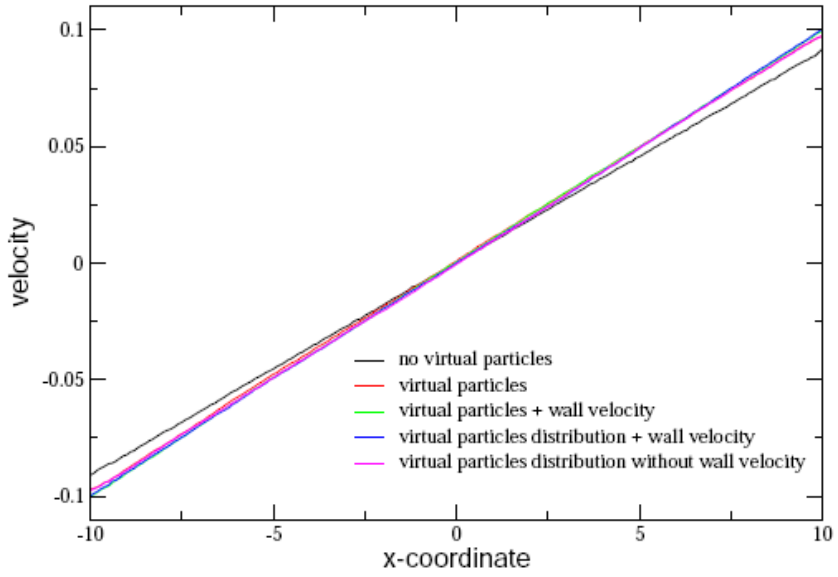
# MPC: boundary conditions

- Example shear flow between plates
  - boundary conditions: no-slip
    - mean velocity of virtual particles in overlapping cell

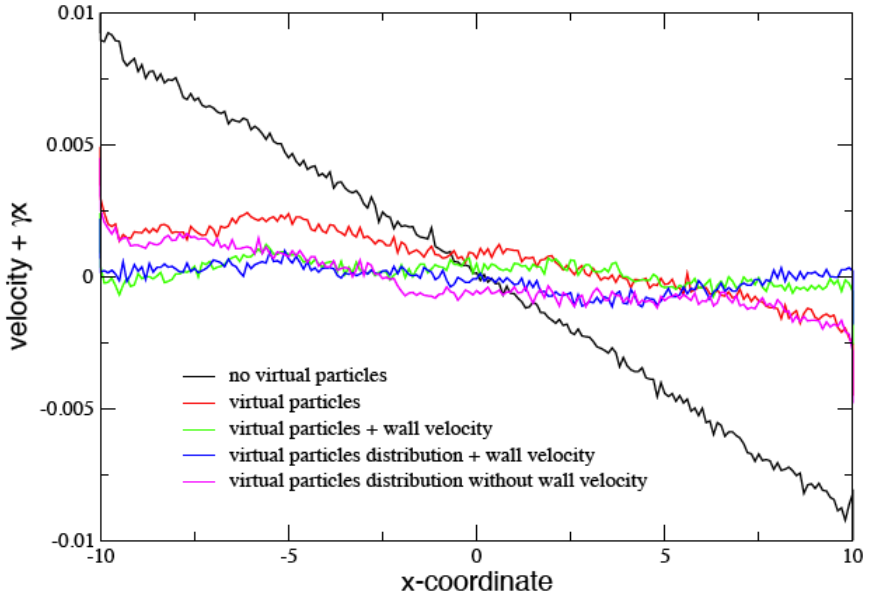
$$\langle v \rangle = \int_{x_{wall}}^{x_{wall}+h-\delta x} dx p(x) v(x) \qquad v = \dot{\gamma} x$$

$$\langle v \rangle = \frac{1}{2} \frac{1}{h-\delta x} \dot{\gamma} \left( (x_{wall} + h - \delta x)^2 - x_{wall}^2 \right)$$

Velocity profile



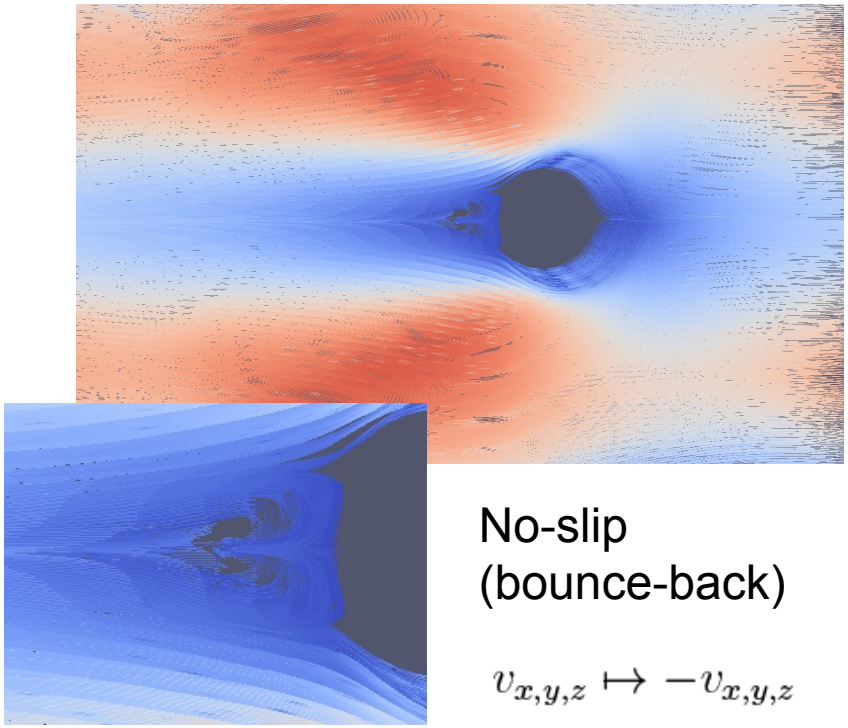

Excess Velocity close to the surface



# Flow around cylinder – boundary conditions

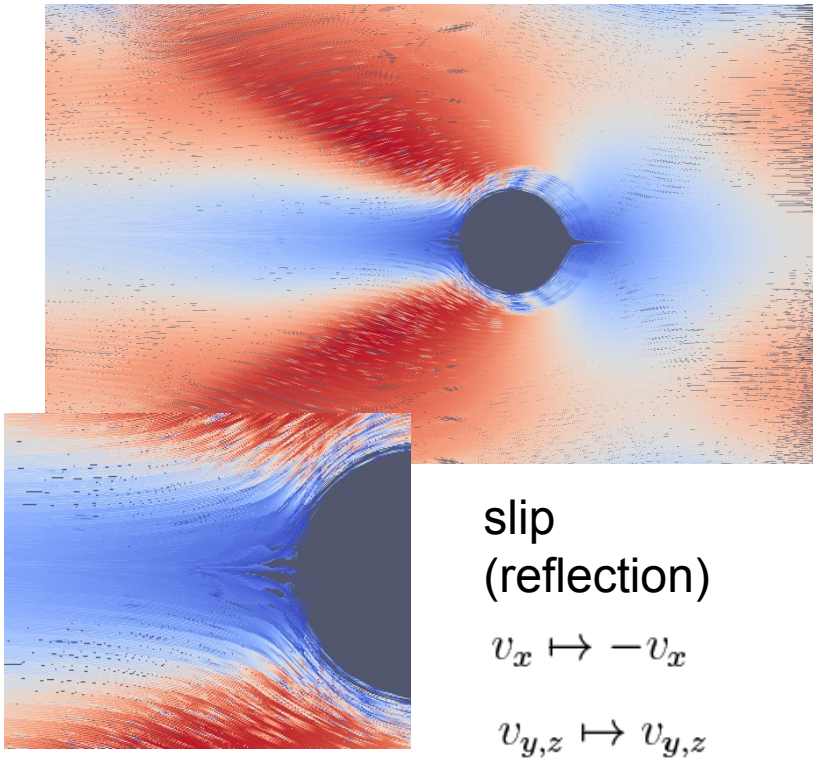
- Influence on flow profile
  - Slip boundary conditions (reflection)
  - No-slip boundary conditions (bounce back)

