# Multiscale Framework via Domain Decomposition

George Em Karniadakis & Xin Bian

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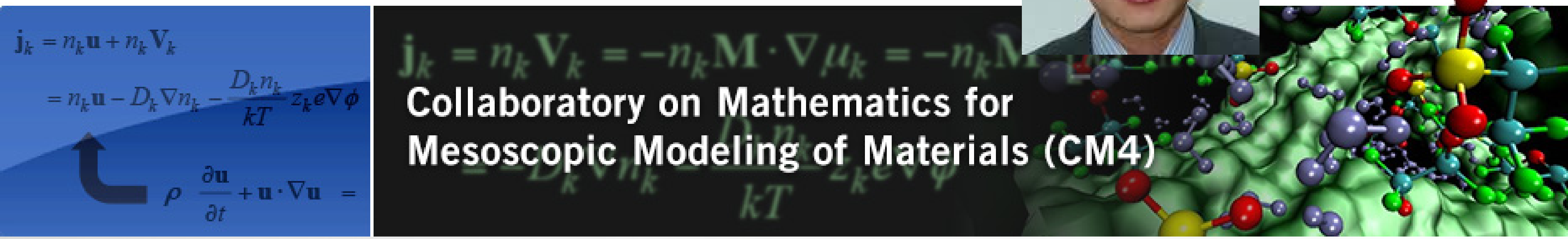


http://www.pnnl.gov/computing/cm4/

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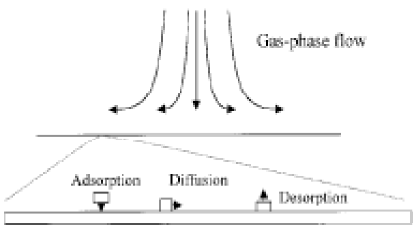
# Surface-Driven Phenomena

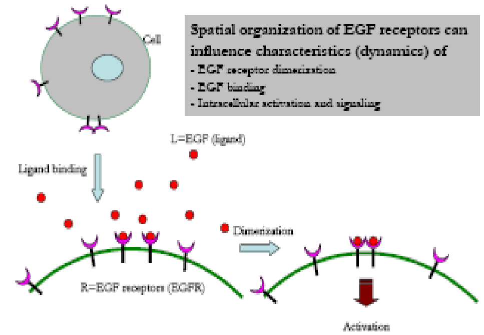
**Surface processes:** Catalysis, Chemical Vapor Deposition, epitaxial growth, etc.




[Lam, Vlachos, PRB 2001]

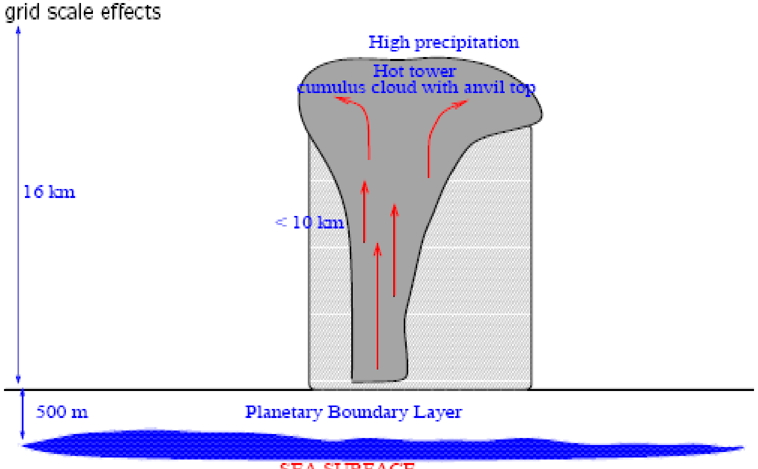
**Cell Biology:** Epidermal Growth Factor binding/dimerization

Early events of EGF signaling



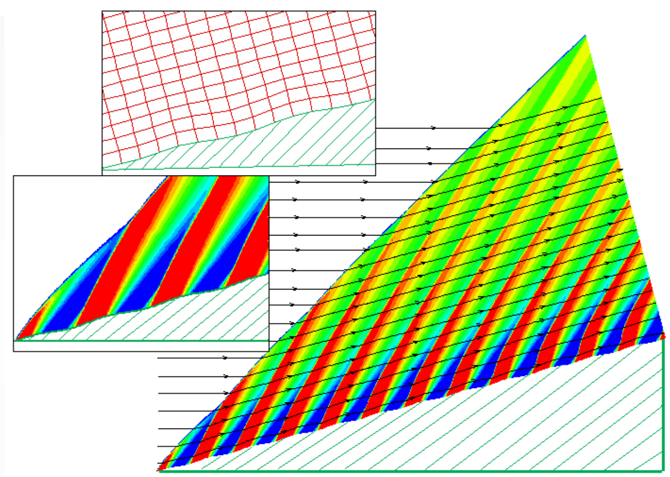

- "noisy" intercellular communication; synchronization

**Atmosphere/Ocean applications:** Tropical convection; sub-grid scale effects




[Majda, Khouider, PNAS 2001],
[Khouider, Majda, Katsoulakis PNAS 2003].

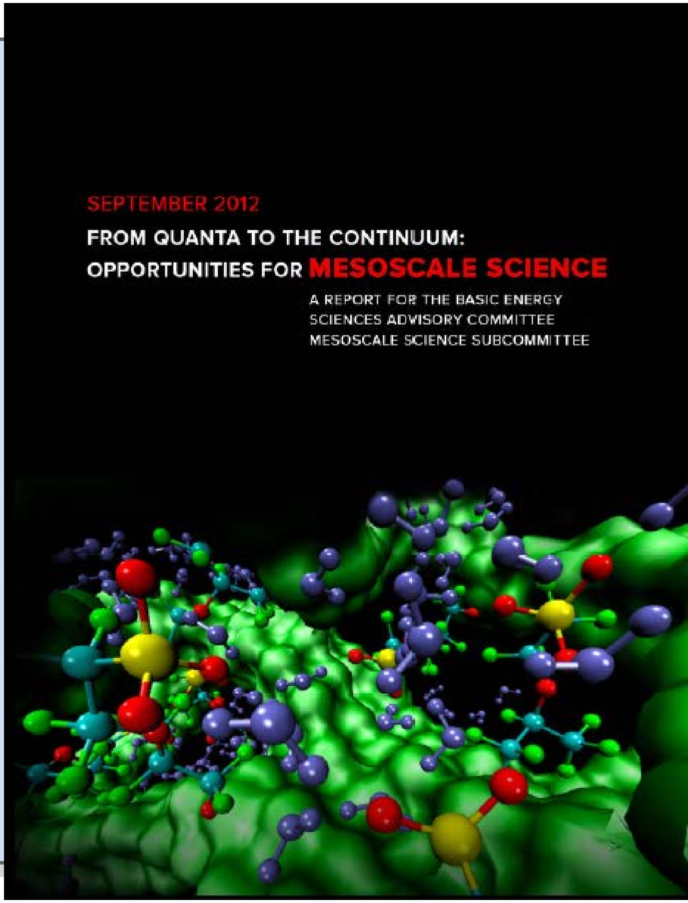
**Shock Dynamics: randomly rough surface**

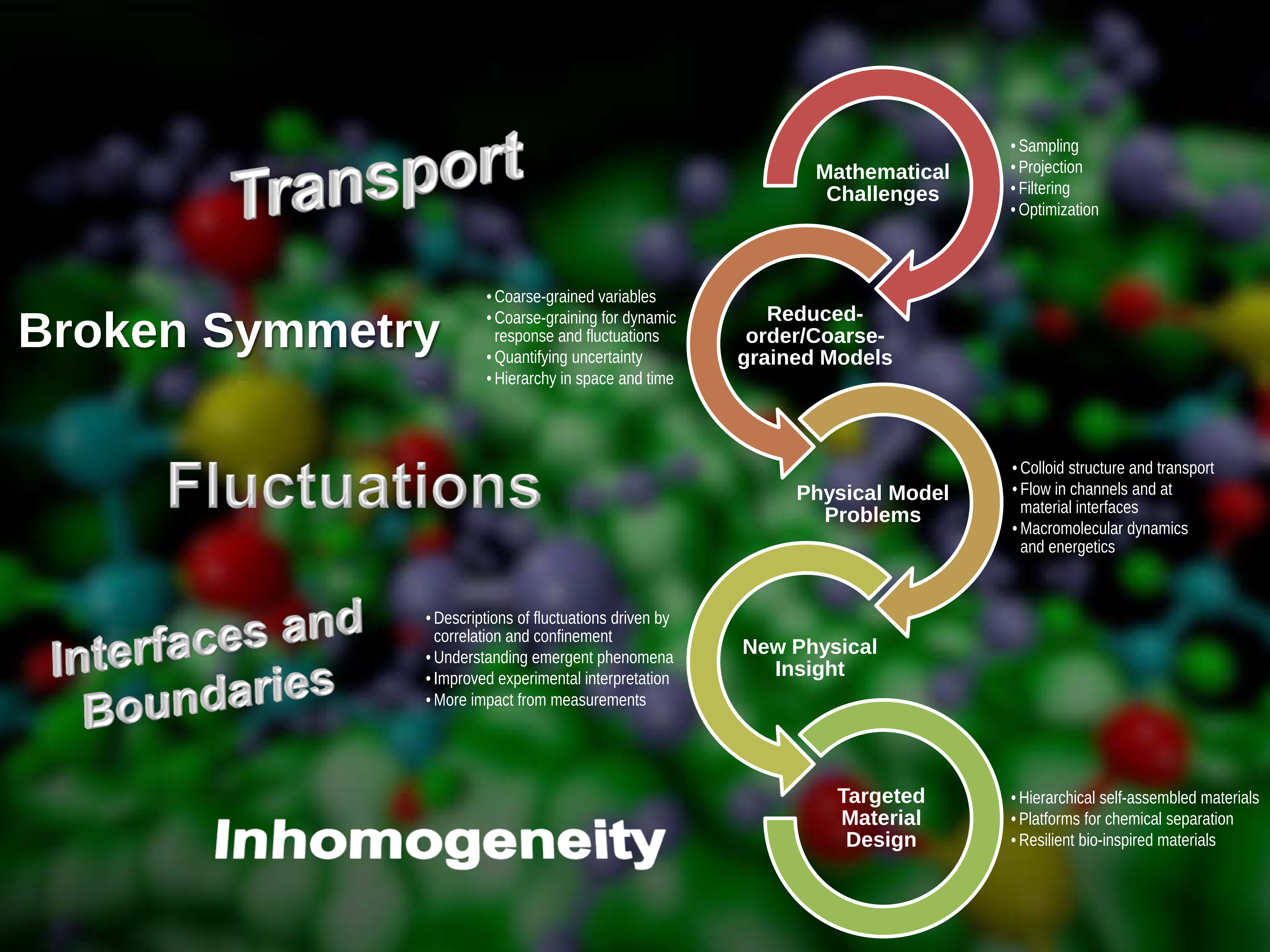


# Imagine the promise of Mesoscale Science

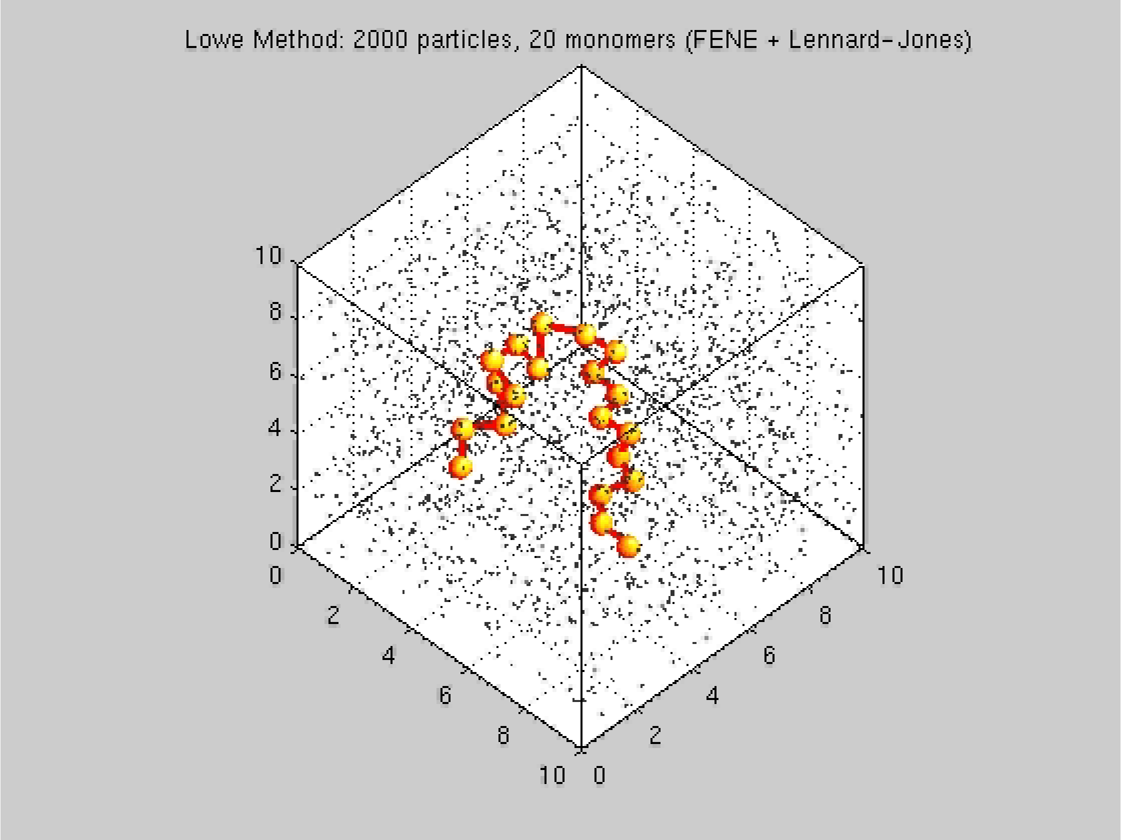
- Imagine the ability to manufacture at the mesoscale: that is, the directed assembly of mesoscale structures that possess unique functionality that yields faster, cheaper, higher performing, and longer lasting products, as well as products that have functionality that we have not yet imagined.
- Imagine the realization of biologically inspired complexity and functionality with inorganic earth-abundant materials to transform energy conversion, transmission, and storage.
- Imagine the transformation from top-down design of materials and systems with macroscopic building blocks to bottom-up design with nanoscale functional units producing next-generation technological innovation.

***This is the promise of mesoscale science.***



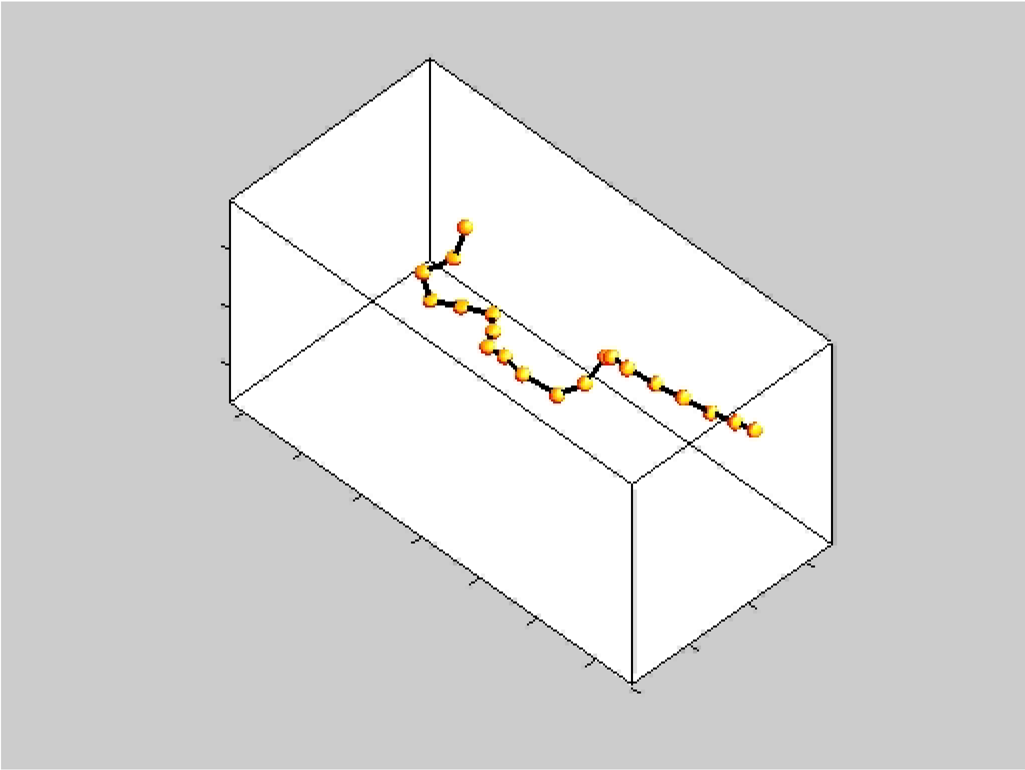


Transport
Broken Symmetry
Fluctuations
Interfaces and Boundaries
Inhomogeneity
Mathematical Challenges
• Sampling
• Projection
• Filtering
• Optimization
Reduced-order/Coarse-grained Models
• Coarse-grained variables
• Coarse-graining for dynamic response and fluctuations
• Quantifying uncertainty
• Hierarchy in space and time
Physical Model Problems
• Colloid structure and transport
• Flow in channels and at material interfaces
• Macromolecular dynamics and energetics
New Physical Insight
• Descriptions of fluctuations driven by correlation and confinement
• Understanding emergent phenomena
• Improved experimental interpretation
• More impact from measurements
Targeted Material Design
• Hierarchical self-assembled materials
• Platforms for chemical separation
• Resilient bio-inspired materials



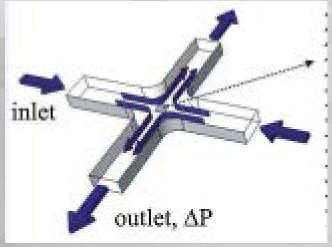

Equilibrium

# Shear Flow

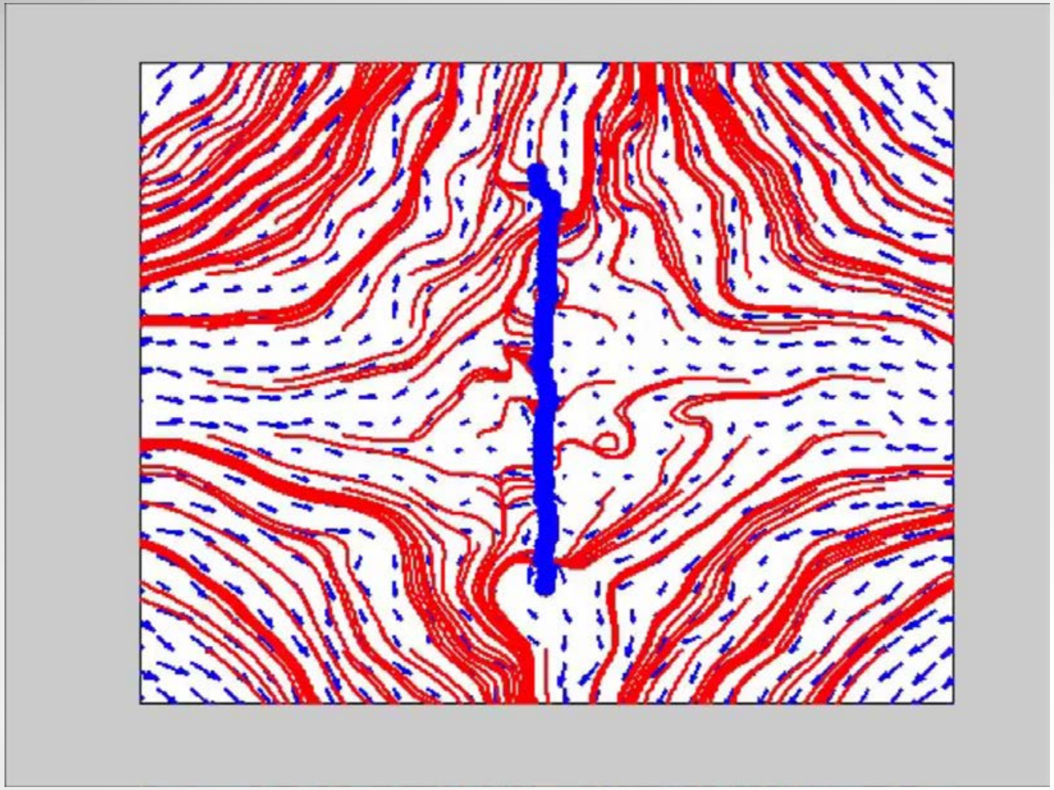


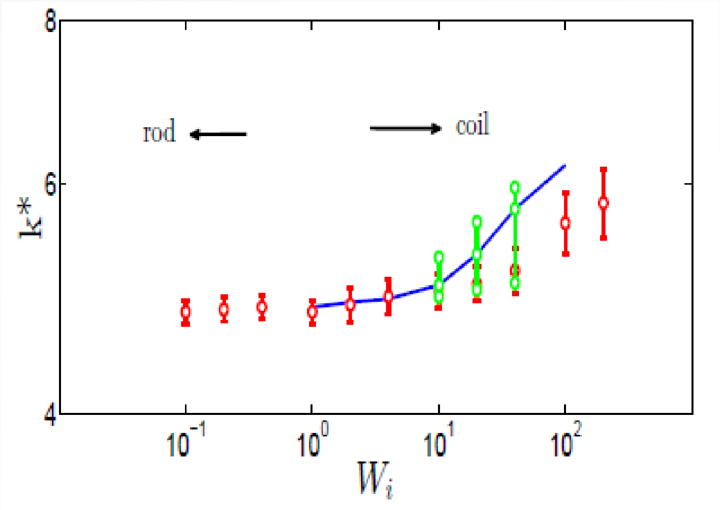
# Buckling Instability due to Thermal Noise Amplification