Re ~ 10



No-slip
(bounce-back)

$$v_{x,y,z} \mapsto -v_{x,y,z}$$



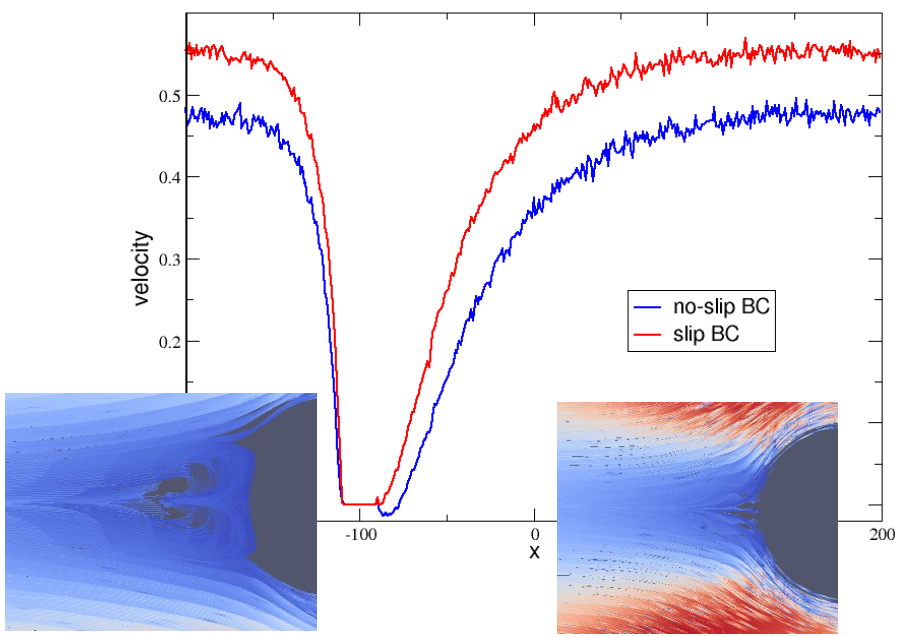
slip
(reflection)

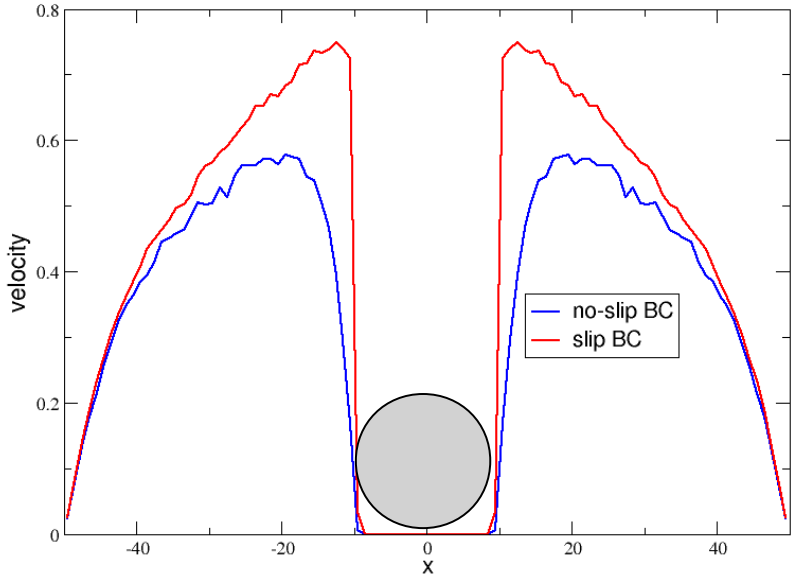
$$v_x \mapsto -v_x$$

$$v_{y,z} \mapsto v_{y,z}$$

# Flow around cylinder – boundary conditions

- Influence on flow profile
  - Slip boundary conditions (reflection)
  - No-slip boundary conditions (bounce back)



# MPC: thermostating the fluid

- MPC is energy and momentum conserving
- in external fields, energy is gained and one has to transfer the energy to a reservoir
- thermostating takes into account a proper temperature distribution
- however, there are differences in local and global temperature corrections
- statistical properties (thermal fluctuations) might be influenced to produce fictitious results

# MPC: thermostating the fluid

- Velocity distribution

$$P(\{\boldsymbol{v}\}) = \left(\frac{m}{2\pi k_B T}\right)^{3N_c/2} \exp\left(-\frac{m}{2k_B T}\sum_{i=1}^{N_c}\boldsymbol{v}_i^2\right)$$

- Kinetic energy distribution (+ momentum conservation)

$$P(E_k) = \frac{1}{Z}\int \delta\left(E_k - \frac{m}{2}\sum_{i=1}^{N_c}\Delta\boldsymbol{v}_i^2\right)\delta\left(\sum_{i=1}^{N_c}\Delta\boldsymbol{v}_i\right)\exp\left(-\frac{m}{2k_B T}\sum_{i=1}^{N_c}\Delta\boldsymbol{v}_i^2\right)d^{N_c}\Delta\boldsymbol{v}$$

$$P(E_k) = \frac{1}{E_k\Gamma(f/2)}\left(\frac{E_k}{k_B T}\right)^{f/2}\exp\left(-\frac{E_k}{k_B T}\right) \qquad f = 3(N_c - 1)$$

- Correction of velocities

$$\Delta\boldsymbol{v}_i' = \alpha\Delta\boldsymbol{v}_i \qquad \alpha = \left(\frac{2E_k'}{m\sum_{i=1}^{N_c}\Delta\boldsymbol{v}_i^2}\right)^{1/2}$$

$E_k'$ from $P(E_k)$ distribution

- Probability for a velocity change to conserve statistics

$$P(\Delta\boldsymbol{v}, N_c) = \left(\frac{m}{2\pi k_B T(1 - 1/N_c)}\right)^{3/2}\exp\left(-\frac{m}{2k_B T(1 - 1/N_c)}\Delta\boldsymbol{v}^2\right)$$

$$P(\Delta\boldsymbol{v}) = \sum_{N_c=2}^{\infty} e^{-\langle N_c\rangle}\frac{\langle N_c\rangle^{N_c}}{N_c!}P(\Delta\boldsymbol{v}, N_c)/\left(1 - (\langle N_c\rangle + 1)e^{-\langle N_c\rangle}\right)$$

# Random Numbers for the Thermostat

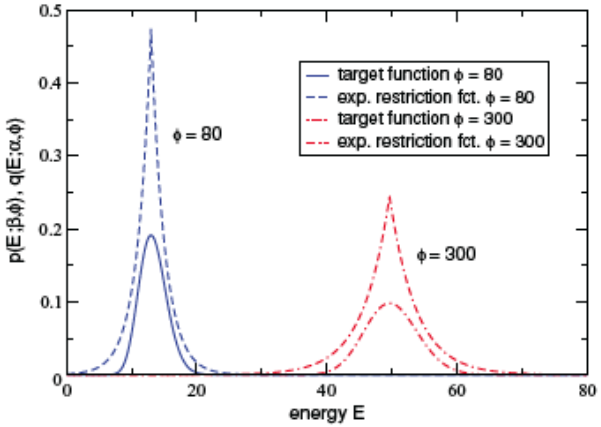
- Acceptance-rejection method

$$c\,g(x) > p(x), \forall x \in \mathbb{R}$$

$$g(E) = \alpha \exp(-\alpha\,|E - E_{\mathrm{m}}|)$$

$$E_{\mathrm{m}} = (\phi/2 - 1)/\beta \qquad \alpha = \beta\sqrt{2/\phi}$$

$$\xi_2 < p(\xi_1)/cg(\xi_1)$$

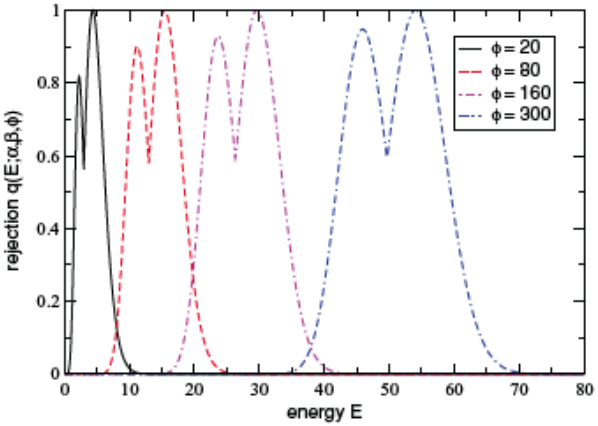



- Rejection function

$$q_0(E;\alpha,\beta,\phi) = \frac{1}{\alpha\Gamma(\phi/2)}\beta^{\phi/2}E^{\phi/2-1}e^{-\beta E}\,e^{|E-(\phi/2-1)/\beta|\alpha}$$

normalized (to maximum)