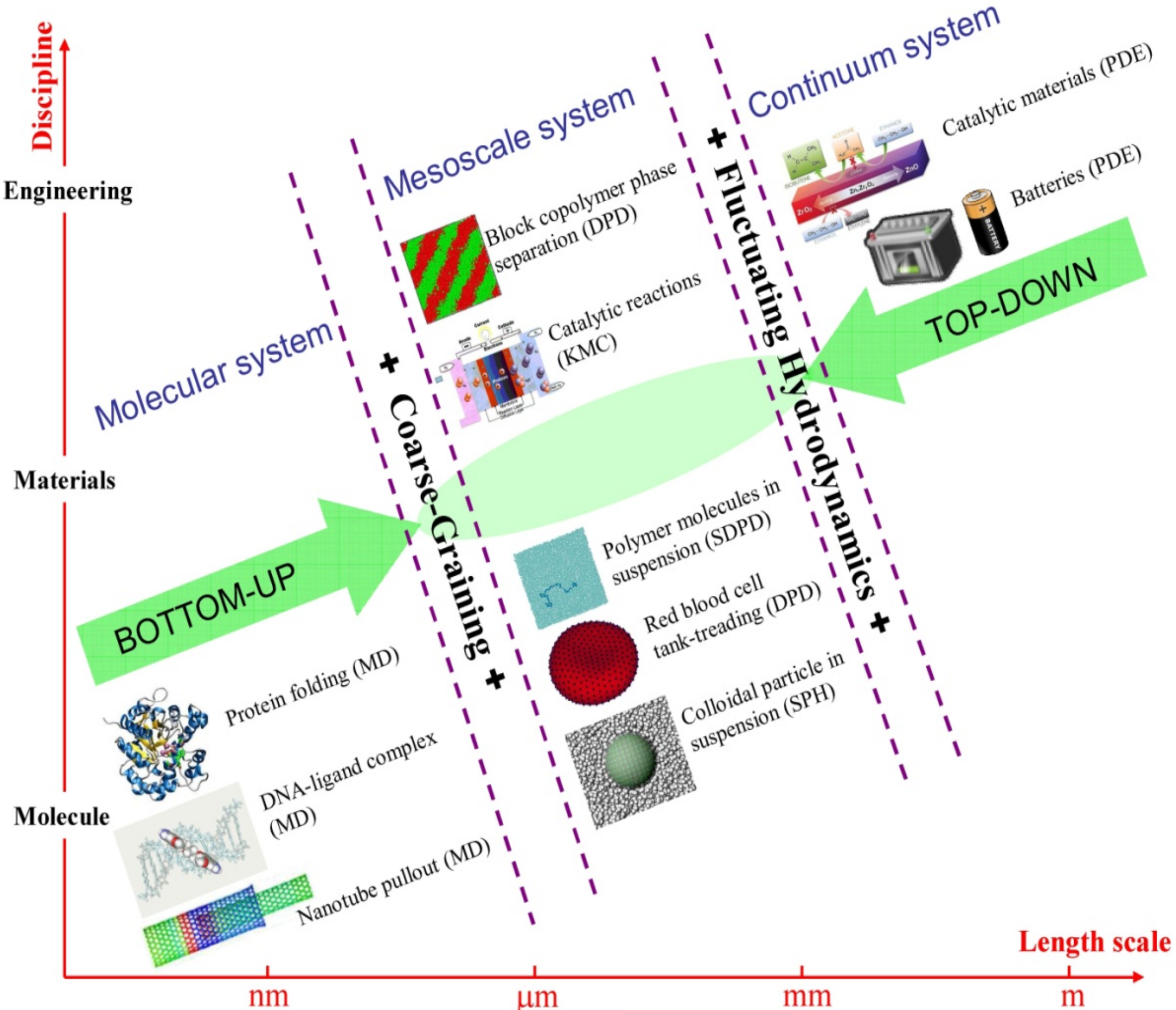



➢ Thermal noise is amplified as a result of stochasticity and nonlinearity competition leading to buckling of elastic fibers in the stagnation flow region.





# Mesoscale Phenomena and Models



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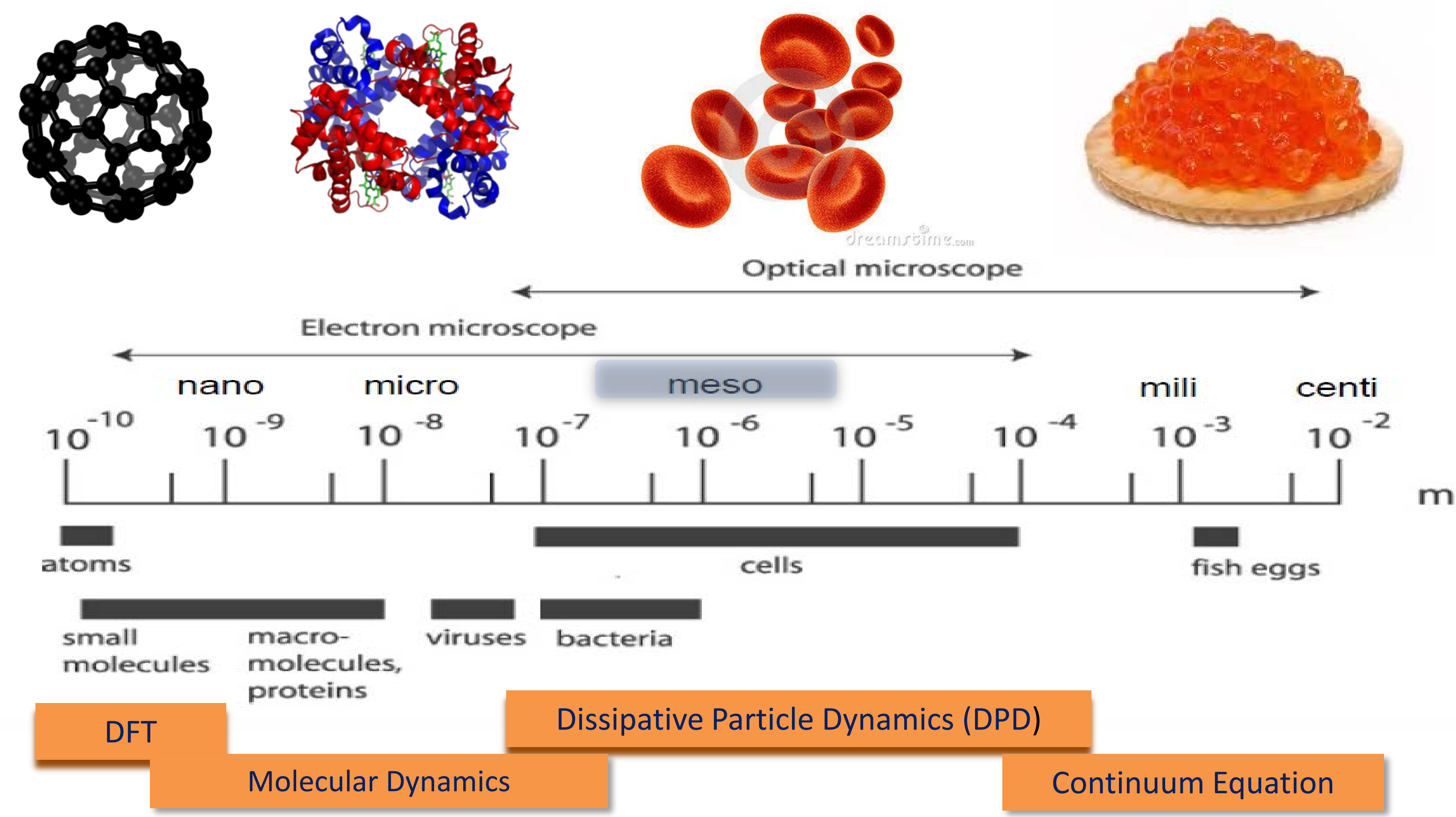
# Multiple Scales – Multiple Methods



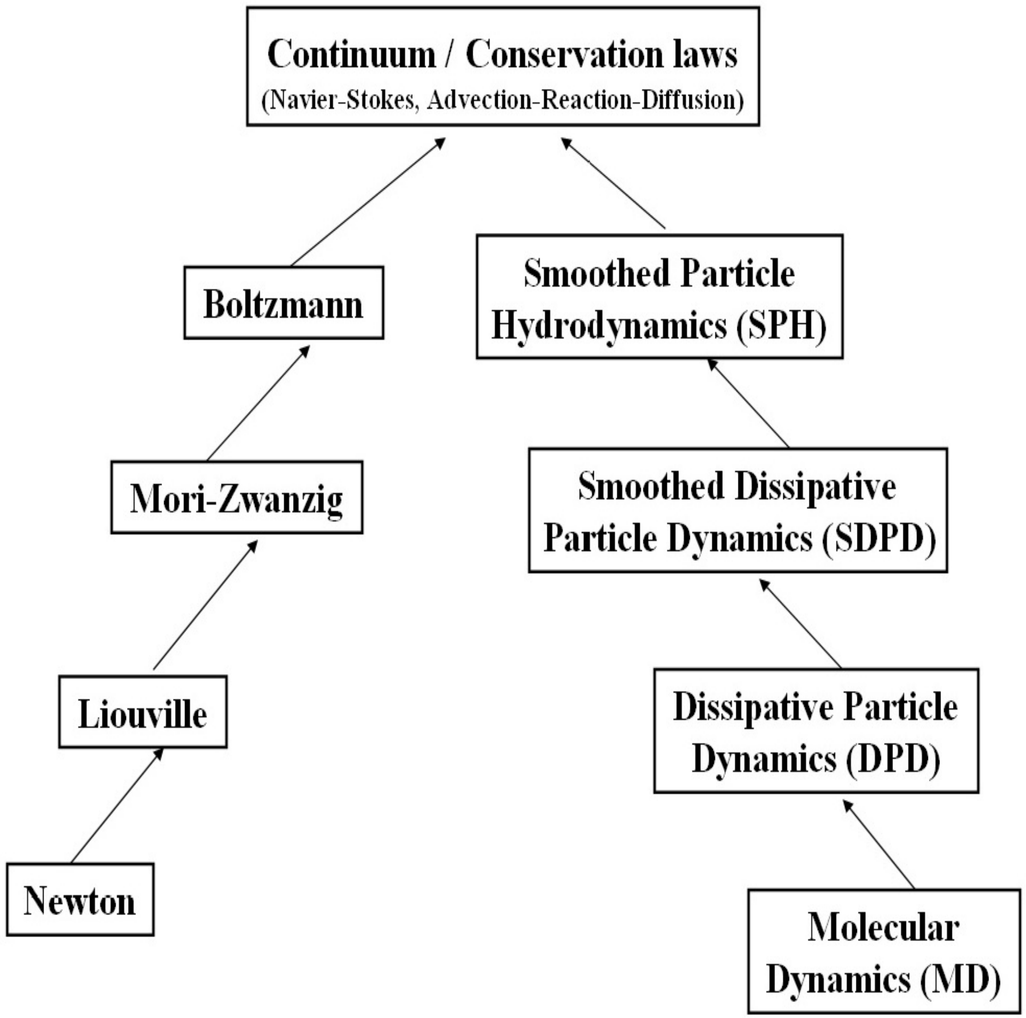
# Outline

**This Lecture: THEORY**

**Next Lecture: Implementation & MUI**

1. Introduction
   - particle methods at various scales
2. Deterministic-deterministic coupling
   - Schwartz alternating method
   - multi-resolution SPH
3. Deterministic-stochastic coupling
   - fluctuations at equilibrium
     - periodic domain
     - truncated domain
   - fluctuations at nonequilibrium
     - periodic domain
     - heterogeneous adjacent multi-domains
4. Stochastic-stochastic coupling
   - the adaptive resolution scheme
     - force-force coupling
     - energy-energy coupling
5. Summary and some perspectives

# Hierarchy of Mathematical & Numerical Models



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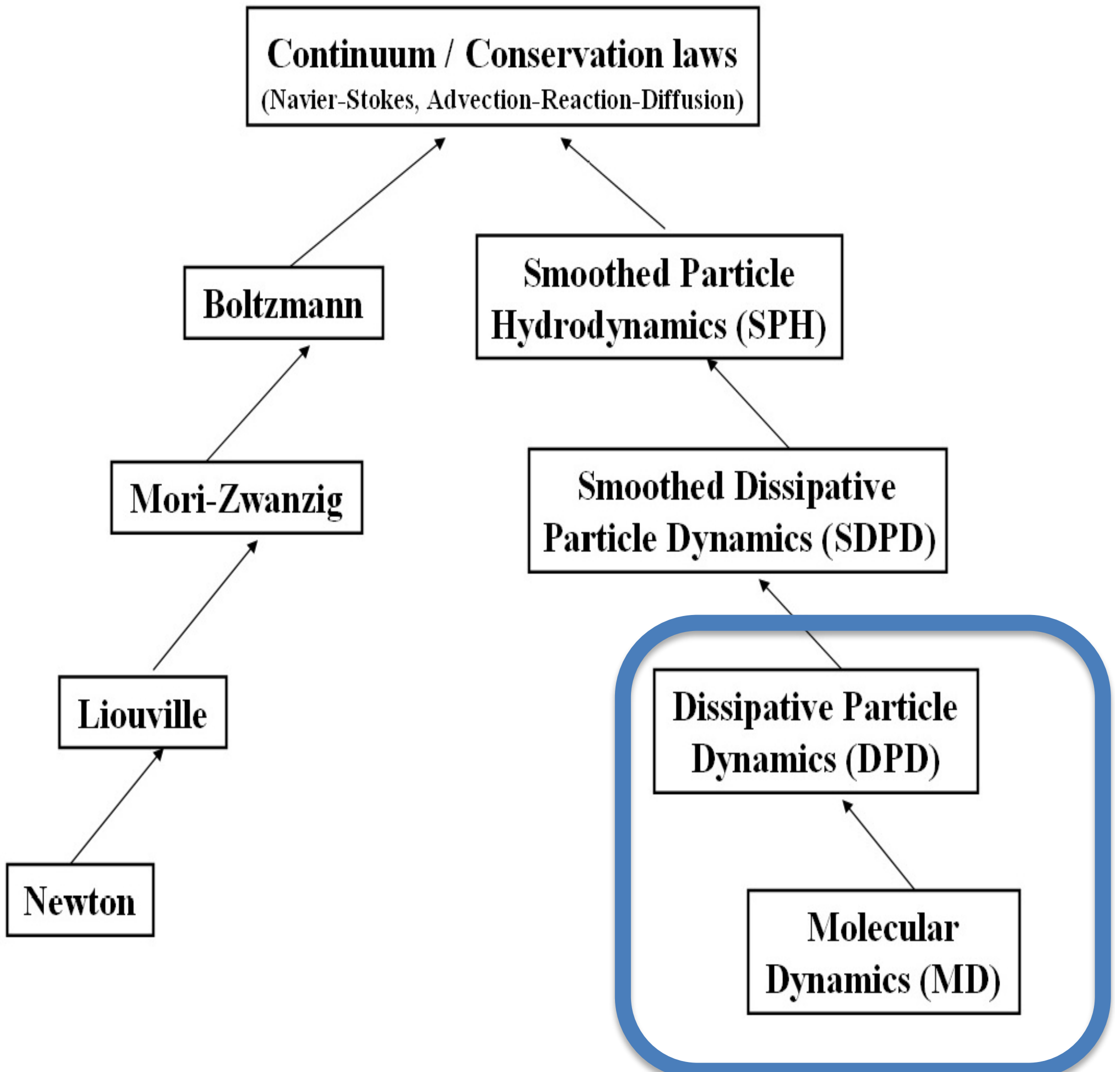
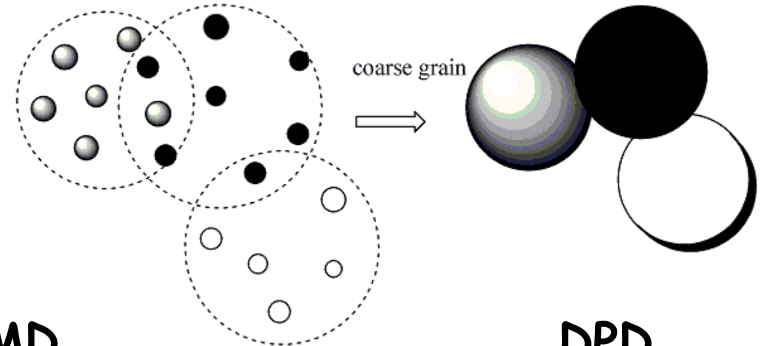
# Hierarchy of Mathematical & Numerical Models



# Dissipative Particle Dynamics (DPD)




**MD**

- MICROscopic level approach

- atomistic approach is often problematic because larger time/length scales are involved

**DPD**

- set of point particles that move off-lattice through prescribed forces

- each particle is a collection of molecules

- MESOscopic scales
- momentum-conserving Brownian dynamics

**Navier-Stokes**

- continuum fluid mechanics

- MACROscopic modeling

Ref on Theory: Lei, Caswell & Karniadakis, Phys. Rev. E, 2010

# Pairwise Interactions

Forces exerted by particle J on particle I:

Fluctuation-dissipation relation:
$\sigma^2 = 2\gamma\kappa_B T$ $\quad \omega^D = [\omega^R]^2$

$$\vec{F}_{ij}^{C} = F_{ij}^{(c)}(r_{ij})\vec{e}_{ij}$$

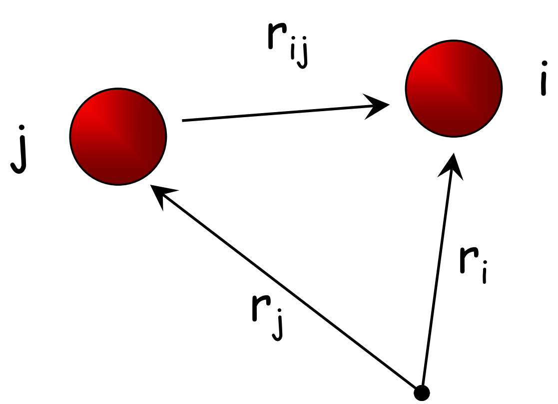
**Conservative**
fluid / system dependent