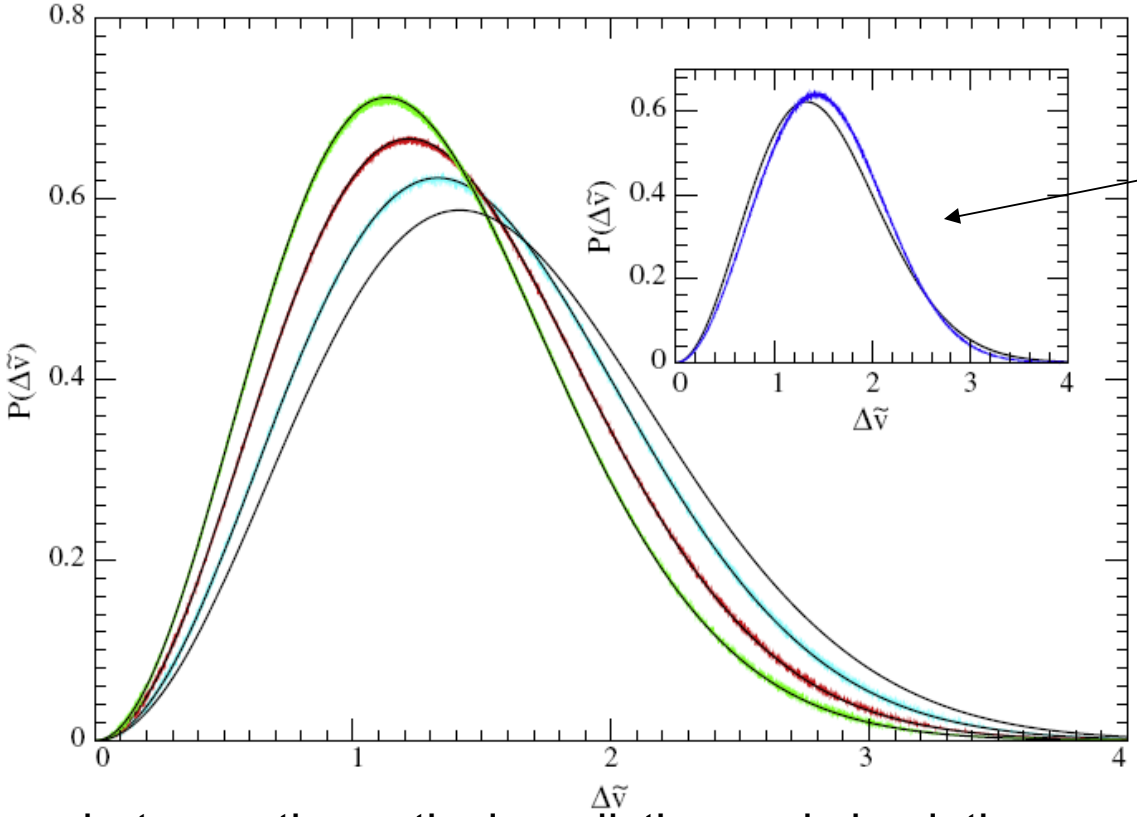
$$q(E;\alpha^*,\beta,\phi) = \frac{E^{\phi/2-1}e^{-\beta E}\,e^{|\beta E-(\phi/2-1)|\alpha^*}}{\left[\frac{\phi/2-1}{\beta(1-\alpha^*)}\right]^{\phi/2-1}e^{(\phi/2-1)(1+\alpha^*)}}$$




$\xi_2 \in [0,1]$

# MPC: thermostating the fluid

- Example: Shear flow




Comparison with strict thermostat

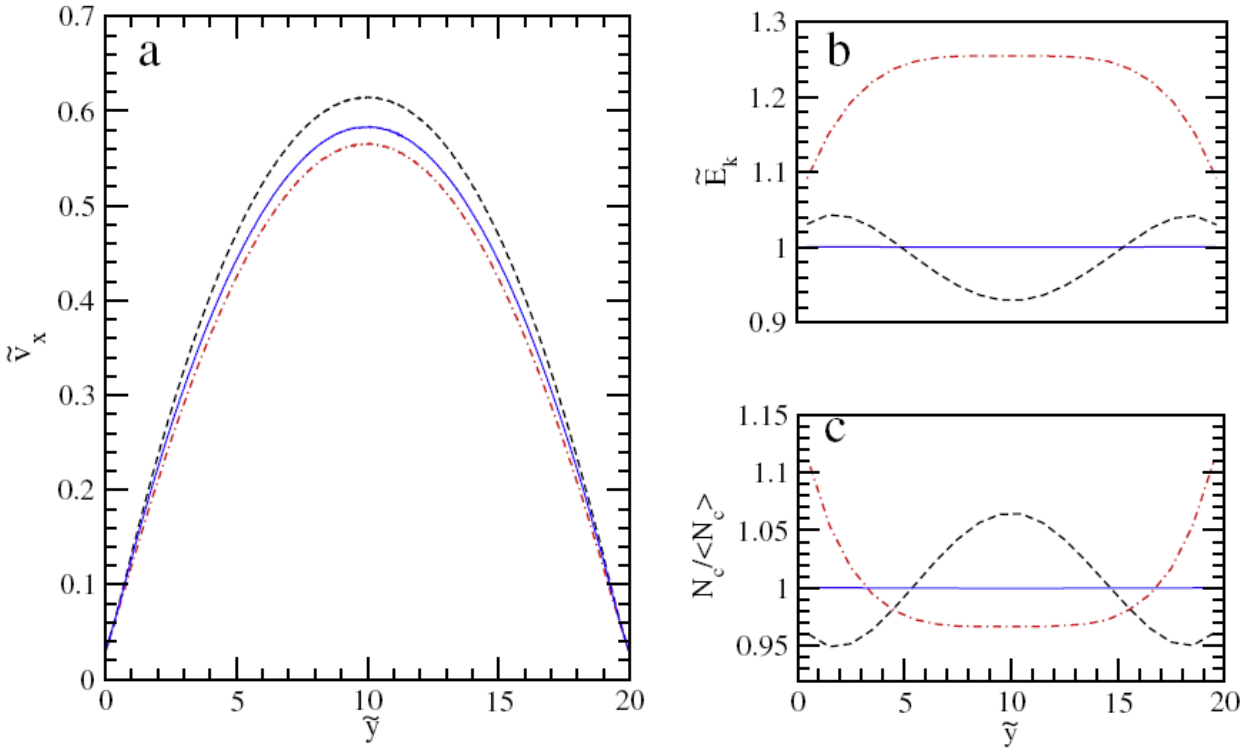
Comparison between theoretical prediction and simulation result for $N_c$ = 3, 5, 10, ∞

# MPC: thermostating the fluid

- Example: Poiseuille flow

$$\hat{v}_{ix}(t+\Delta t) = v_{ix}(t) + g\Delta t \qquad r_{ix}(t+\Delta t) = r_{ix}(t) + v_{ix}(t)\Delta t + \frac{1}{2}g\Delta t^2$$

Velocity profile $$v_x(y) = \frac{4v_{max}(H-y)y}{H^2} \qquad v_{max} = \frac{mN_c g H^2}{8\eta}$$

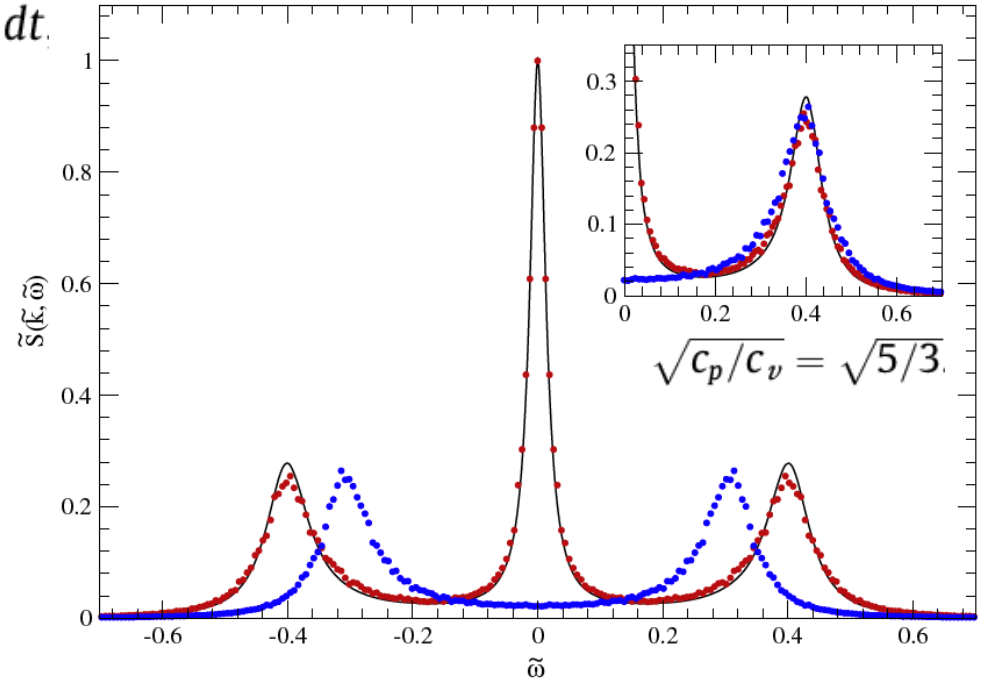


# Dynamic Structure Factor

- MPC with constant energy vs constant temperature

$$S(\boldsymbol{k},\omega) = \int \langle \rho(\boldsymbol{k},t)\rho(-\boldsymbol{k},0)\rangle e^{-i\omega t}\, dt$$

$$\rho(\boldsymbol{k},t) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\boldsymbol{k}\boldsymbol{r}_j(t)}$$

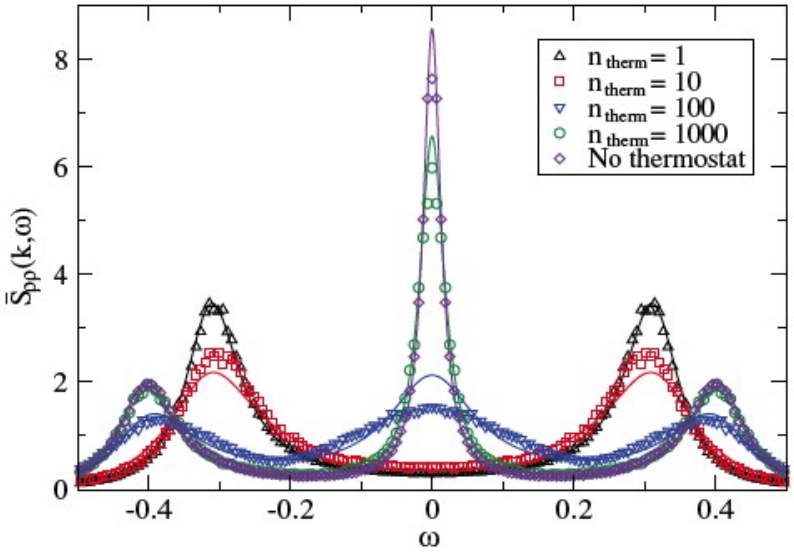


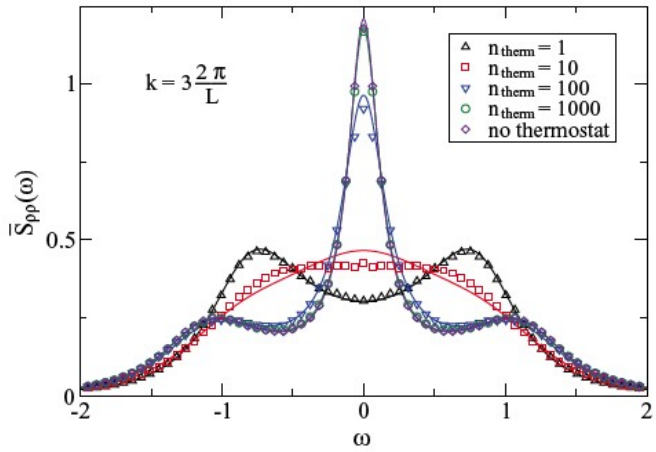

$$S(\boldsymbol{k},\omega) = k_B T N_c \left\{ \left(\frac{c_v}{c_p}\right) \frac{c^2 k^4 \Gamma}{(\omega^2 - c^2k^2)^2 + (\omega k^2 \Gamma)^2} + \left(1 - \frac{c_v}{c_p}\right) \frac{D_T k^2}{\omega^2 + (k^2 D_T)^2} - \left(1 - \frac{c_v}{c_p}\right) \frac{(\omega^2 - c^2k^2) D_T k^2}{(\omega^2 - c^2k^2)^2 + (\omega k^2 \Gamma)^2} \right\}$$

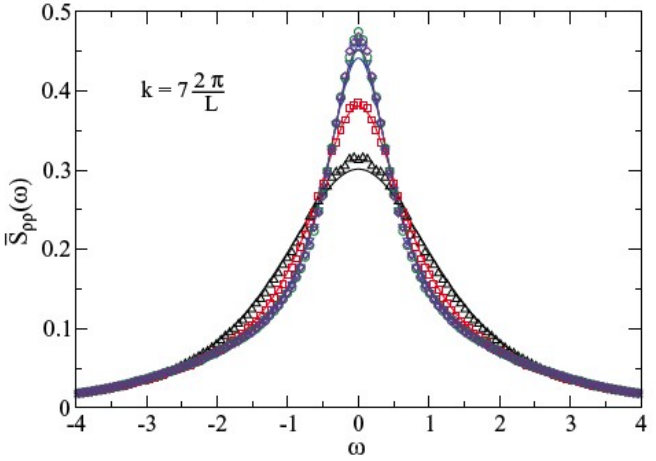
# Dynamic Structure Factor

- MPC partially thermostated

$$S_{\rho\rho}(\vec{k},\omega) = 2(2\pi)^3 \delta_{\vec{k}}(0) k_B T_0 \rho_0 D_l k^4 \left\{ \frac{\bar{\alpha}}{\omega^2 + \omega_T^2} + \bar{\beta} \left[ \frac{1}{(\omega+\omega_s)^2 + \omega_\Gamma^2} + \frac{1}{(\omega-\omega_s)^2 + \omega_\Gamma^2} \right] + \bar{\gamma} \left[ \frac{\omega+\omega_s}{(\omega+\omega_s)^2 + \omega_\Gamma^2} - \frac{\omega-\omega_s}{(\omega-\omega_s)^2 + \omega_\Gamma^2} \right] \right\}$$



# Solute/Solvent interactions: coupling to MD

- Every n MD steps sort solutes together with solvent particles into collision cells
- Calculate common com-velocity

$$\mathbf{v}_{c,cm} = \frac{1}{M_C^{(A)} + M_C^{(B)}} \left( \sum_{a \in C}^{N_A} m_a \mathbf{v}_a + \sum_{b \in C}^{N_B} m_b \mathbf{v}_b \right)$$

$$\tilde{\mathbf{v}}_i = \mathbf{v}_i - \mathbf{v}_{c,cm} \qquad i \in \{A, B\}$$

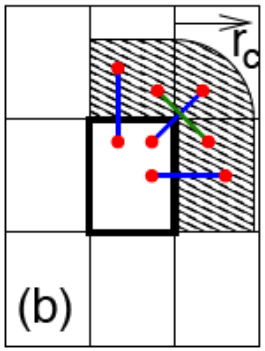
  and perform a rotation in velocity space for both solvent and solute particles around the same random axis