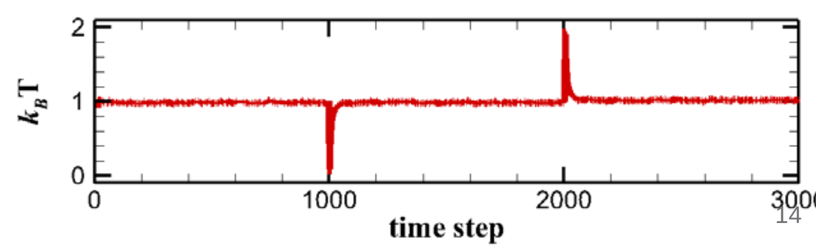
$$\vec{F}_{ij}^{D} = -\gamma\omega^{D}(r_{ij})(\vec{v}_{ij}\cdot\vec{e}_{ij})\vec{e}_{ij}$$

**Dissipative**
frictional force, represents viscous resistance within the fluid – accounts for energy loss

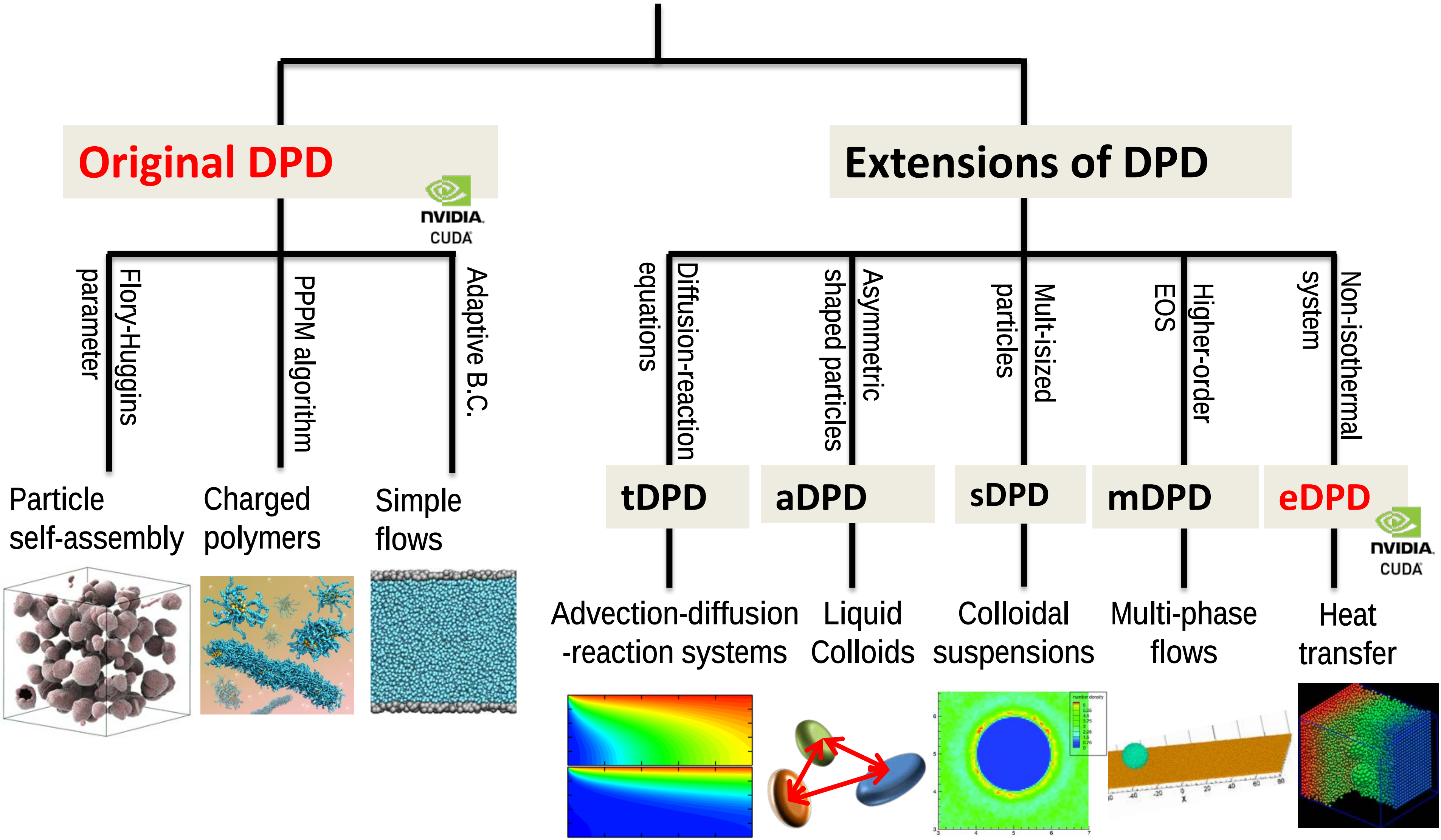
$$\vec{F}_{ij}^{R} = \sigma\omega^{R}(r_{ij})\xi_{ij}\vec{e}_{ij}$$

**Random**
stochastic part, makes up for lost degrees of freedom eliminated after the coarse-graining



# Dissipative Particle Dynamics (DPD)



# Algorithmic similarity: pairwise forces within short range $r_c$

- in a nutshell, ∀ particle $i$ in **SPH**, **SDPD**, **DPD**, or **MD**, the EoM:

$$m_i \dot{\mathbf{v}}_i = \sum_{j \neq i} \left( \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \right) \tag{1}$$

- options for different components
  - weighting kernel or potential gradient in MD
  - equation of state
  - density field
  - thermal fluctuations
  - NVT: thermostat
  - ... ...

top-down/continuum-based

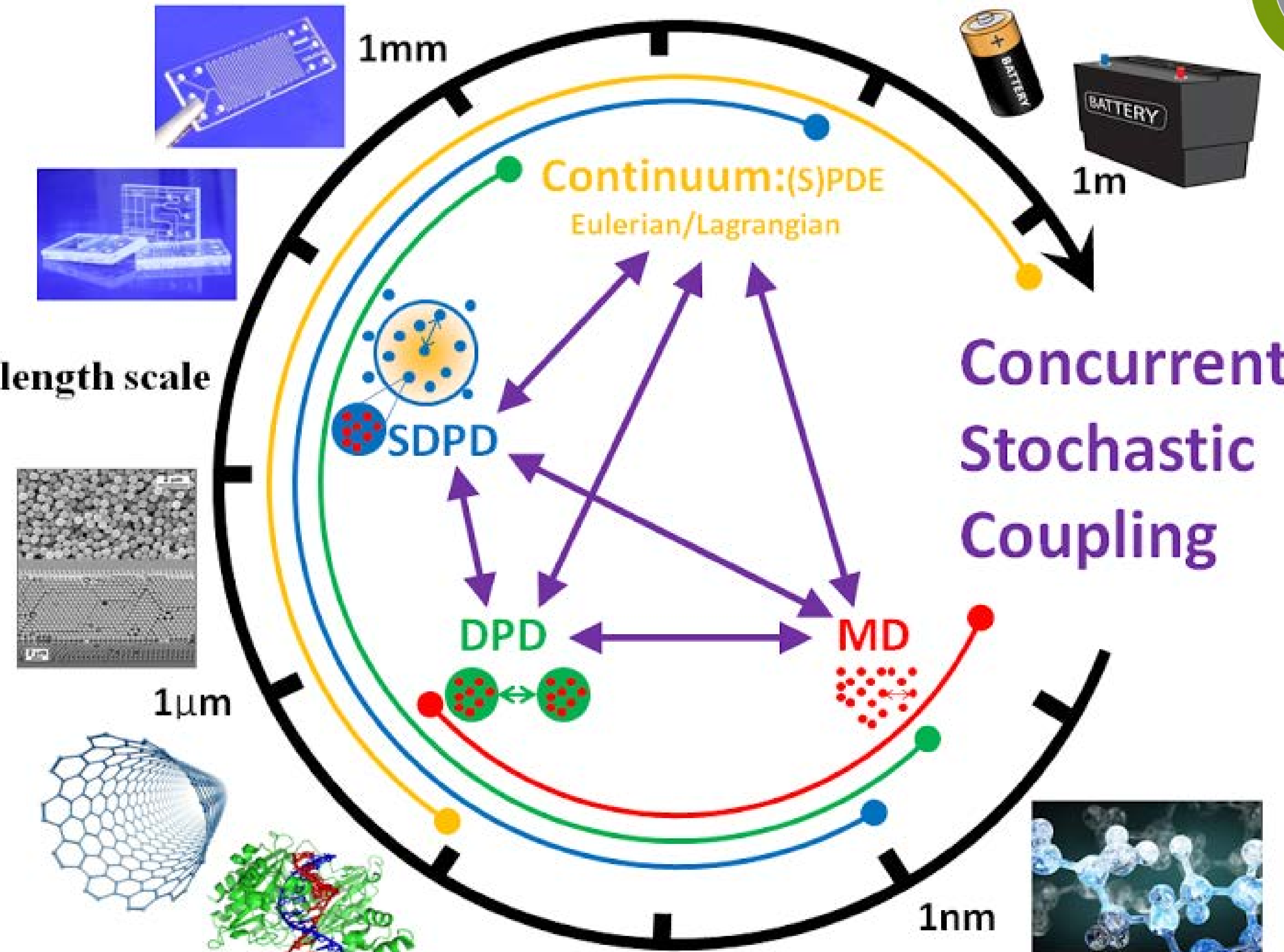
- SPH: Gingold et al. 1977, *Mon. Not. R. Astron. Soc.* Lucy 1977, *Astron. J.*
- SDPD: Español et al. 2003, *Phys. Rev. E*

bottom-up/coarse-grained/semi-empirical

- DPD: Hoogerbrugge et al. 1992, *Europhys. Lett.* Groot et al. 1997, *J. Chem. Phys.*
- MD: Allen et al. 1989; Frenkel et al. 2002; Evans et al. 2008; Tuckerman 2010

# Grid-Based Methods

| Immersive Grid-Based | | Particle – Based (meshless) |
|---|---|---|
| FCM<br>Coarse-grained dynamics<br>Small particles, simple shapes<br>Efficient for many particles<br>Mesh independent | Macro | SPH<br>Lower-order continuum scheme<br>Based on local smoothing kernel<br>Easy to configure<br>Galilean invariant |
| SPM<br>Finer resolution<br>Larger or compound particles | | SPH + Thermal fluctuations<br>Pan & Tartakovsky (PNNL) |
| SELM<br>Thermal fluctuations<br>Finer resolution<br>Deformable bodies or interfaces<br>Atzberger (UCSB) | | Smoothed DPD<br>Continuum terms from SPH<br>Thermal fluctuations |
| | | DPD<br>Coarse-grained MD<br>Thermal fluctuations |
| Higher-order schemes | Micro | Classical MD |

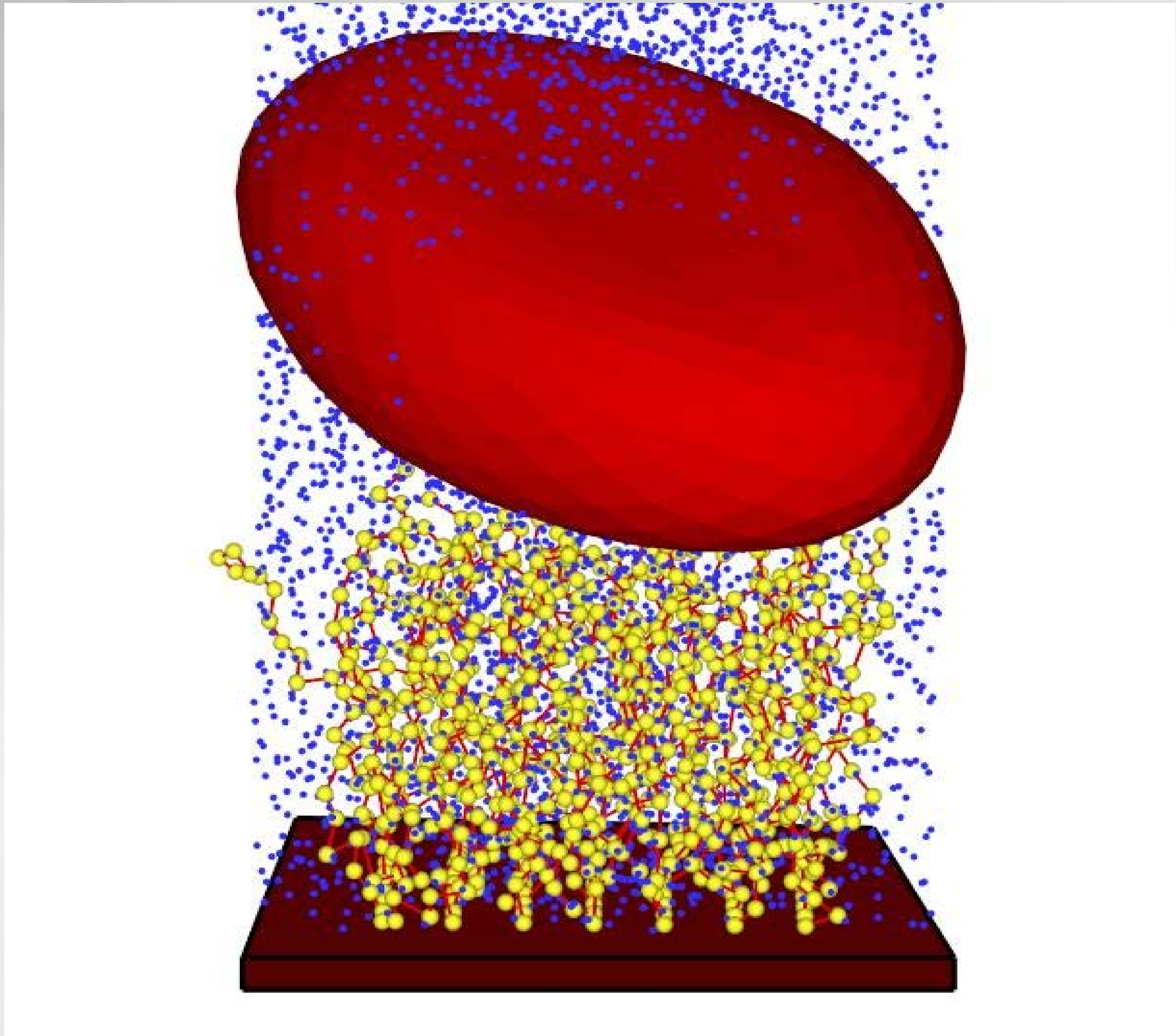

1mm
1m
Continuum:(S)PDE
Eulerian/Lagrangian
length scale
SDPD
DPD
MD
1μm
1nm
Concurrent
Stochastic
Coupling

# Overview on multiscale coupling *(incomplete list)*

- domain decomposition method:
  - coupling state variable
    - relaxation dynamics O'Connell et al. 1995, *Phys. Rev. E*
    - Maxwell buffer Hadjiconstantinou et al. 1997, *Int. J. Mod. Phys. C*
    - least constraint dynamics Nie et al. 2004, *J. Fluid Mech.*
  - coupling flux Flekkøy et al. 2000, *Europhys. Lett.* Delgado-Buscalioni et al. 2003, *Phys. Rev. E*
  - adaptive resolution scheme
    - coupling force Praprotnik et al. 2005, *J. Chem. Phys.*
    - coupling energy Potestio et al. 2013, *Phys. Rev. Lett.*
- CONNFFESSIT: Laso et al. 1993, *J. Non-Newton Fluid Mech.* Öttinger et al. 1997, *J. Non-Newton Fluid Mech.* Hulsen et al. 1997, *J. non-Newton Fluid Mech.* (FEM + Brownian dynamics)
- heterogeneous multiscale method: E et al. 2003, *Comm. Math. Sci.* Ren et al. 2005, *J. Comput. Phys.* (continuum + molecular dynamics)
- equation-free: Kevrekidis et al. 2003, *Comm. Math. Sci.* Kevrekidis et al. 2009, *Annu. Rev. Phys. Chem.* (molecular dynamics + spatial interpolation/temporal projection)
- adaptive mesh & algorithm refinement: Garcia et al. 1999, *J. Comput. Phys.* Donev et al. 2010, *Multiscale Model Simul.* (AMR + DSMC)

# Red blood cell and surface interacions





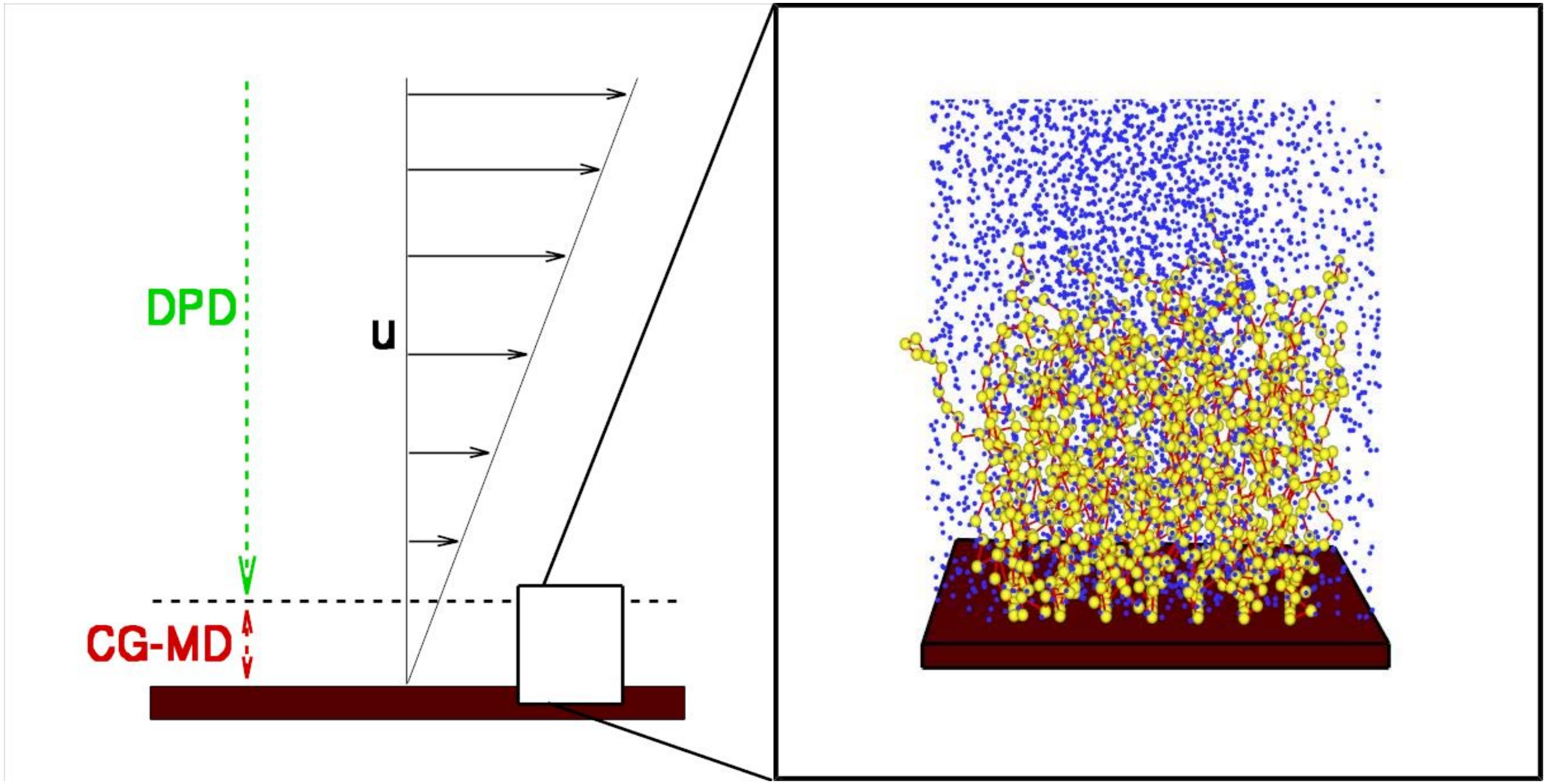
RBC-surface interactions

Adhesion of RBCs

Vessel wall modelling

RBC migration

# Coarse-grained multiscale descriptions



# Triple-Decker Algorithm

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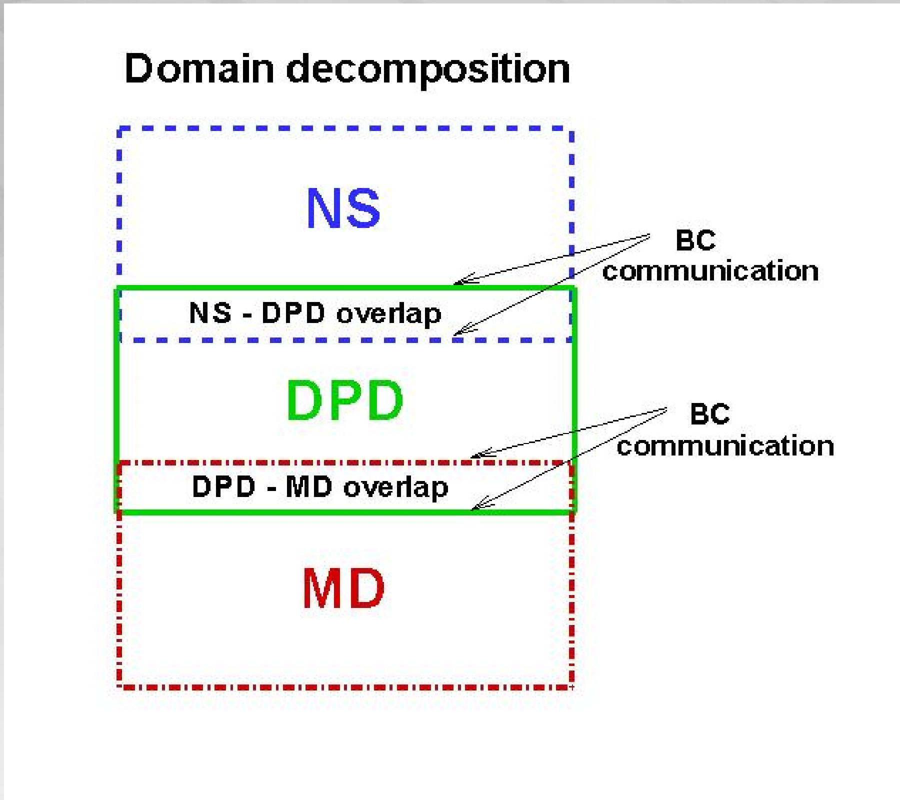