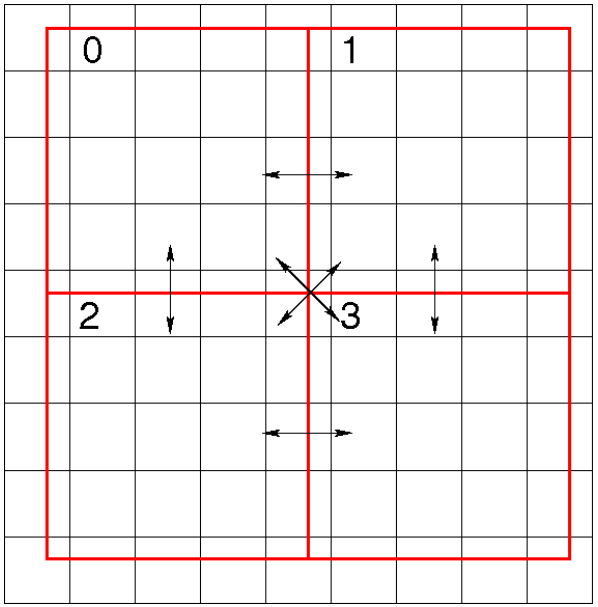
- Results in a stochastic momentum change of the solutes while conserving the overall momentum and kinetic energy in the system
- Inclusion of hydrodynamic modes into solute dynamics

# Domain Decomposition

MD and MPC methods are local – no long range interactions (not yet)

- Every processor is responsible for a certain region
  Domain Decomposition
- In 3 dimensions every domain has 26 neighbors (if decomposition is not time dependent – load balanced)
- Communication parts
  - MPC
    - *Collision cell properties*
    - *Import/Export of particles due to diffusion*



# Hardware

- Implementation into MP2C (not designed for special hardware platform)
- Running with MPI on several machines (hybrid in progress)
- Target platforms for present benchmark:

## JUROPA

2208 / 1080 compute nodes
2 PEs (Intel Nehalem quad core)
17664 / 8640 cores total
207 / 101 Tflop/s peak,

79 TByte main memory,
**24 GByte per node**

## JUGENE

73720 compute nodes
294912 compute cores
1 PetaFlop / Peak
825.5 TeraFlop / Linpack

147 Tbyte main memory
**2 GByte per node**

## JUQUEEN

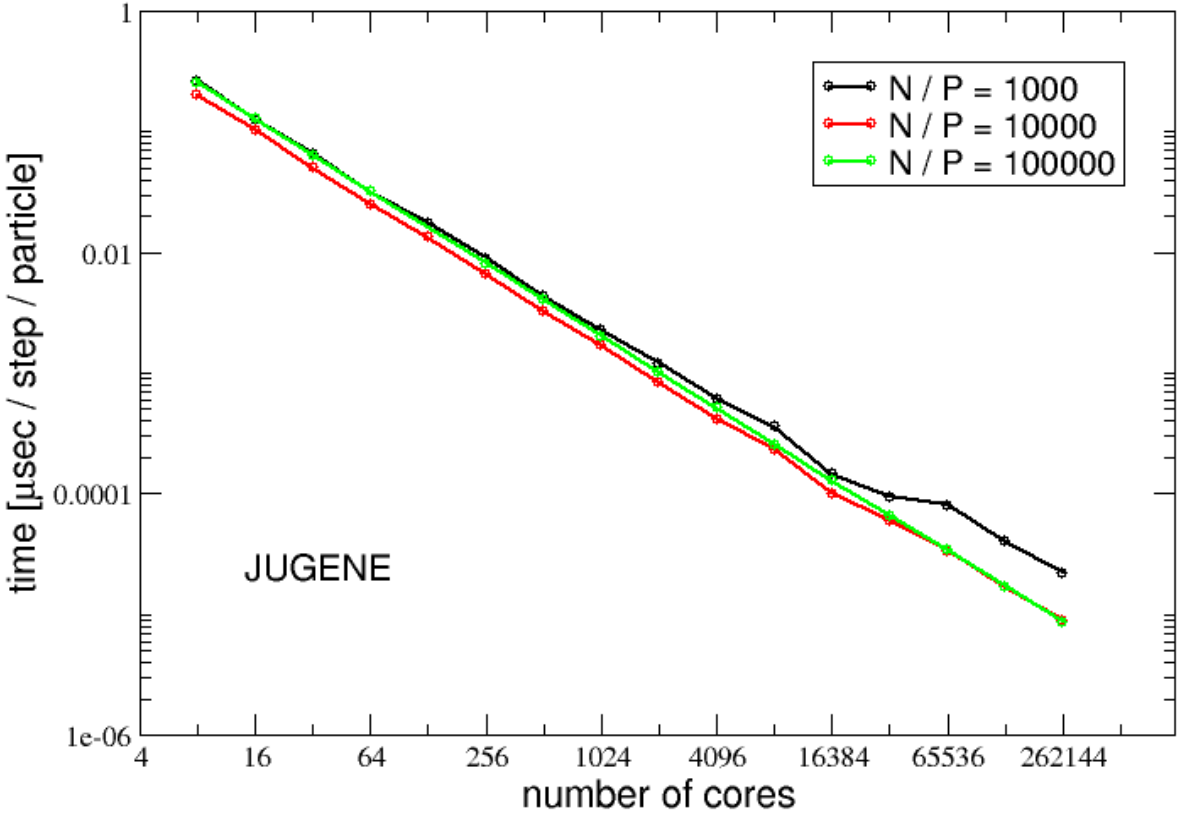
28672 compute nodes
458752 compute cores
5.9 PetaFlop / Peak
4.141 PetaFlop / Linpack

448 Tbyte main memory
**16 GByte per node**

No. 5 world  No. 1 Europe
(Nov. 2012)