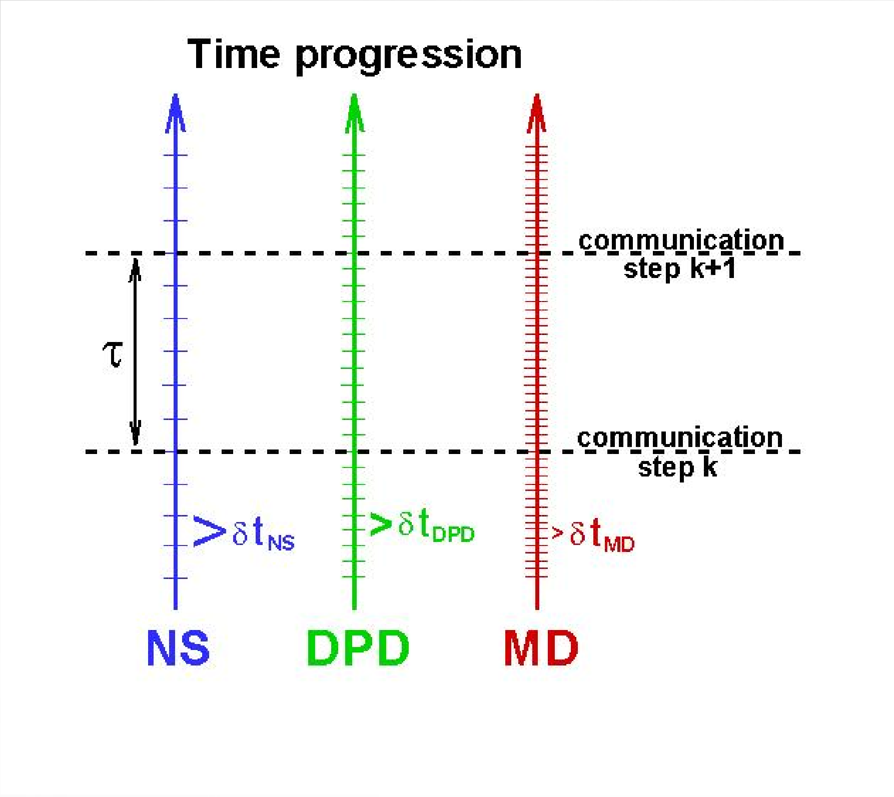


- Atomistic-Mesoscopic-Continuum Coupling
- Efficient time and space decoupling
- Subdomains are integrated independently and are coupled through the boundary conditions every time $\tau$

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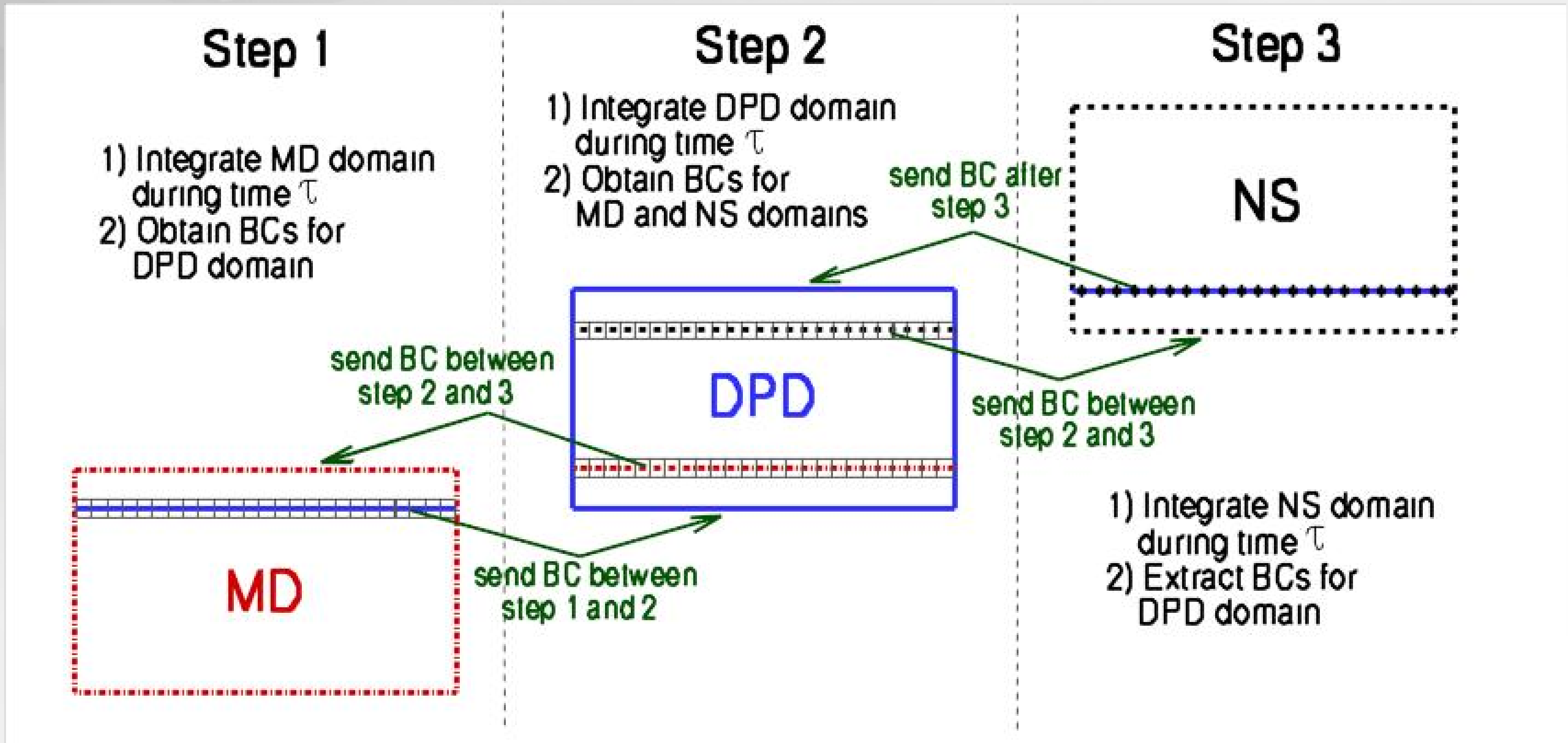
# Communication among domains

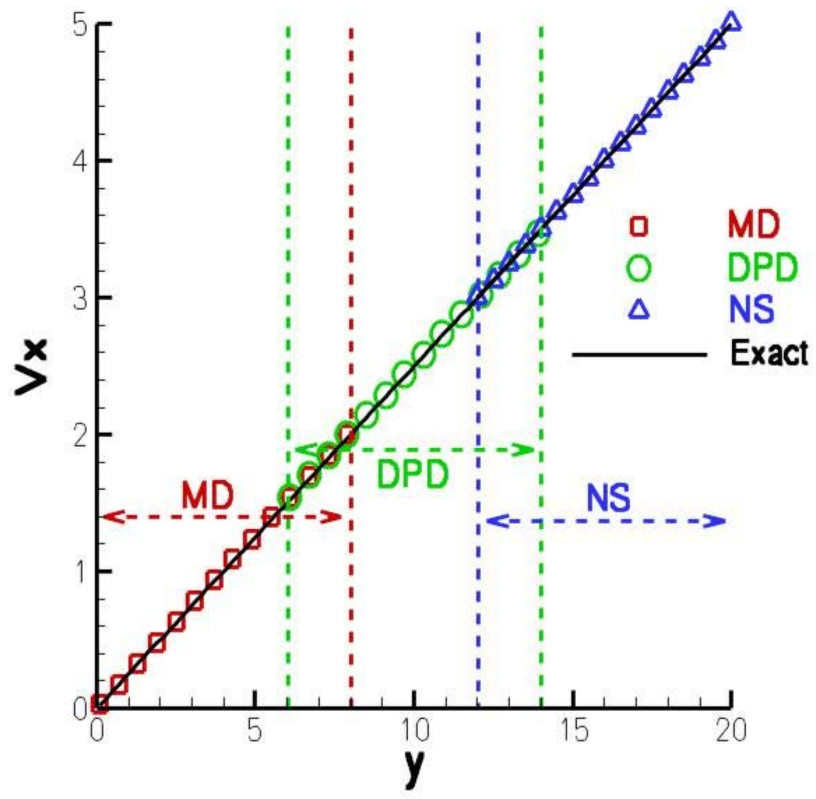



**1.D. A. Fedosov** and G. E. Karniadakis, "Triple-decker: Interfacing atomistic-mesoscopic-continuum flow regimes", [*Journal of Computational Physics*, 228(4), 1157-1171, 2009]().

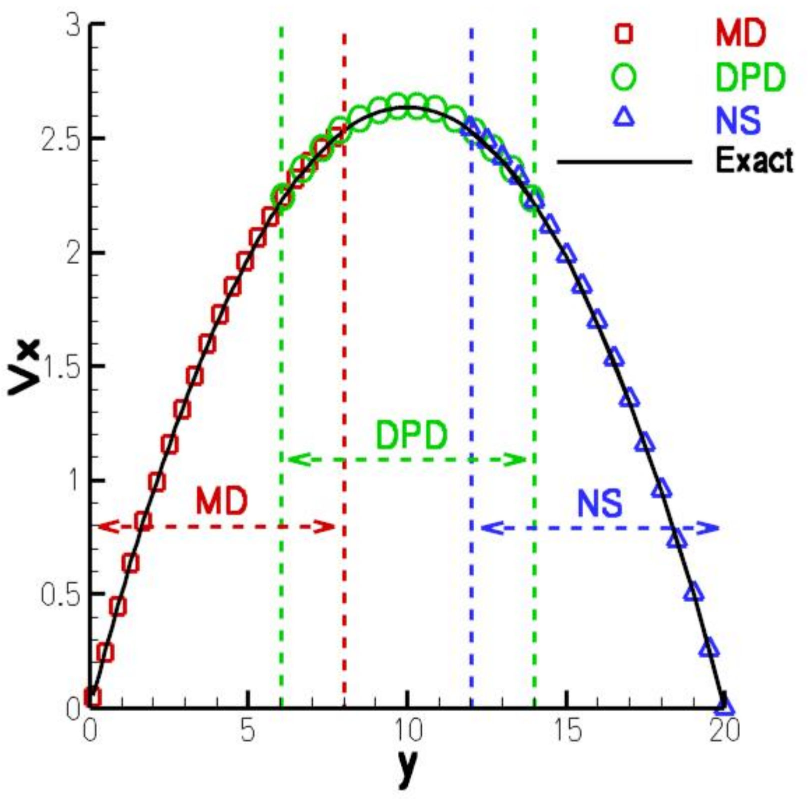
# Algorithm validation: 1D flows



## Couette flow




## Poiseuille flow



# Square cavity flow

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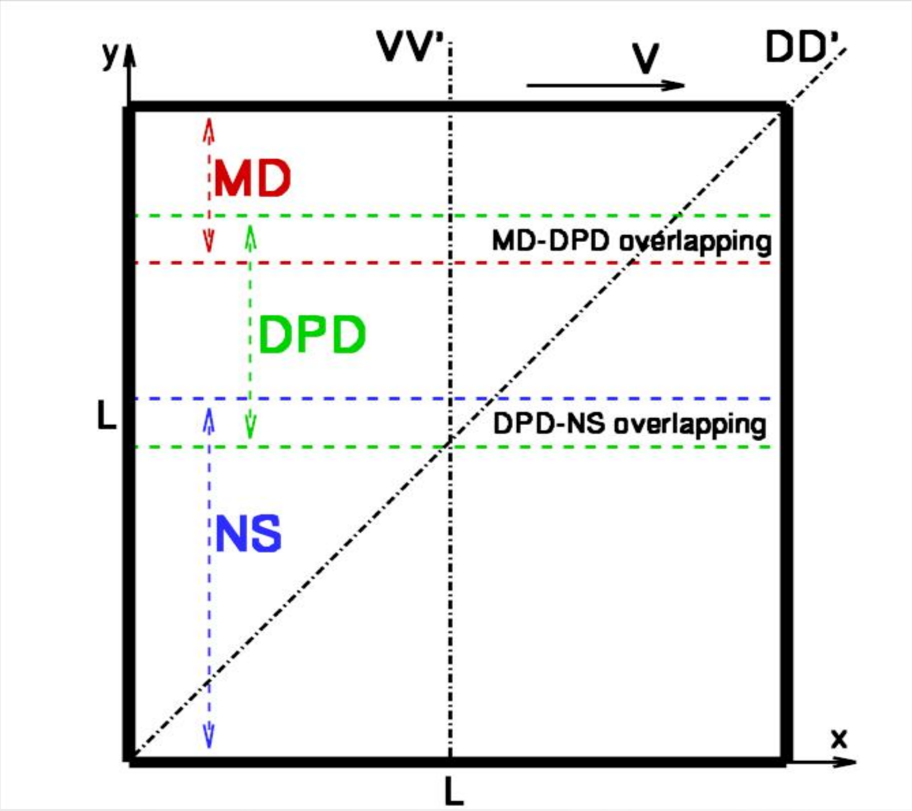
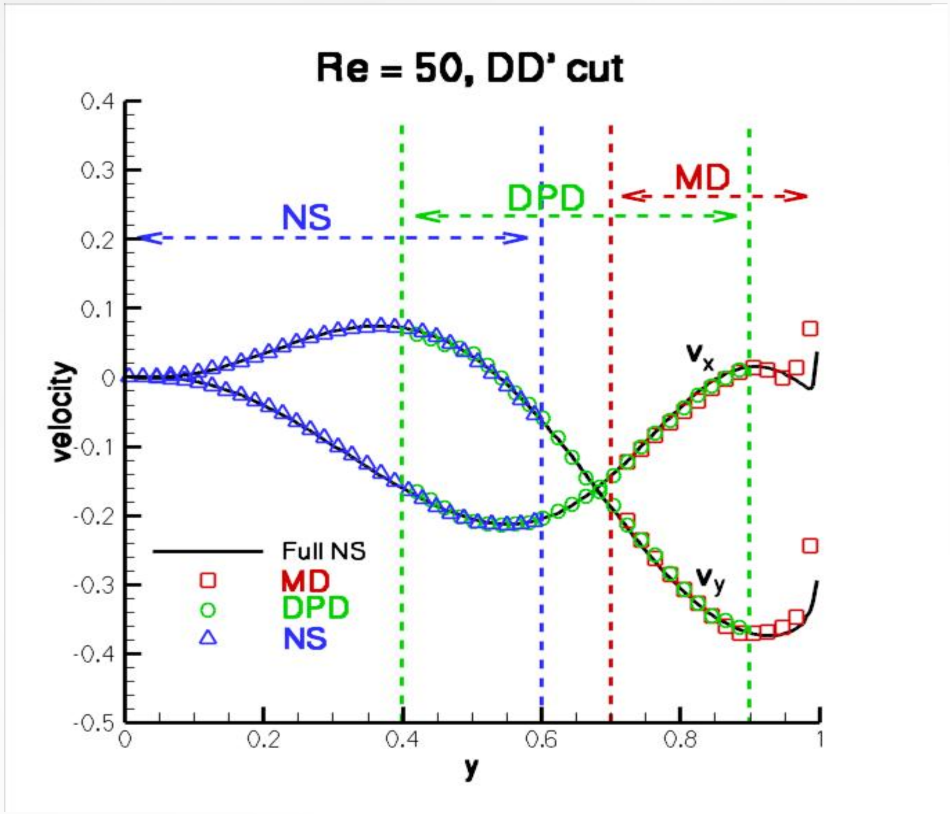
Square cavity, upper wall is moving to the right



# The Triple-Decker algorithm:Summary



- Triple-Decker algorithm is able to glue together atomistic, mesoscopic, and continuum regimes
- Effective space and time decoupling
- Algorithm is tested on well-known prototype flows such as Couette, Poiseuille and lid-driven square cavity
- Certain types of flows allow zero thickness of domain overlap
- Extension to complex fluids…

1.**D. A. Fedosov** and G. E. Karniadakis, "Triple-decker: Interfacing atomistic-mesoscopic-continuum flow regimes", *Journal of Computational Physics, 228(4), 1157-1171, 2009*.

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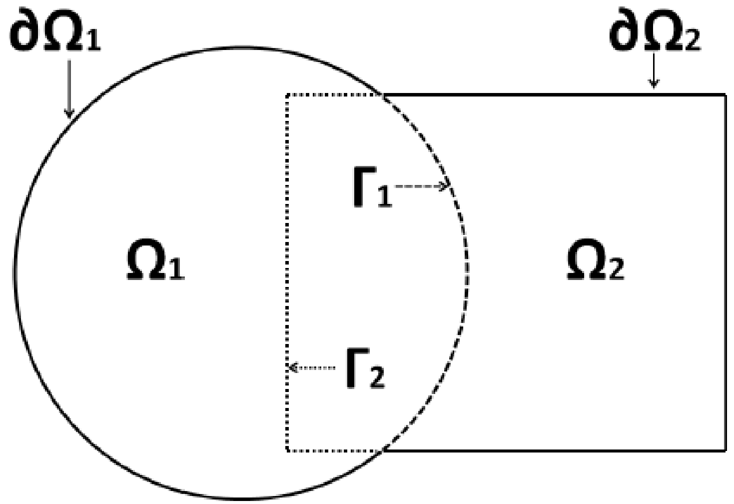
# Schwartz alternating method[1]

- DDM: overlapping sub-domains
  - domain $\Omega = \Omega_1 \cup \Omega_2$
  - external b.c. $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$
  - artificial b.c. $\Gamma = \Gamma_1 \cup \Gamma_2$




- *Dirichlet* b.c. on $\partial\Omega_1$, and $\partial\Omega_1$
- *Dirichlet* b.c. on $\Gamma_1$ and $\Gamma_2$

1. ($k = 1$) solve elliptic PDF in $\Omega_1$

$$\begin{aligned} Lu_1^k &= f && in\ \Omega_1, && (2) \\ u_1^k &= g && on\ \partial\Omega_1, && (3) \\ u_1^k &= u_2^{k-1}|\Gamma_1 && on\ \Gamma_1. && (4) \end{aligned}$$

"|" is the restriction onto $\Gamma_1$.