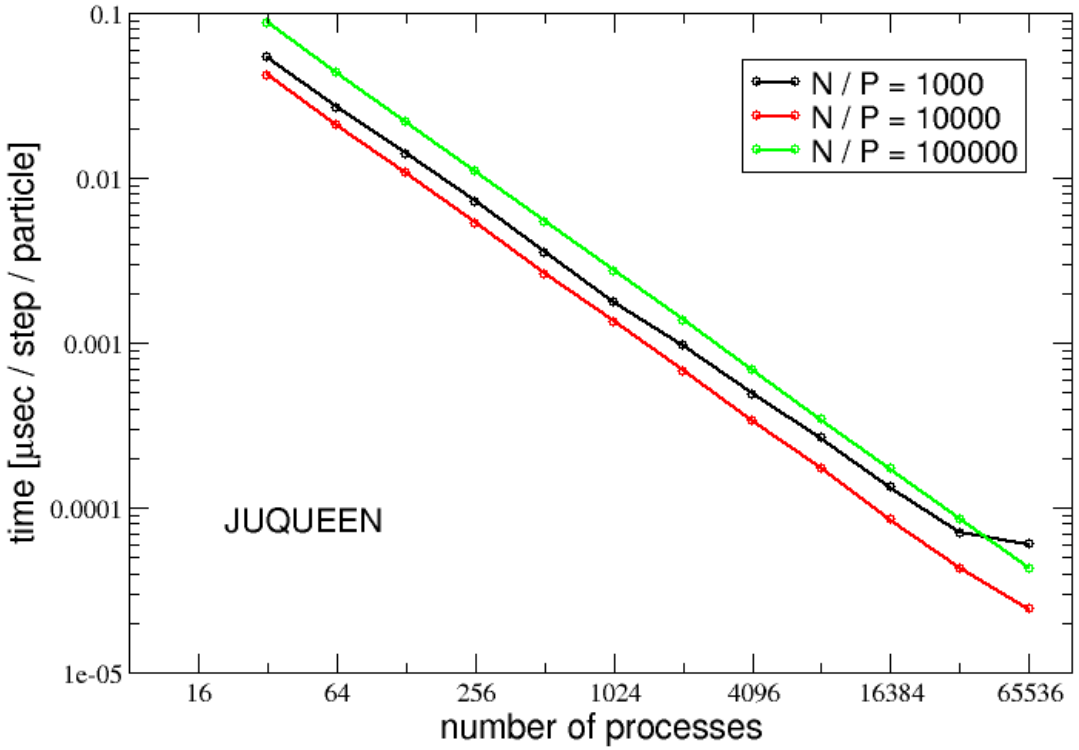
# MPC: Weak scaling BG/P

- Keep number of particles/processor constant



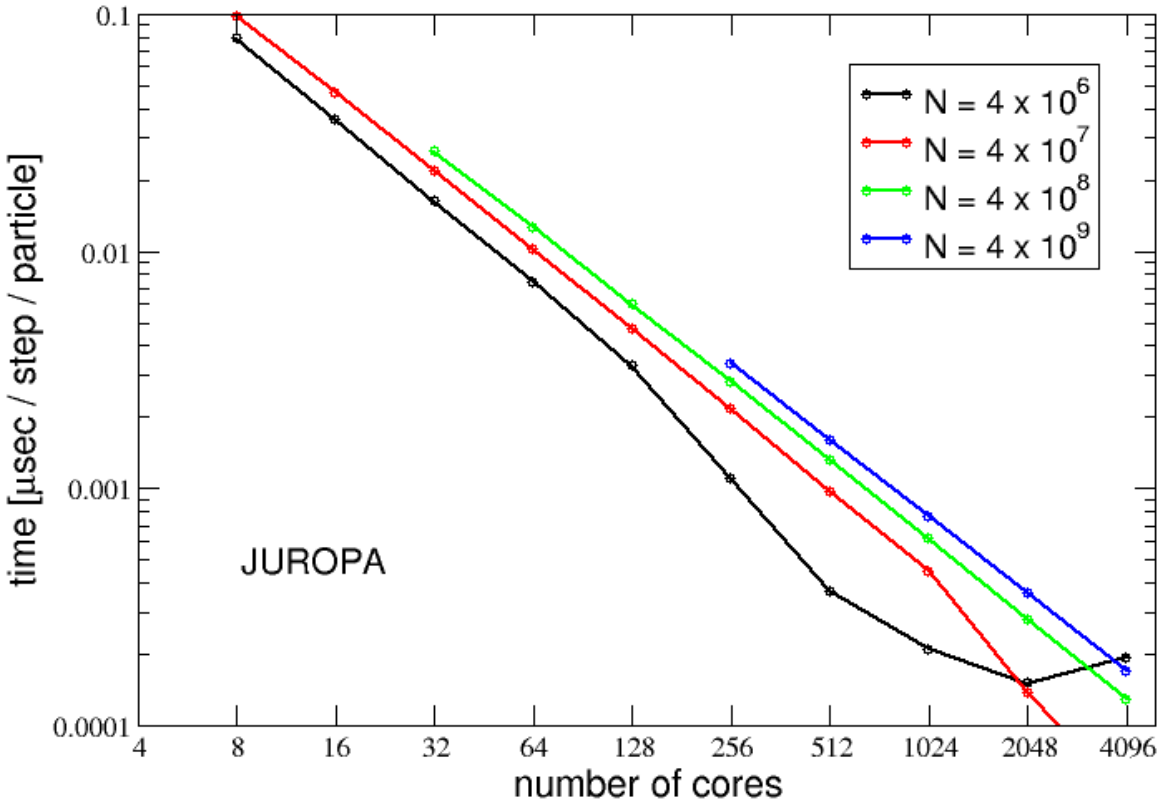
# MPC: Weak scaling BQ/Q

- Keep number of particles/processor constant



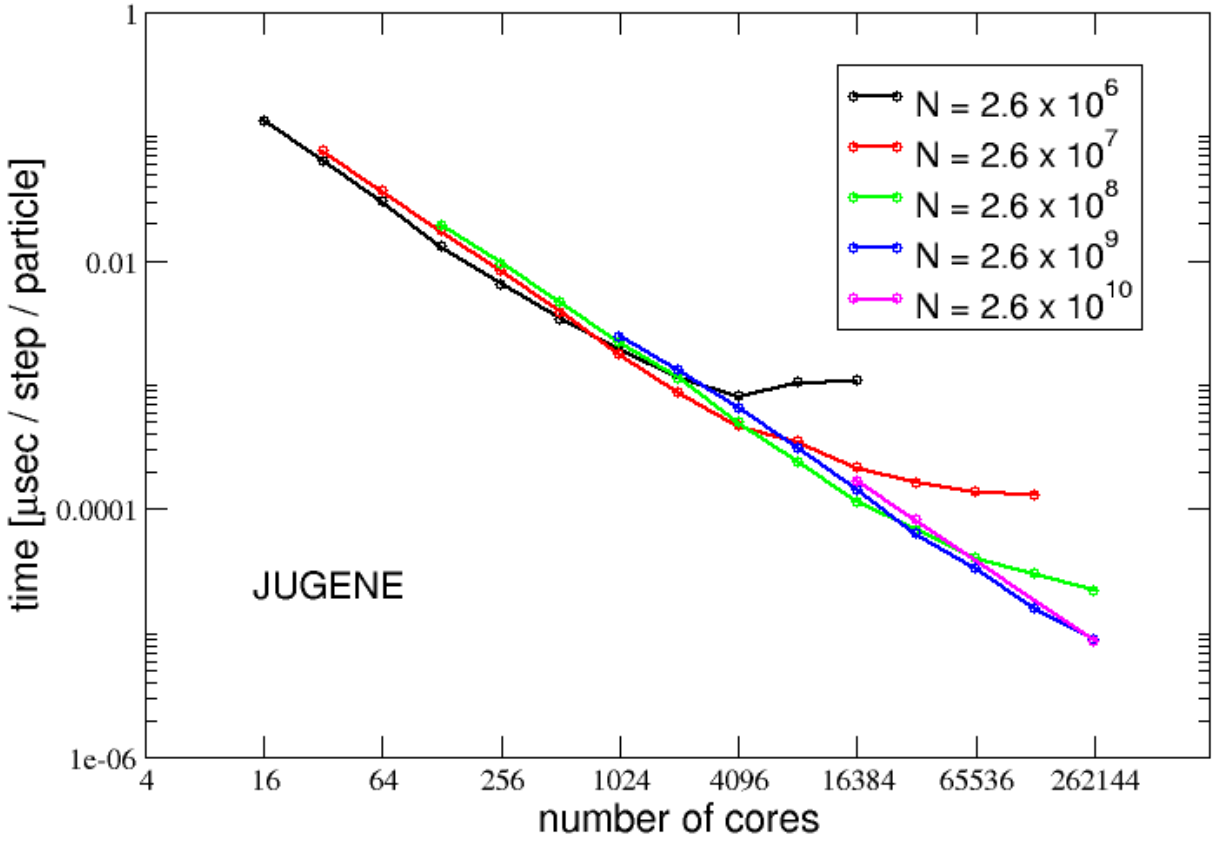
# Strong scaling on JUROPA

- Keep total problem size constant



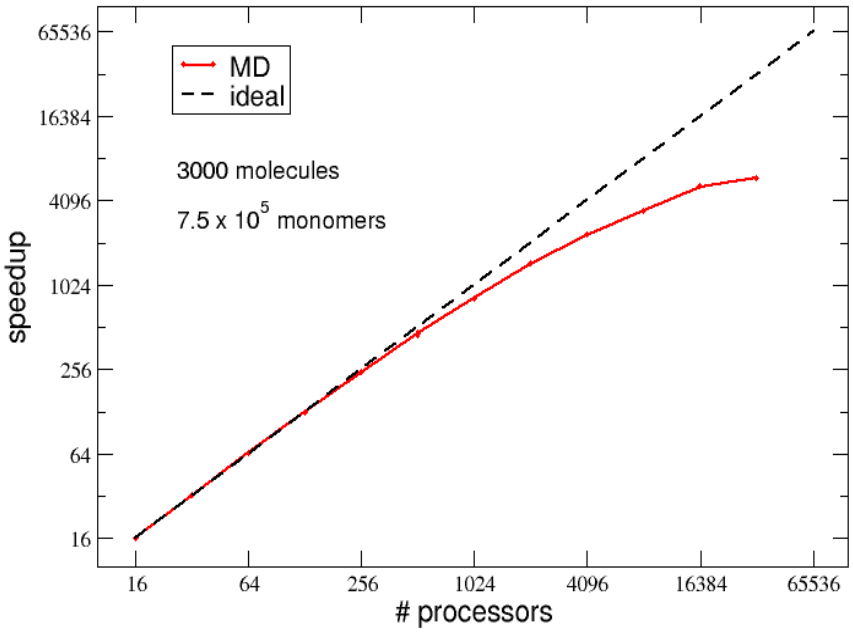
# Strong scaling JUGENE

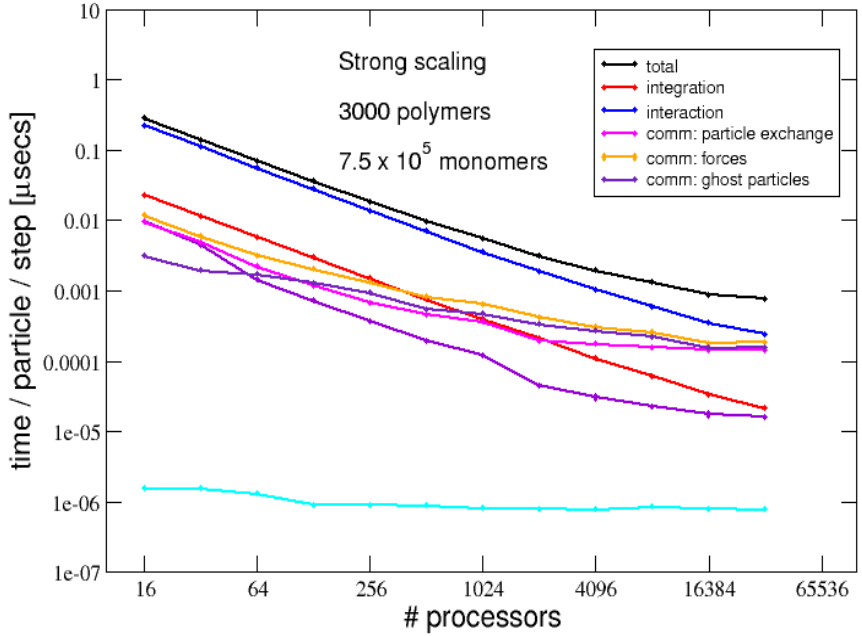
- Keep total problem size constant



# MD: Strong scaling

- Keep total number of particles constant
- Benchmark system: 3000 Polymer chains with 250 monomers

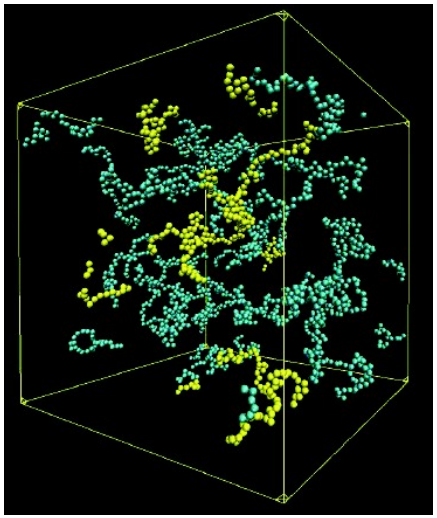


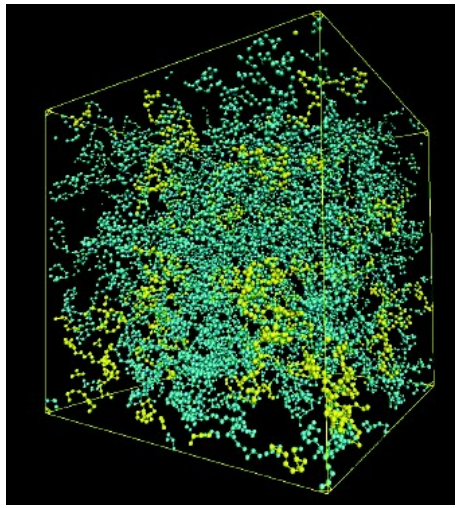
# Expl: Semi-diluted Polymer solutions under Shear

- Problem with polymers is the increasing relaxation time with number of monomers ($O(N^2)$)
- Simplifications through coarse grain potentials and coarse grain solvent
- Interesting phenomena, like shear thinning, occur from c/c* > 1

$$c^* = \frac{L}{V_p} = L\left(\frac{4}{3}\pi R_g^3\right)^{-1} \propto L^{-0.8}$$



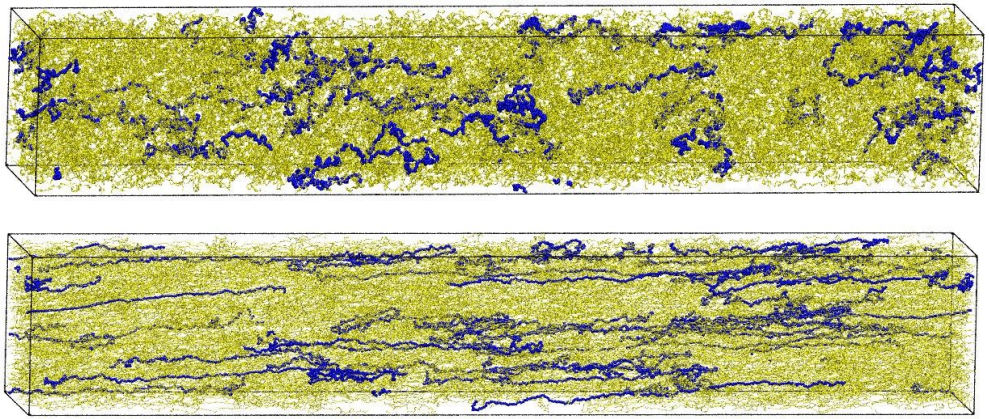
L=50 c/c*=0.1



L=50 c/c*=1.04

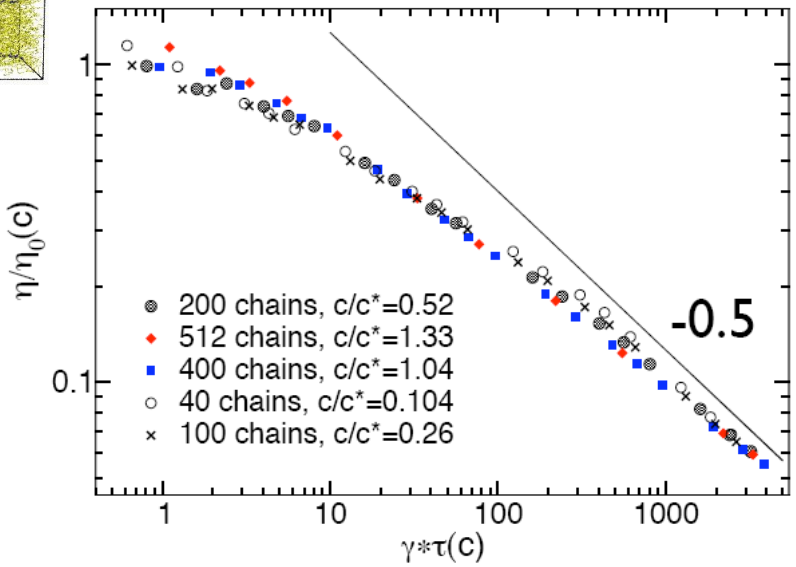
# Expl: Semi-diluted Polymer solutions under Shear