2. solve elliptic PDF in $\Omega_2$

$$\begin{aligned} Lu_2^k &= f && in\ \Omega_2, && (5) \\ u_2^k &= g && on\ \partial\Omega_2, && (6) \\ u_2^k &= \begin{cases} u_1^k|\Gamma_2 \\ u_1^{k-1}|\Gamma_2 \end{cases} && on\ \Gamma_2. && (7) \end{aligned}$$

   - multiplicative Schwartz
   - additive Schwartz

3. $k+ = 1$ repeat until convergence

[1] Smith et al. 1996.

# DDM with non-overlapping: Robin-Robin algorithm[2]

1. ($k = 1$) solve PDF in $\Omega_1$

$$\begin{aligned} Lu_1^k &= f && \textit{in } \Omega_1, && (8)\\ u_1^k &= g && \textit{on } \partial\Omega_1, && (9)\\ \frac{\partial u_1^k}{\partial n} + \gamma_1 u_1^k &= \frac{\partial u_2^{k-1}}{\partial n} + \gamma_1 u_2^{k-1} && \textit{on } \Gamma. && (10) \end{aligned}$$

2. solve PDF in $\Omega_2$

$$\begin{aligned} Lu_2^k &= f && \textit{in } \Omega_2, && (11)\\ u_2^k &= g && \textit{on } \partial\Omega_2, && (12)\\ \frac{\partial u_2^k}{\partial n} + \gamma_2 u_2^k &= \begin{cases} \frac{\partial u_1^k}{\partial n} + \gamma_2 u_1^k \\ \frac{\partial u_1^{k-1}}{\partial n} + \gamma_2 u_1^{k-1} \end{cases} && \textit{on } \Gamma. && (13) \end{aligned}$$

   - $u_2^0$ is assigned
   - $\gamma_1$, $\gamma_2$ are non-negative acceleration parameters that satisfy $\gamma_1 + \gamma_2 > 0$
   - for parallelization

3. $k+ = 1$ repeat until convergence

[2] Quarteroni et al. 1999.

# SPH: isothermal Navier-Stokes equations

- continuity equation: Monaghan 2005, *Rep. Prog. Phys.*

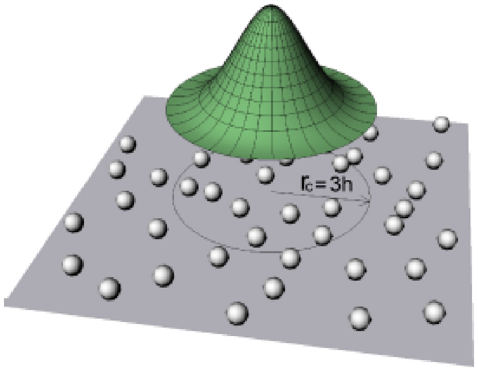
$$d_i = \frac{\rho_i}{m_i} = \sum_j W_{ij}, \quad \dot{\mathbf{r}}_i = \mathbf{v}_i \tag{14}$$

- momentum equation: Español et al. 2003, *Phys. Rev. E*; . Hu et al. 2006, *J. Comput. Phys.*

$$m_i \dot{\mathbf{v}}_i = \sum_{j \neq i} \left( \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D \right) + \mathbf{F}_i^b, \tag{15}$$

$$\mathbf{F}_{ij}^C = -\left( \frac{P_i}{d_i^2} + \frac{P_j}{d_j^2} \right) \frac{\partial W}{\partial r_{ij}} \mathbf{e}_{ij}, \tag{16}$$

$$\mathbf{F}_{ij}^D = \frac{\eta}{d_i d_j r_{ij}} \frac{\partial W}{\partial r_{ij}} \left( \frac{2D-1}{D} \mathbf{v}_{ij} + \frac{D+2}{D} \mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \mathbf{e}_{ij} \right) \tag{17}$$



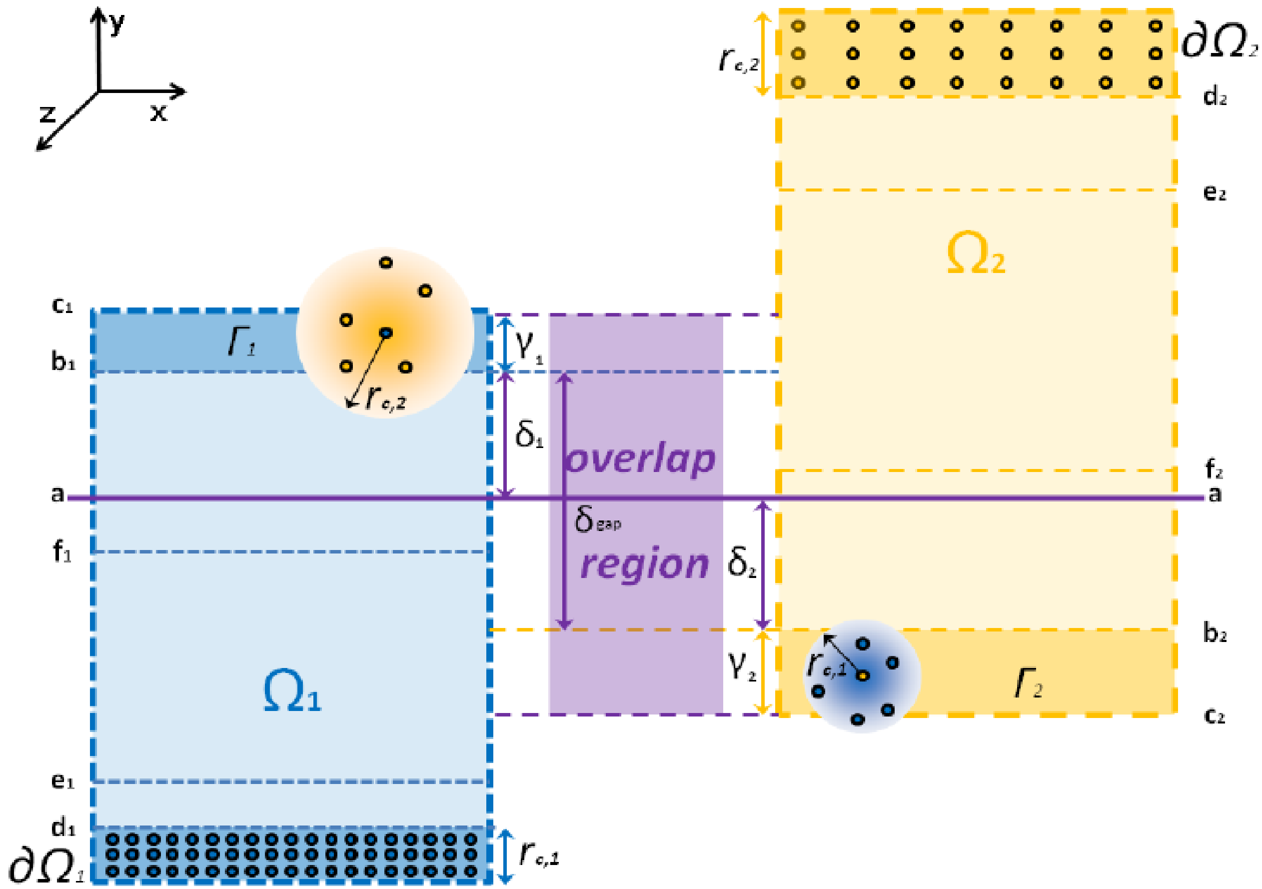

$W(r_{ij})$: B-Splines, Gaussian, Wendland functions ...

- weakly compressible: Batchelor 1967; Monaghan 1994, *J. Comput. Phys.*

$$p = p_0 \left[ \left( \frac{\rho}{\rho_r} \right)^\gamma - 1 \right] \tag{18}$$

$p_0$ relates to an artificial sound speed $c_T$

# Overlapping sub-domains of particles: hybrid interface[3]




- $\Gamma_1$ and $\Gamma_2$: constraint dynamics for $v$ (and $\rho$)
- $c_1$ and $c_2$: pressure correction and deletion-insertion of particles
- $a$: hybrid reference line for combining two results

[3] X. Bian et al. (2015b). "Multi-resolution flow simulations by smoothed particle hydrodynamics via domain decomposition". In: *J. Comput. Phys.* 297.0, pp. 132 –155.

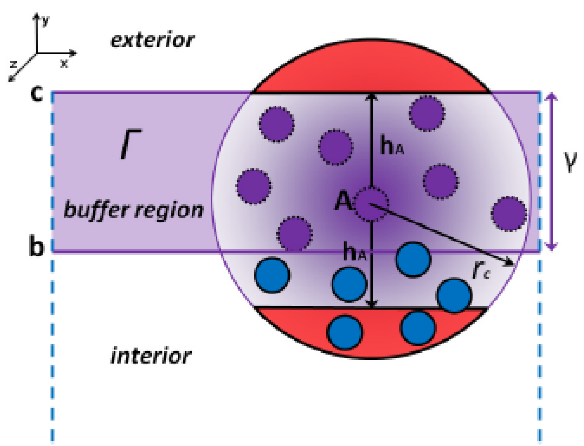
# Hybrid interface region: identified tasks[4]

- **velocity, density constraint in $\Gamma_1, \Gamma_2$: targeting the other side**
  - Lagrangian interpolation from the other sub-domain

$$\mathbf{u}_k^{constr} = \sum_l \frac{\mathbf{v}_l}{d_l} W_{kl},\ d_k^{cons} = \sum_l \frac{m_2}{m_1} W_{kl},\ k \in \Gamma_1, \quad l \in \Omega_2|_{y:[f_2,e_2]} \quad (19)$$

$$\mathbf{v}_k^{constr} = \sum_l \frac{\mathbf{u}_l}{d_l} W_{kl},\ d_k^{cons} = \sum_l \frac{m_1}{m_2} W_{kl},\ k \in \Gamma_2, \quad l \in \Omega_1|_{y:[e_1,f_1]} \quad (20)$$

- **pressure correction**: keep conditionally $\mathbf{F}_{ij}^C \cdot \mathbf{e}_n$ in $\Gamma_1$, $\Gamma_2$




- **particle deletion/insertion**
  - deletion: leave sub-domain
  - insertion: according to (*integer*) mass accumulated along $c_1$, $c_2$

$$N_{A_i}^{t_1^n} = N_{A_i}^{t_1^{n-1}} + d_{A_i} u_{A_i,y} \Delta x_1 \Delta t_1, \quad (21)$$

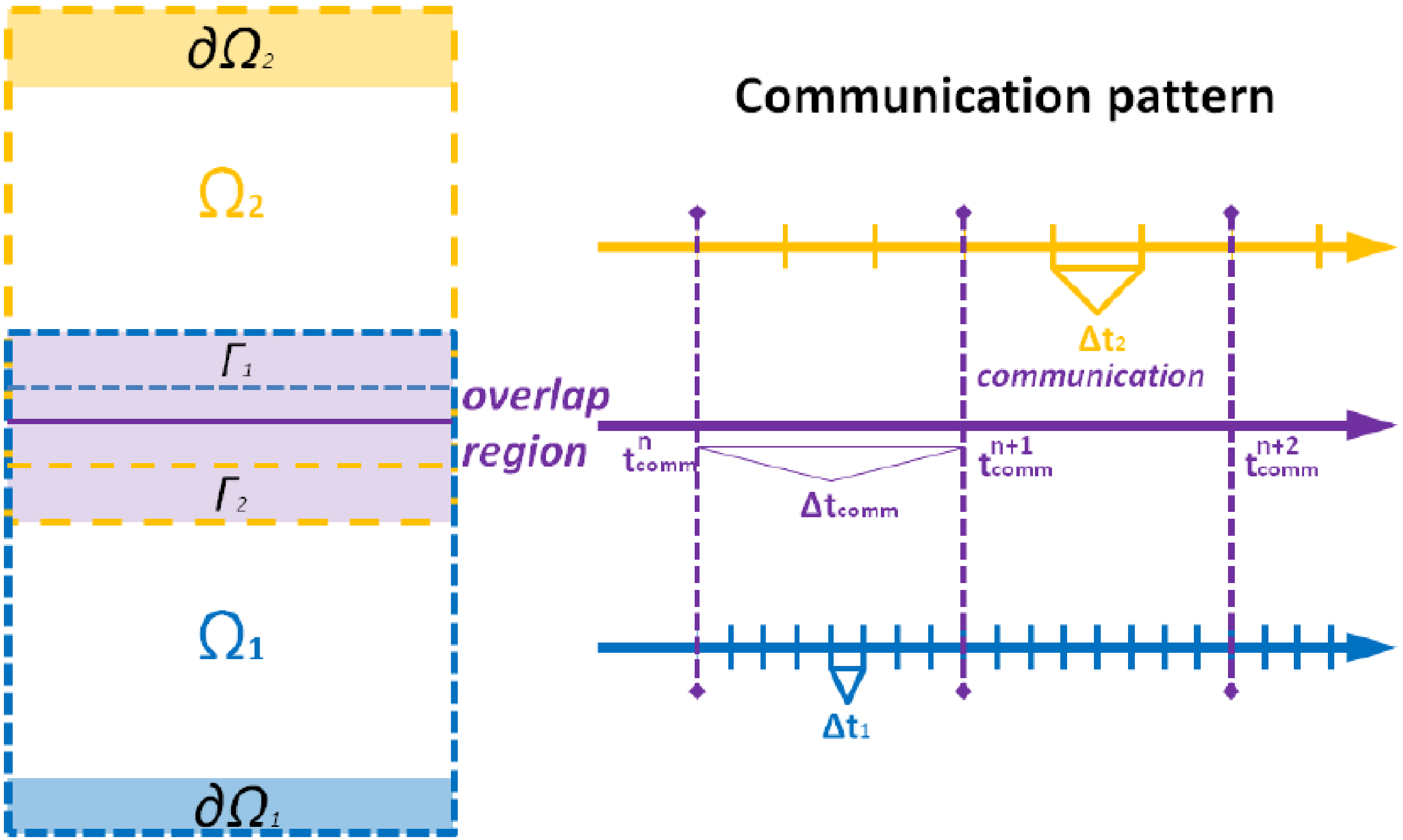
$$N_{B_i}^{t_2^n} = N_{B_i}^{t_2^{n-1}} + d_{B_i} v_{B_i,y} \Delta x_2 \Delta t_2. \quad (22)$$

$A_i$ are regular points spaced $\Delta x_1$ along $c_1$,
$B_i$ are regular points spaced $\Delta x_2$ along $c_2$.
when $N^t > 1$ insert one particle and $N^t - = 1$

[4] Bian et al. 2015b, *J. Comput. Phys.*

# Parallel integrations/intermediate communications

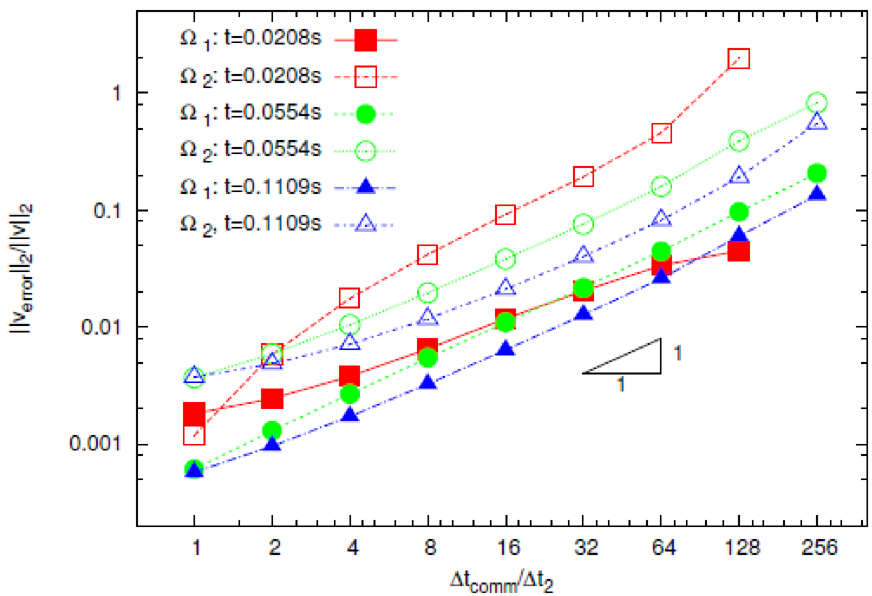
- $\Delta t_2 = N_s \Delta t_1$ and $\Delta t_{comm} = N_c \Delta t_2$



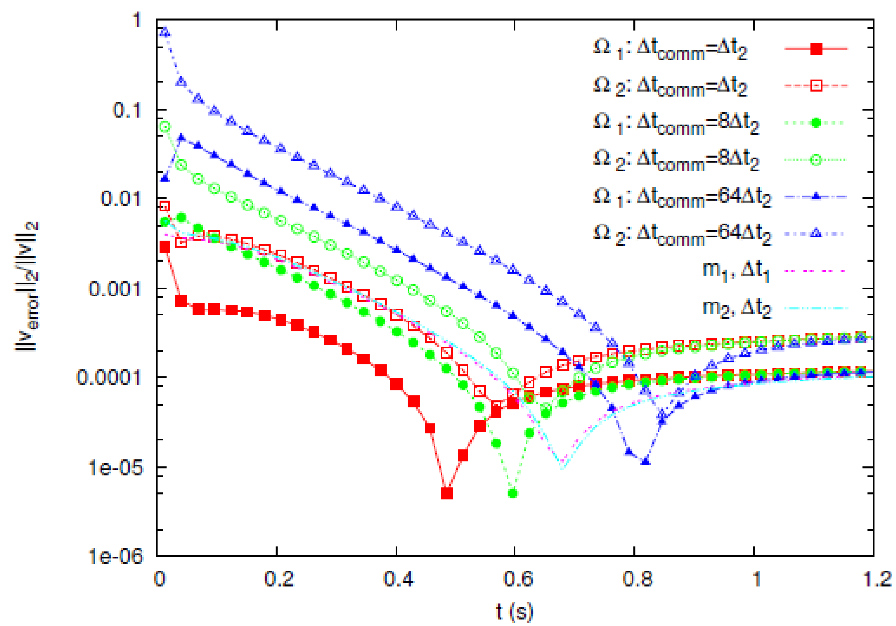

- at each $\Delta t_{comm}$, a quasi-steady state is assumed

# Numerical errors due to intermediate communications

- Transient Couette flow:
  - $v_x \neq 0$ and $\partial v_x / \partial y > 0$
  - hybrid reference line $y_a = L_y/2$
  - $m_2 = 8m_1$ and $\Delta t_2 = 4\Delta t_1$