- Shear thinning for large shear rates



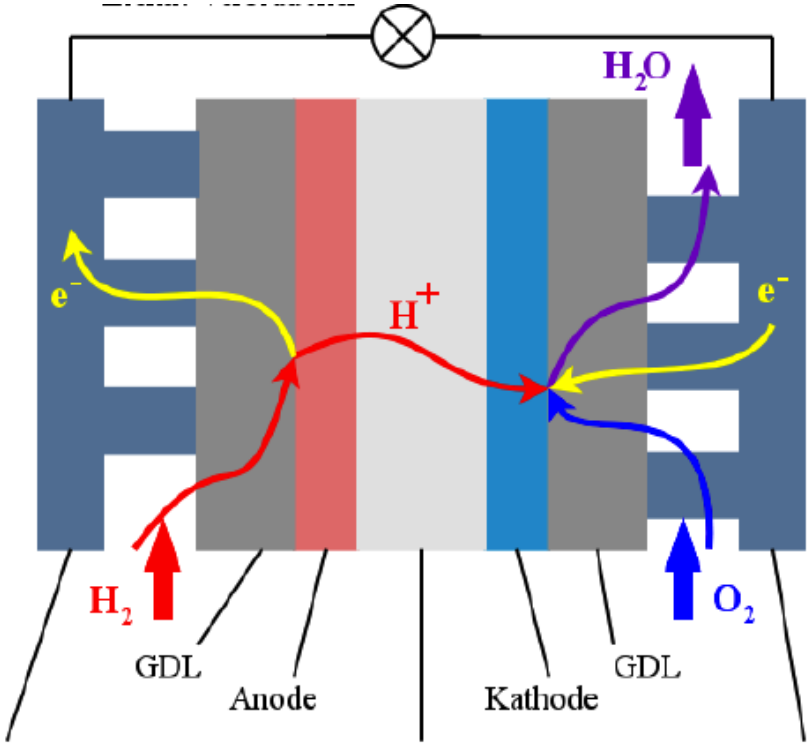
$$\eta = \eta_s + \eta_{bond} + \eta_{intra} + \eta_{inter}$$

$$\eta_s = \frac{1}{Vh}\sum_{i=1}^{N_s} m v_{ix} v_{iy} - \frac{1}{Vh}\sum_{i=1}^{N_s} \Delta p_{ix} r_{iy}$$

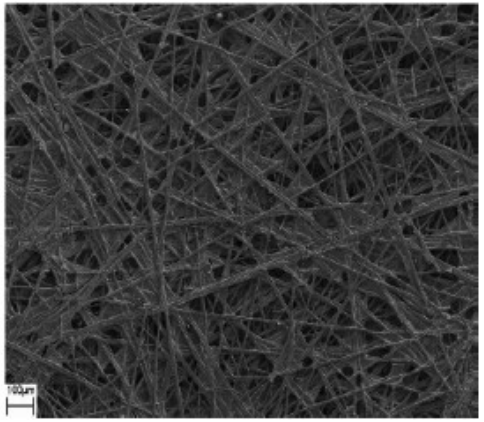


# Flow in stochastic geometries

- High Temperature – Polymer Electrolyte Fuel Cell (HT-PEFC)




$$H_2 \longrightarrow 2\,H^+ + 2\,e^-$$
$$O_2 + 4\,e^- \longrightarrow 2\,O^{2-}$$
$$4\,H^+ + 2\,O^{2-} \longrightarrow 2\,H_2O$$



GDL

Bipolar plate Membrane Bipolar plate

# Flow in stochastic geometries

- Effective path length: tortuosity
  - Fick's law

$$j_A = -c\, D_{AB}^{(f)} \nabla x_A$$

  - Diffusion in porous media

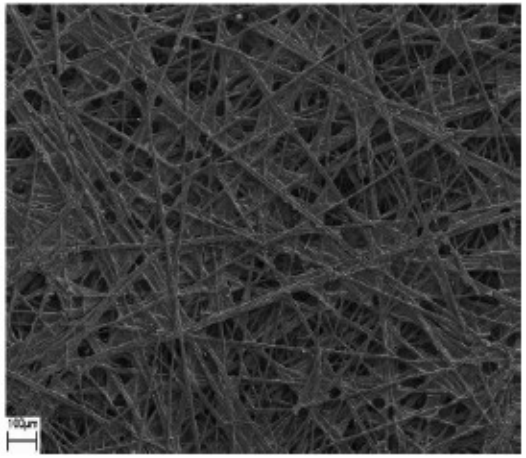
$$D_{AB}^{(p)} = \beta D_{AB}^{(f)} \qquad \beta = \phi S_g \tau$$

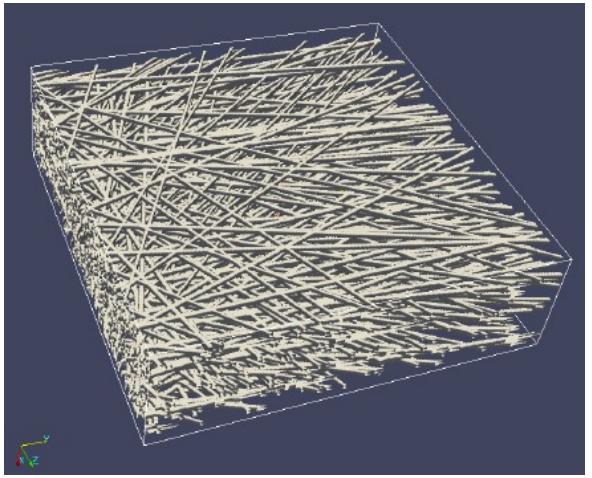
$\phi$ porosity

$S_g$ gas saturation

$\tau$ tortuosity

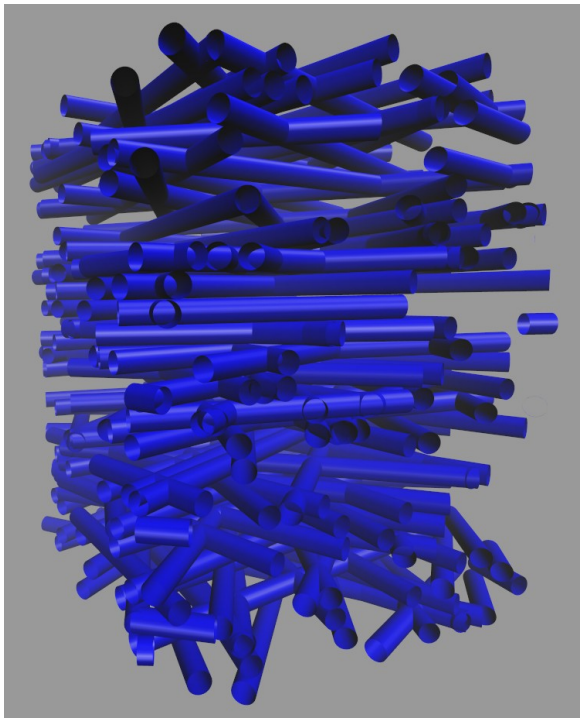
GDL

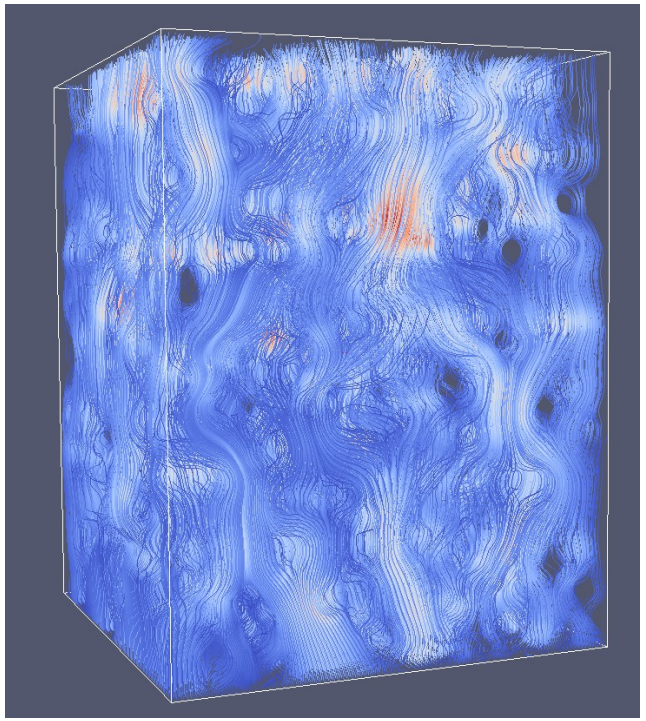




# Flow in stochastic geometries

- Flow in Gas Diffusion Layer (GDL) of fuel cells





Tortuosity: $\tau = 1.149 \pm 0.03$ $\tau_v = 1.187$ $\tau_v = \frac{\langle |\mathbf{v}| \rangle}{\langle |v_z| \rangle}$

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# Thank you for your attention !