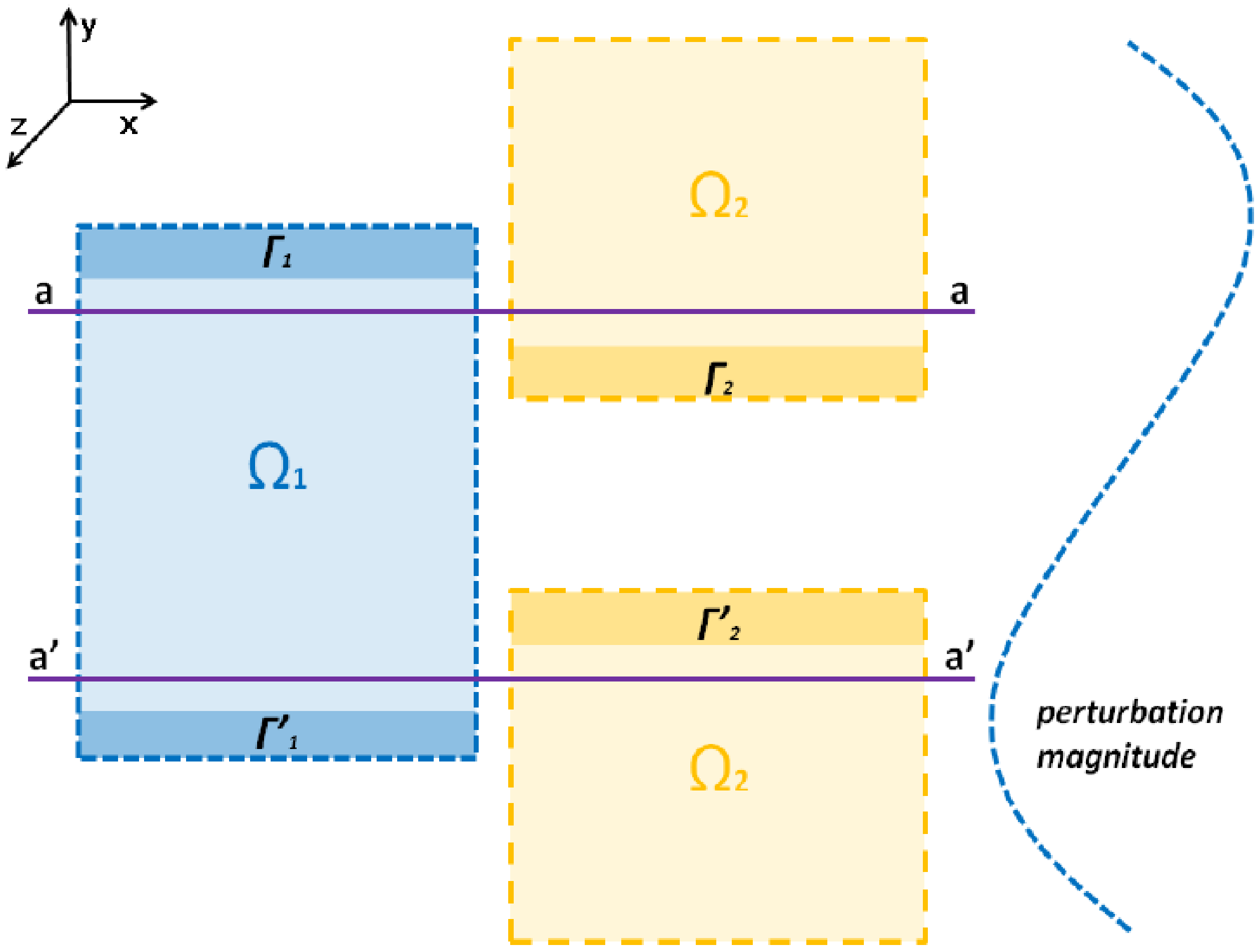

errors vs. $t_{comm}$ at three snapshots




errors vs time for three $t_{comm}$s.

solid symbols for $\Omega_1$ (fine resolution) and empty for $\Omega_2$ (coarse resolution)

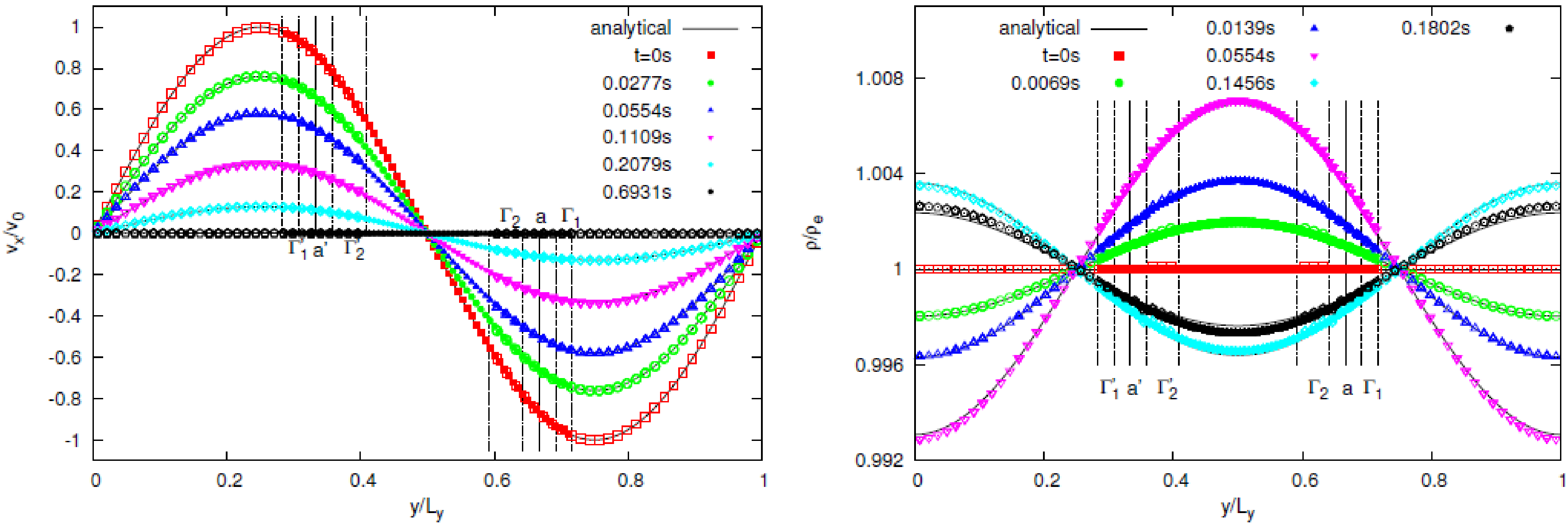
# Perturbations on coupled sub-domains




- periodic in all directions
- initial velocity either in $x$ (transversal) or in $y$ (longitudinal)

# Vorticity diffusion and sound wave across hybrid interface

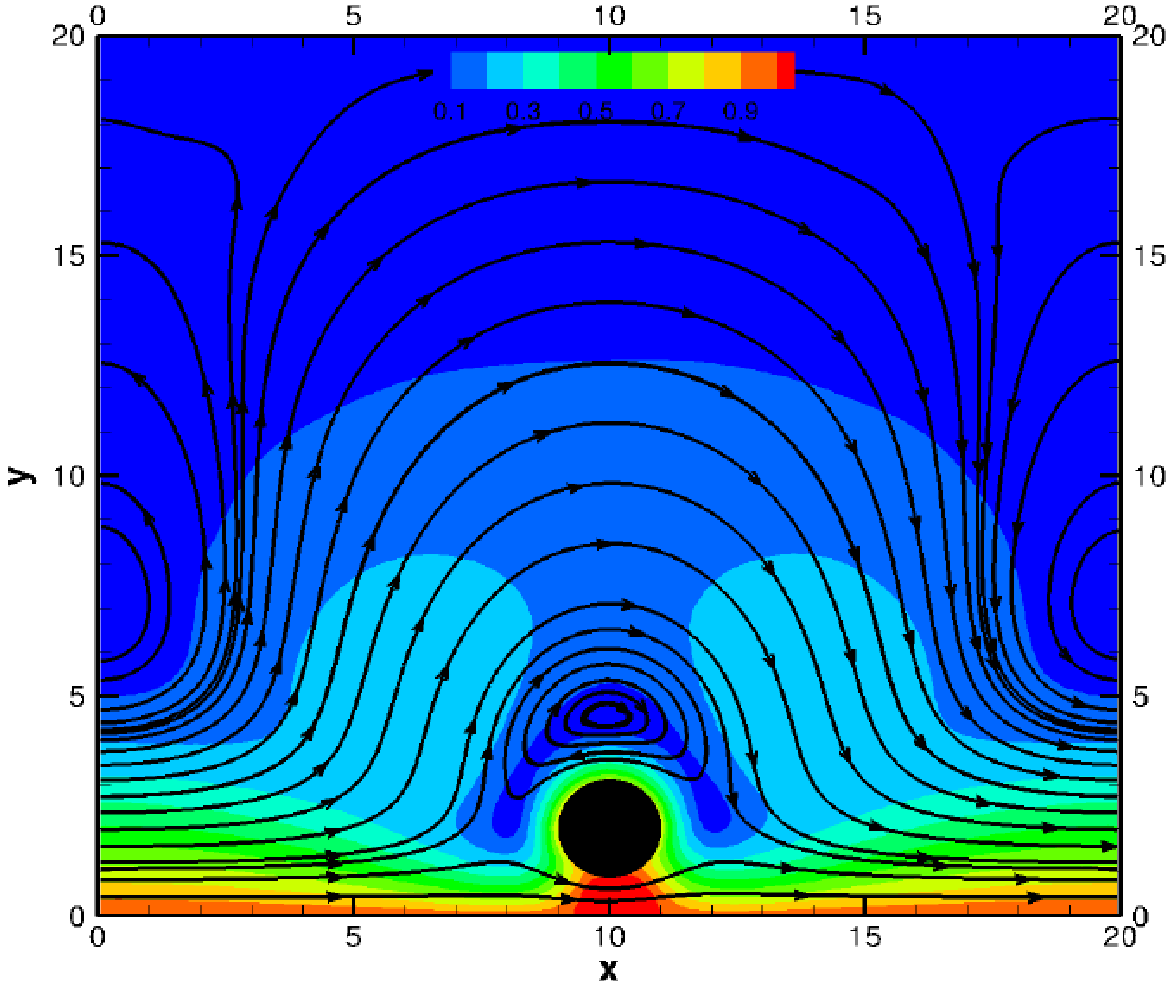
- multi-resolution SPH: $m_2 = 8m_1$ and $\Delta t_2 = 4\Delta t_1$




transversal perturbation ($v_x \neq 0$) longitudinal perturbation ($v_y \neq 0$)

# Wannier-like flow: $Re = 0.0946$

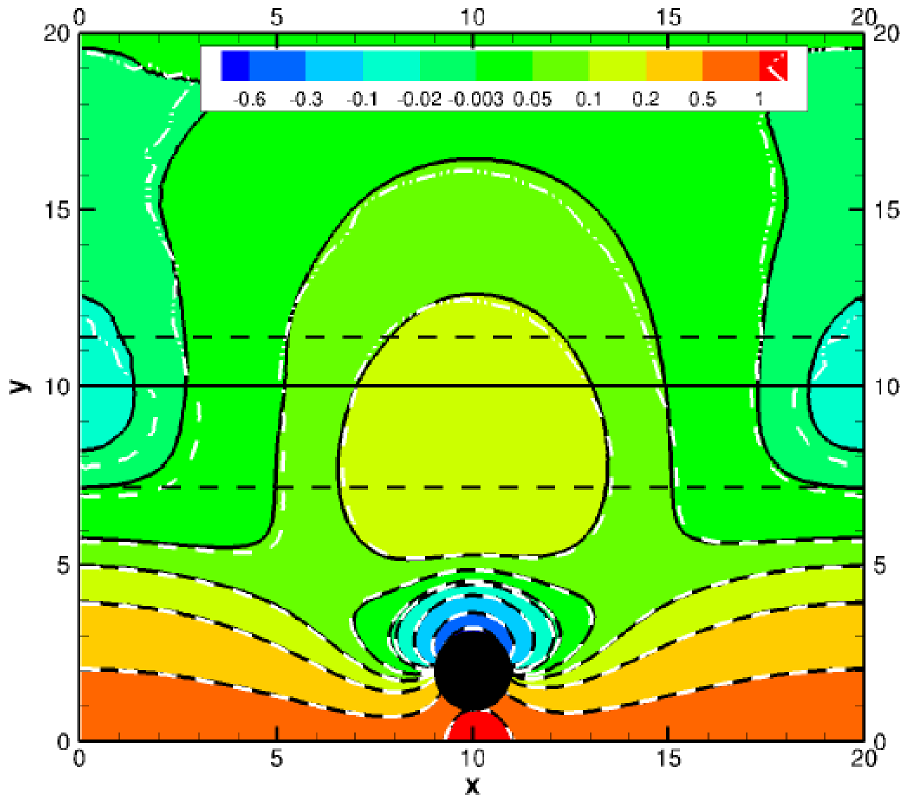
- single high resolution SPH: $N = 41504$



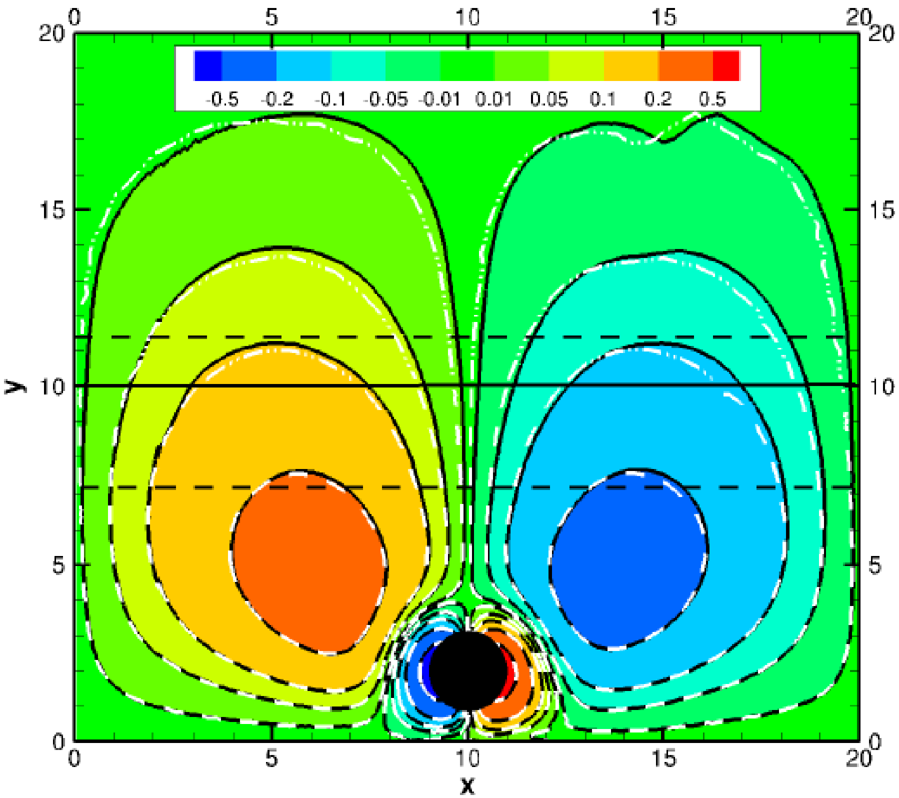

A cylinder confined in channel flow: streamlines

# Wannier-like flow: two and single resolutions[5]

- $m_2 = 16m_1$ and $\Delta t_2 = 16\Delta t_1$
- $N_1 = 23704$ and $N_2 = 1850$




velocity contour: $v_x$




velocity contour: $v_y$

[5]Bian et al. 2015b, *J. Comput. Phys.*

# Outline

# The Landau-Lifshitz-Navier-Stokes (LLNS) equations[6]

The equations of continuity and dynamics for an isothermal fluid read as,

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\rho + \rho\nabla\cdot\mathbf{v} = 0, \tag{23}$$

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\mathbf{v} + \nabla\cdot\mathbf{\Pi} = 0, \tag{24}$$

where the stress tensor consist of three components

$$\Pi_{\mu\sigma} = \Pi^{C}_{\mu\sigma} + \Pi^{D}_{\mu\sigma} + \Pi^{R}_{\mu\sigma}. \tag{25}$$

$$\Pi^{C}_{\mu\sigma} = p\delta_{\mu\sigma}, \tag{26}$$

$$\Pi^{D}_{\mu\sigma} = -\eta\left(\frac{\partial v_\mu}{\partial x_\sigma} + \frac{\partial v_\sigma}{\partial x_\mu} - \frac{2}{3}\delta_{\mu\sigma}\frac{\partial v_\epsilon}{\partial v_\epsilon}\right) - \zeta\delta_{\mu\sigma}\frac{\partial v_\epsilon}{\partial x_\epsilon}, \tag{27}$$

$$< \Pi^{R}_{\mu\sigma} > = 0, \tag{28}$$

$$< \Pi^{R}_{\mu\sigma}(\mathbf{x},t)\Pi^{R}_{\epsilon\iota}(\mathbf{x}',t') > = 2k_B T\Delta_{\mu\sigma\epsilon l}\delta(\mathbf{x}-\mathbf{x}')\delta(t-t'), \tag{29}$$

$$\Delta_{\mu\sigma\epsilon\iota} = \eta\left(\delta_{\mu\epsilon}\delta_{\sigma\iota} + \delta_{\mu\iota}\delta_{\sigma\epsilon}\right) + \left(\zeta - \frac{2}{3}\eta\right)\delta_{\mu\sigma}\delta_{\epsilon\iota} \tag{30}$$

# Linearization of LLNS

The fluctuations on the state variables are defined as

$$\mathbf{z}(\mathbf{x},t) = [\delta\rho(\mathbf{x},t), \delta\mathbf{v}(\mathbf{x},t)], \tag{31}$$

with $\rho = \rho_0 + \delta\rho =< \rho > +\delta\rho$ and $\mathbf{v} = \mathbf{v}_0 + \delta\mathbf{v} = \delta\mathbf{v}$.
Neglecting the second order in fluctuations we get

$$\begin{aligned} \frac{\partial \delta\rho}{\partial t} + \rho_0 \nabla \cdot \delta\mathbf{v} &= 0, & (32) \\ \frac{\partial \delta v_\mu}{\partial t} + \frac{c_T^2}{\rho_0}\frac{\partial}{\partial x_\mu}\delta\rho - \nu\nabla^2\delta v_\mu - \left(\kappa + \frac{\nu}{3}\right)\frac{\partial}{\partial x_\mu}\nabla\cdot\delta\mathbf{v} &= -\frac{1}{\rho_0}\frac{\partial}{\partial x_\mu}\sigma^R_{\mu\sigma}, \end{aligned}$$

After spatial Fourier transform, we write in a compact form

$$\frac{\partial \widehat{z}_\epsilon(\mathbf{k},t)}{\partial t} = -\mathcal{L}_{\epsilon\iota}(\mathbf{k},t)\widehat{z}_\iota(\mathbf{k},t) \tag{33}$$

where $\mathcal{L}$ is the hydrodynamic matrix. Solve Eq. (33) to get evolutions and correlations of fluctuations.

# Summary of theory: correlation functions of fluctuations[7]

- in k-space: spatial Fourier transform of fluctuations

$$\frac{< g_\perp(k,t) g_\perp(k,t+\tau) >}{\sigma^2[g_\perp(k,t)]} = e^{-\nu k^2 \tau}, \quad (34)$$

$$\frac{< g_{||}(k,t) g_{||}(k,t+\tau) >}{\sigma^2\left[g_{||}(k,t)\right]} = e^{-\Gamma_T k^2 \tau} cos(c_T k\tau), \quad (35)$$

$$\frac{< \rho(k,t) \rho(k,t+\tau) >}{\sigma^2\left[\rho(k,t)\right]} = e^{-\Gamma_T k^2 \tau} cos(c_T k\tau), \quad (36)$$

$$\frac{< g_{||}(k,t) i\rho(k,t+\tau) >}{\sigma^2\left[g_{||}(k,t)\right]/c_T} = e^{-\Gamma_T k^2 \tau} sin(c_T k\tau), \quad (37)$$

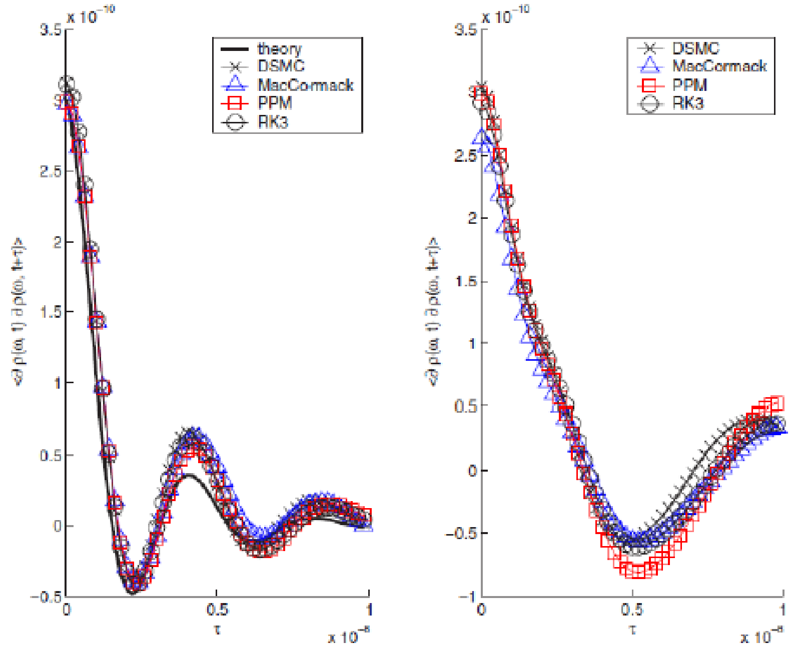
$$\frac{< \rho(k,t) i g_{||}(k,t+\tau) >}{\sigma^2\left[g_{||}(k,t)\right]/c_T} = -e^{-\Gamma_T k^2 \tau} sin(c_T k\tau), \quad (38)$$

- $\Gamma_T = (4\eta/3 + \zeta)/2\rho$: sound attenuation coefficient

[7] Ernst et al. 1971, *Phys. Rev. A*; . Boon et al. 1991; Hansen et al. 2013.

# Discretization of the LLNS equations.

- Eulerian discretization of SPDE




FVM with various temporal schemes (periodic versus specular wall)

- no guarantee of thermodynamic consistency on the discrete level
- some improvement has been done recently

- Lagrangian mesoscopic particle methods: thermodynamic consistency
  - dissipative particle dynamics
  - smoothed dissipative particle dynamics
- GENERIC framework[a]
  - discrete form easily cast into its formulation

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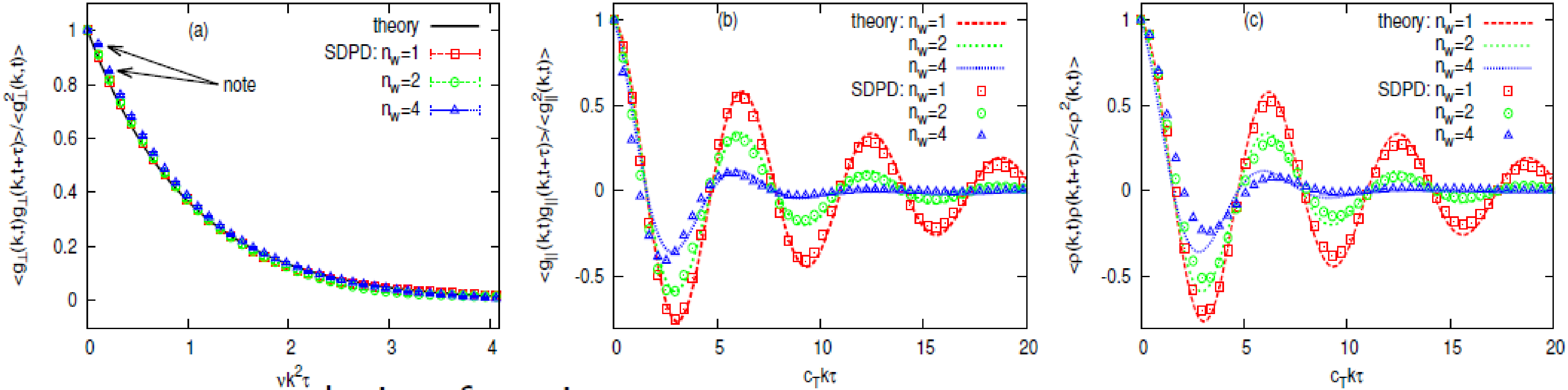
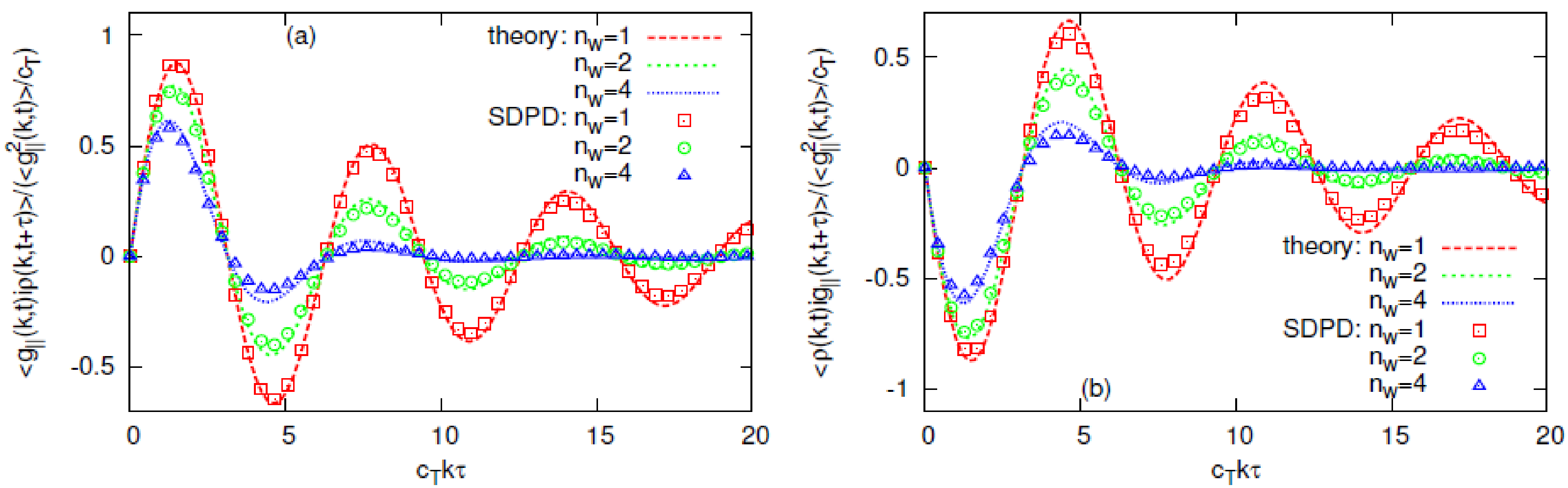
[a] Öttinger et al. 1997b, *Phy. Rev. E*.

# SDPD simulation: correlation of fluctuations in pbc[7]

- autocorrelation functions




- cross-correlation functions




[7] X. Bian et al. (2015a). "Fluctuating hydrodynamics in periodic domains and heterogeneous adjacent multidomains: Thermal equilibrium". In: *Phys. Rev. E* 92 (5), p. 053302. DOI: 10.1103/PhysRevE.92.053302.

# DPD fluid properties: measured by correlation functions[8]

Given trajectories, we calculate

$$< u(k,t) w(k,t+\tau) >=$$

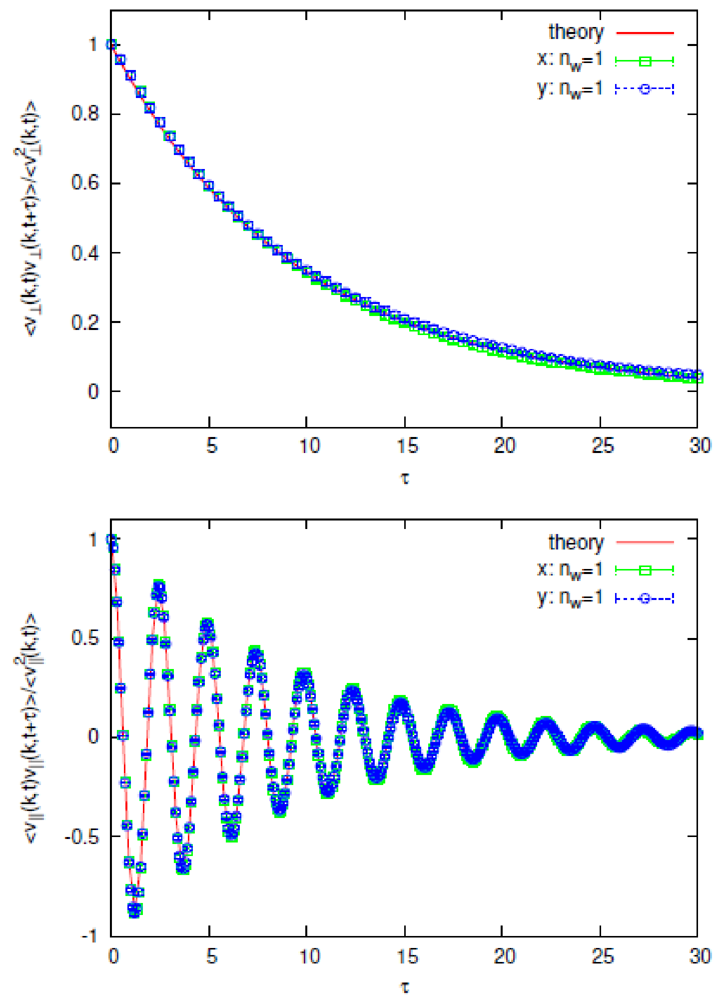
$$\frac{1}{N_s}\sum_{s=1}^{N_s} \hat{f}_k(u(\mathbf{x},t))\hat{f}_k(w(\mathbf{x},t+\tau)), \quad (28)$$

where Fourier transform is defined as

$$\hat{f}_k(u(\mathbf{x},t)) = \frac{1}{N_p}\sum_{j=1}^{N_p} u(\mathbf{x_j},t)e^{-i\mathbf{k}\cdot\mathbf{x}_j(t)}. \quad (29)$$

From Eqs.(23) and (24), we infer the fluid properties as

- $\eta = 1.077$, $c_T = 4.085$, $\zeta = 0.718$

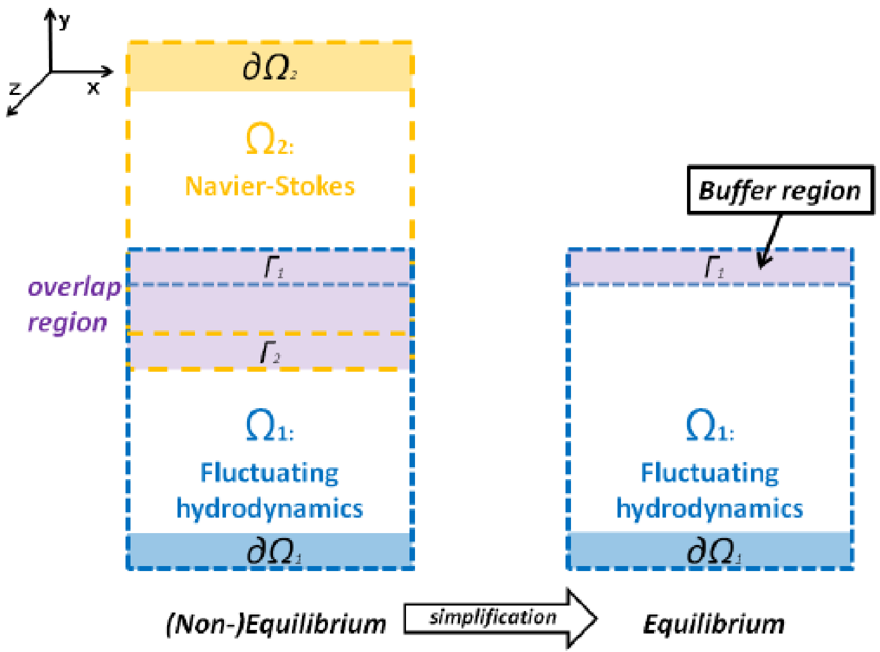


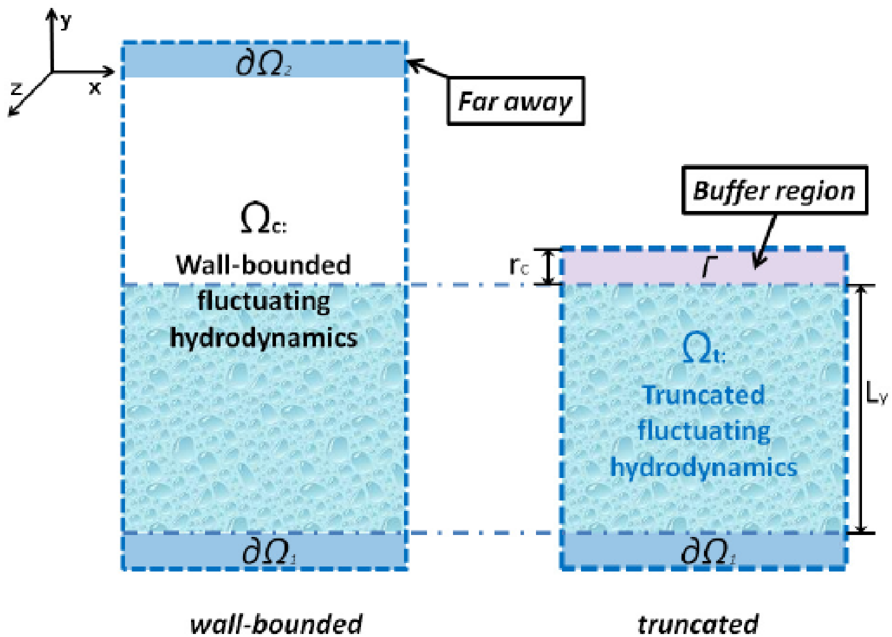

Transversal and longitudinal CFs

[8] Bian et al. 2015a, *Phys. Rev. E*.

# Fluctuations in a truncated domain at equilibrium

- continuum-particle coupling may be simplified by a truncated domain



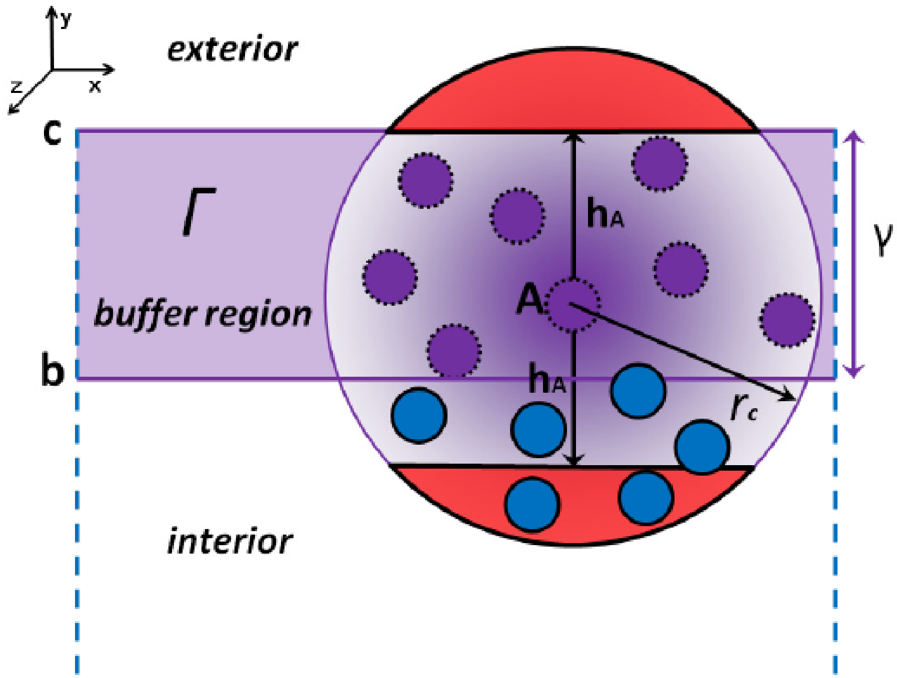




simplification of coupling    examined zone

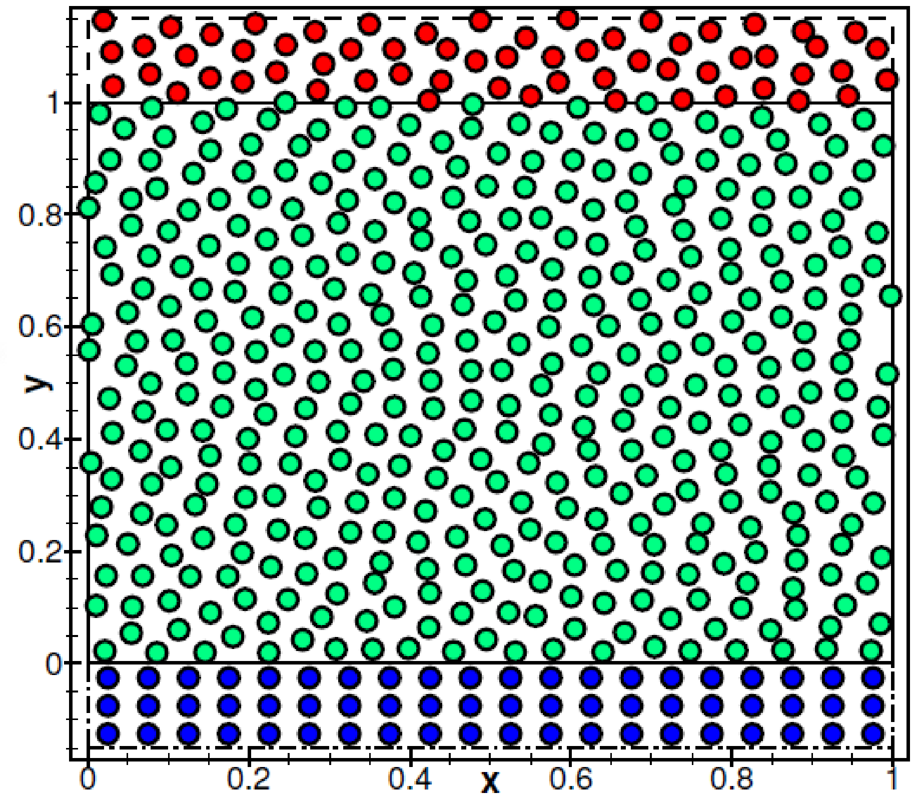
- we quantify the fluctuations in the shadowed zone

# A buffer boundary for the truncated domain

- velocity is from a Gaussian distribution
- density is from
  - a Gaussian distribution or
  - a conditional Gaussian distribution using Kriging
- missing pressure: conditional conservative force

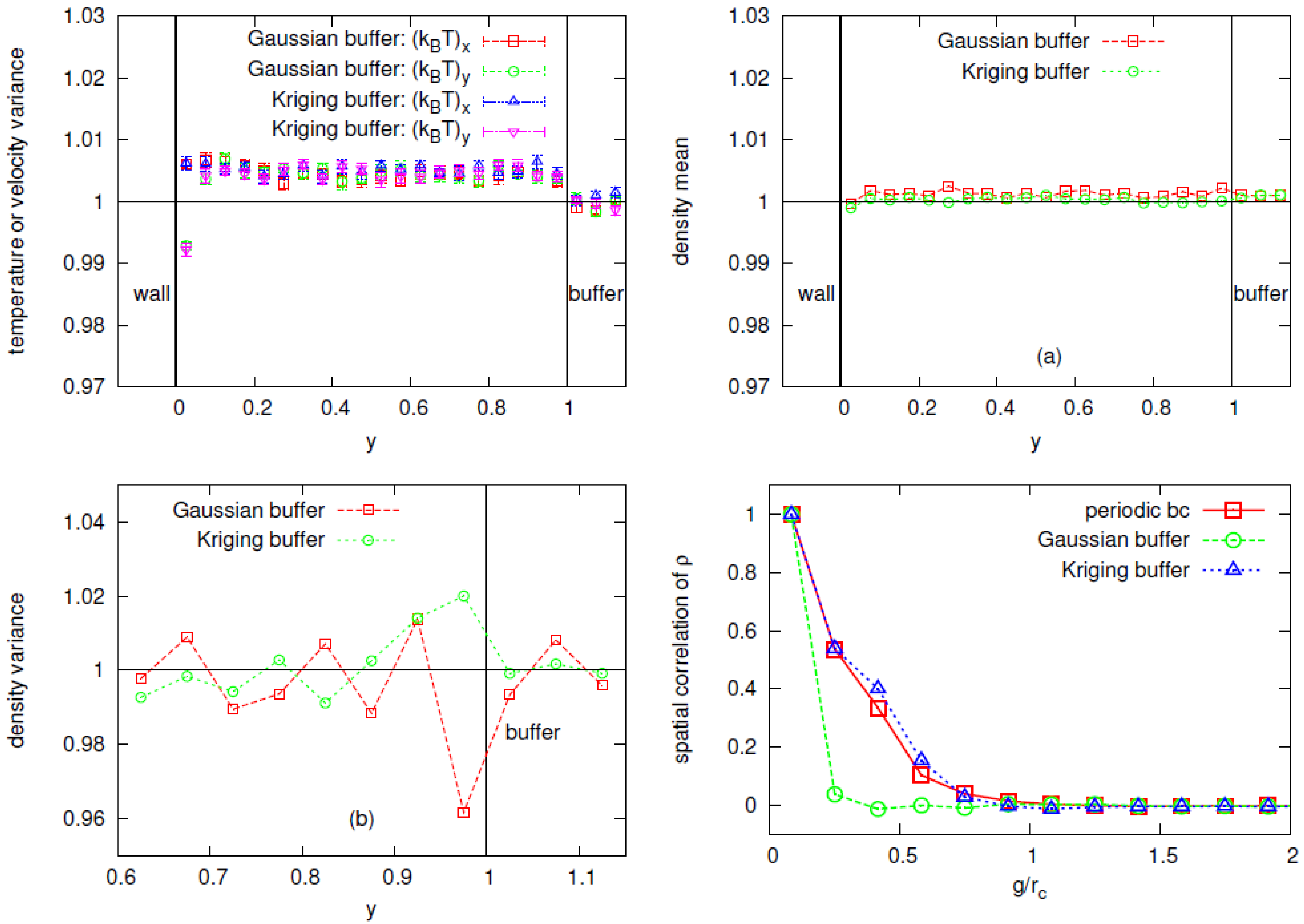



conditional conservative force

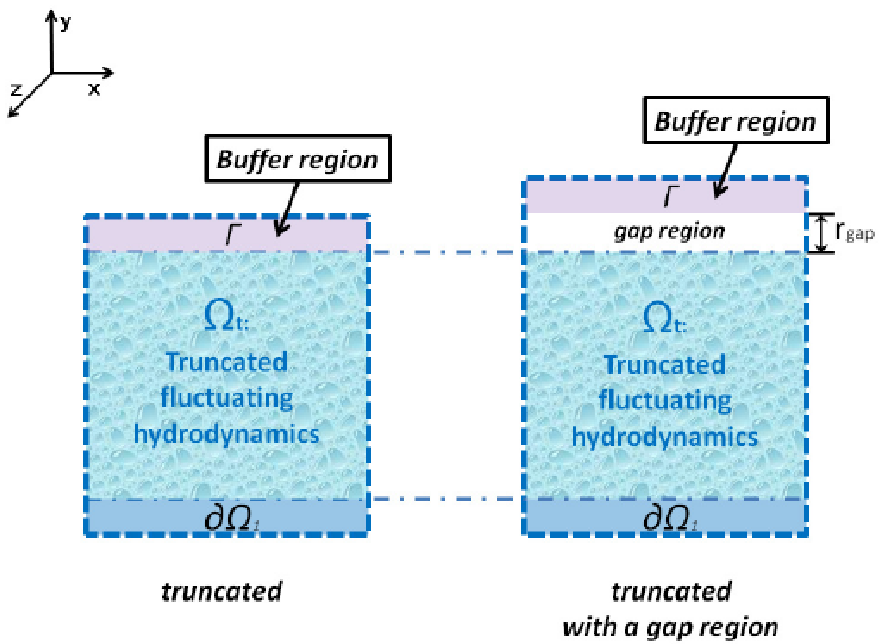



regular particle distribution

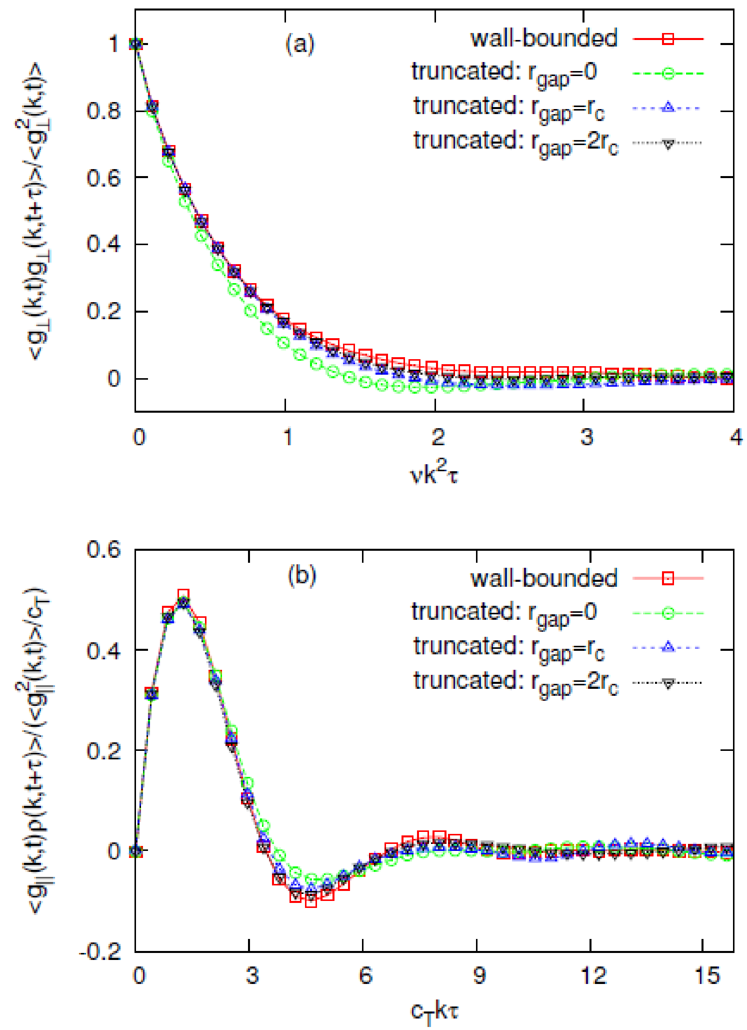
# Temperature, density, its variance, and spatial correlation



# Correlation functions of fluctuations in truncated domain[9]




introducing a gap to reduce errors




transversal and longit.-density CFs

[9]Bian et al. 2015a, *Phys. Rev. E.*

# Outline

# Perturbation theory at stationary state: ACFs of fluctuations in Lees-Edwards bc

- $\mathbf{k}(t) = (k_x, k_y - \dot{\gamma} t k_x, k_z)$: time-dependent
- $\mathbf{e}_1 = \mathbf{k}(t)/k(t), \mathbf{e}_2 = [\mathbf{e}_y - (\mathbf{e}_1 \cdot \mathbf{e}_y)\mathbf{e}_1]/k_\perp, \mathbf{e}_3 = \mathbf{e}_1 \times \mathbf{e}_2$
- $k_\perp = (k_x^2 + k_z^2)^{1/2}/k_0$, $k(t) = |\mathbf{k}(t)|$, $\mathbf{k}_0 = \mathbf{k}(0)$

$$C_{T_1}(\mathbf{k}, \tau) = \left(\frac{k_0}{k(\tau)}\right) e^{-\nu\alpha(\mathbf{k},\tau)}, \tag{30}$$

$$C_{T_2}(\mathbf{k}, \tau) = e^{-\nu\alpha(\mathbf{k},\tau)}, \tag{31}$$

$$C_L(\mathbf{k}, \tau) = \left(\frac{k(\tau)}{k_0}\right)^{1/2} e^{-\Gamma_T\alpha(\mathbf{k},\tau)} cos(c_T\beta(\mathbf{k}, \tau)). \tag{32}$$

$\alpha$ and $\beta$ are defined as

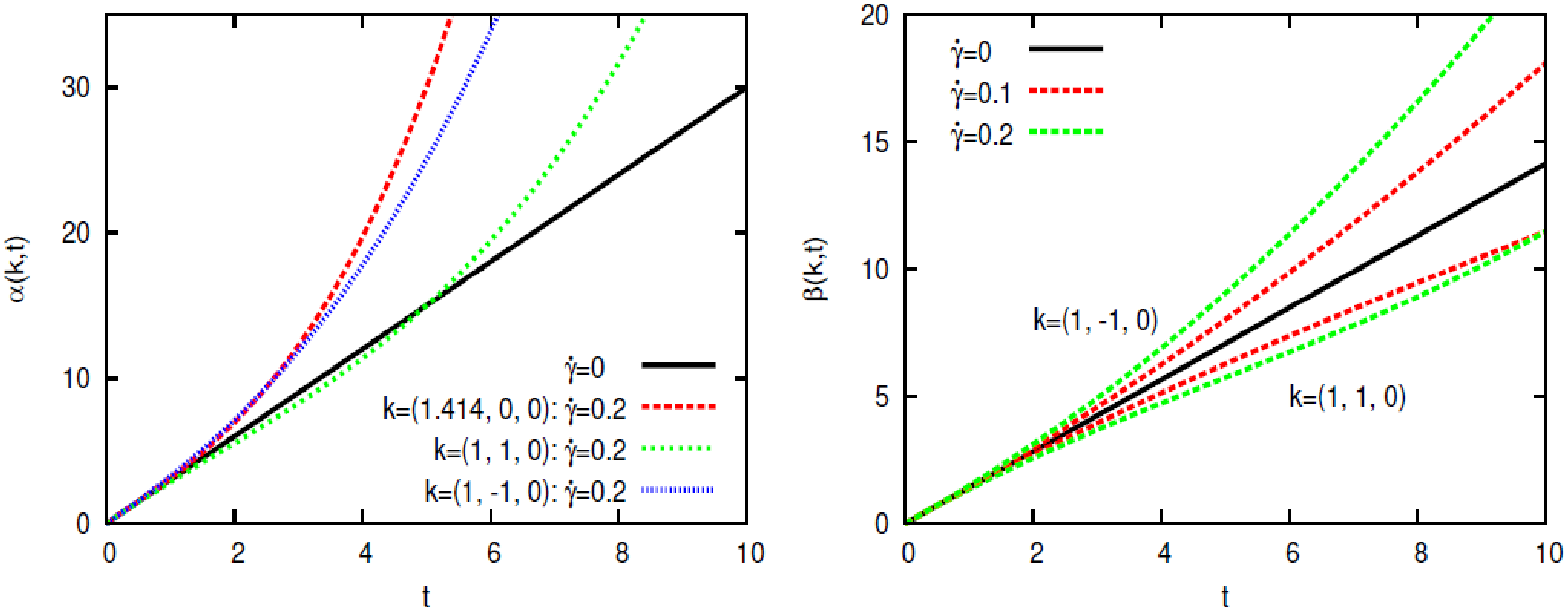
$$\alpha(\mathbf{k}, t) = k_0^2 t - \dot{\gamma} k_x k_y t^2 + \frac{1}{3}\dot{\gamma}^2 k_x^2 t^3, \tag{33}$$

$$\beta(\mathbf{k}, t) = \frac{1}{2\dot{\gamma} k_x}\left\{k_y k_0 - k_y(t)k(t) - k_\perp^2 ln\left[\frac{k_y(t) + k(t)}{k_y + k_0}\right]\right\}. \tag{34}$$

Lutsko et al. 1985, *Phys. Rev. A*; . Otsuki et al. 2009, *Phys. Rev. E*; . Varghese et al. 2015, *Phys. Rev. E*

# Exponent $\alpha(\mathbf{k}, t)$ and frequency $\beta(\mathbf{k}, t)$

- $\dot{\gamma} > 0$ versus $\dot{\gamma} = 0$ (equilibrium)

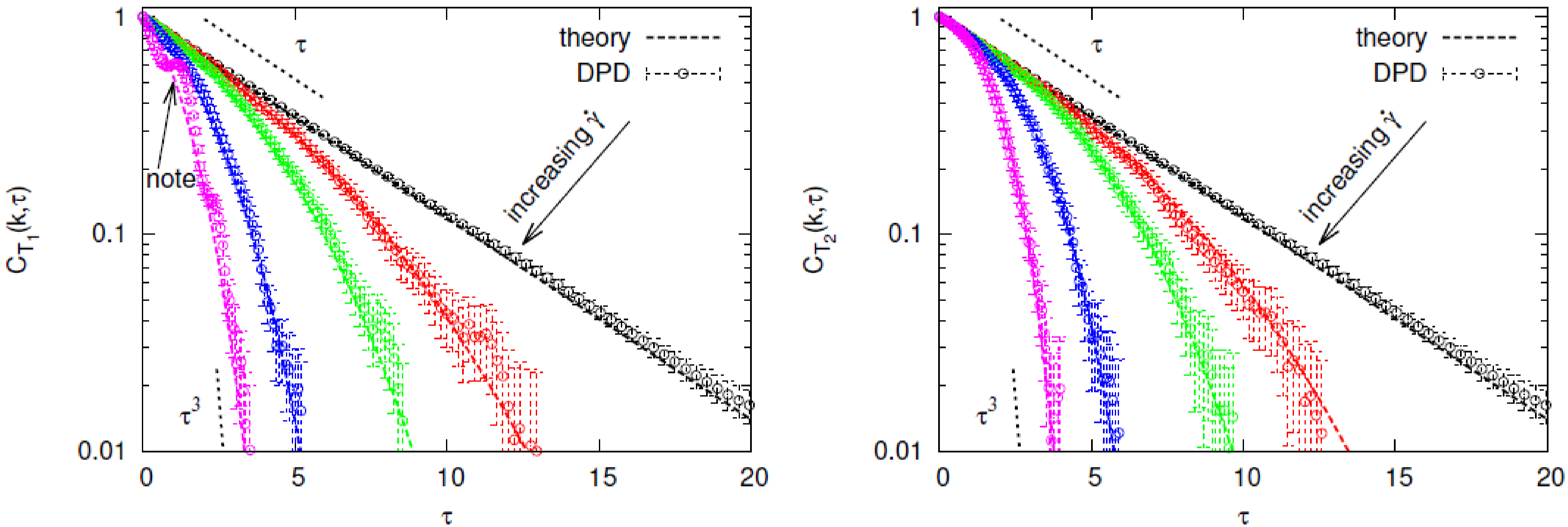



- transversal ACF: may decay faster or slower
- longitudinal ACF: sound frequency may be higher or lower

# DPD simulation 1: transversal ACFs of fluctuations[10]

- $\mathbf{k}_1 = (2\pi/L_x, 0, 0)$:

$$\alpha(\mathbf{k}, t) = k_0^2 t + \frac{1}{3}\dot{\gamma}^2 k_x^2 t^3 \quad (35)$$



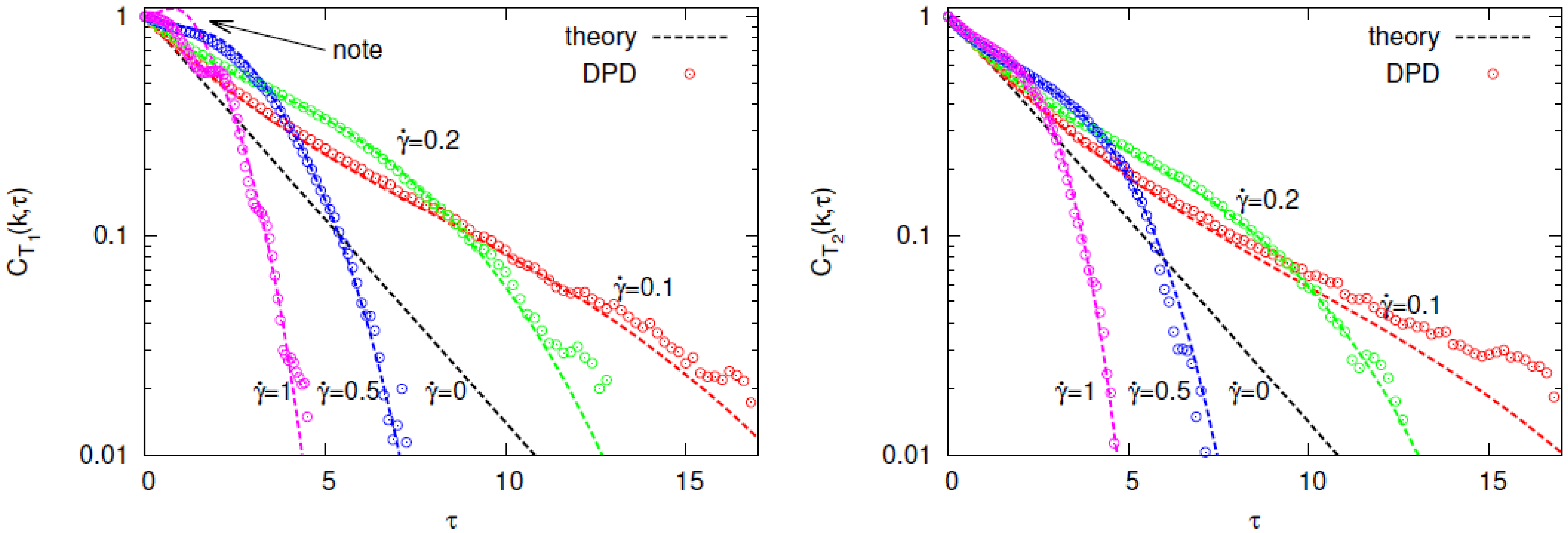

$\dot{\gamma} = 1.0, 0.5, 0.2, 0.1$ and 0 (at equilibrium)

[10] X. Bian et al. (2016c). "Correlations of hydrodynamic fluctuations in shear flow". In: *J. Fluid Mech. submitted*.

# DPD simulation 2: transversal ACFs of fluctuations[11]

- $\mathbf{k}_1 = (2\pi/L_x, 2\pi/L_y, 0)$

$$\alpha(\mathbf{k}, t) = k_0^2 t - \dot{\gamma} k_x k_y t^2 + \frac{1}{3}\dot{\gamma}^2 k_x^2 t^3 \quad (36)$$



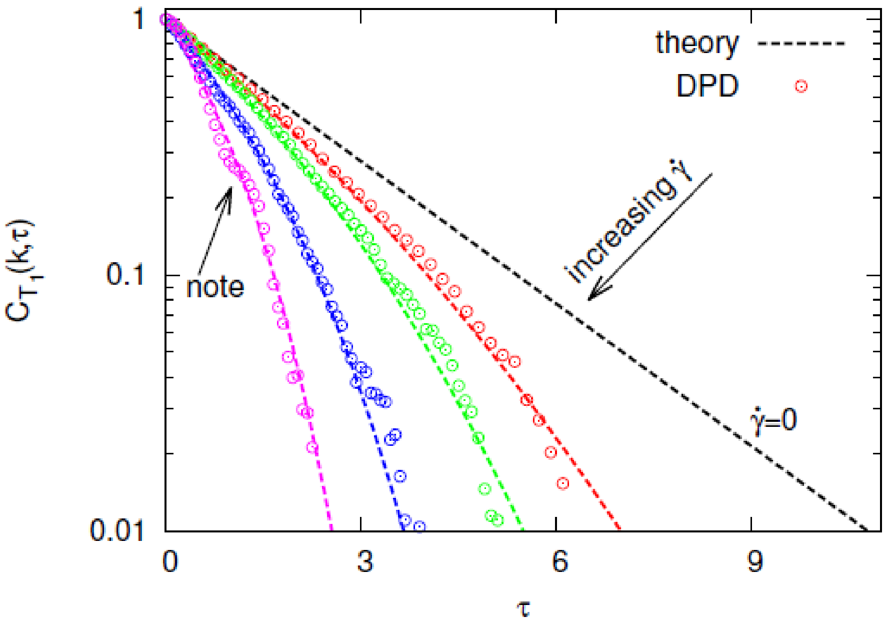

$\dot{\gamma} = 1.0, 0.5, 0.2, 0.1$ and 0 (at equilibrium)

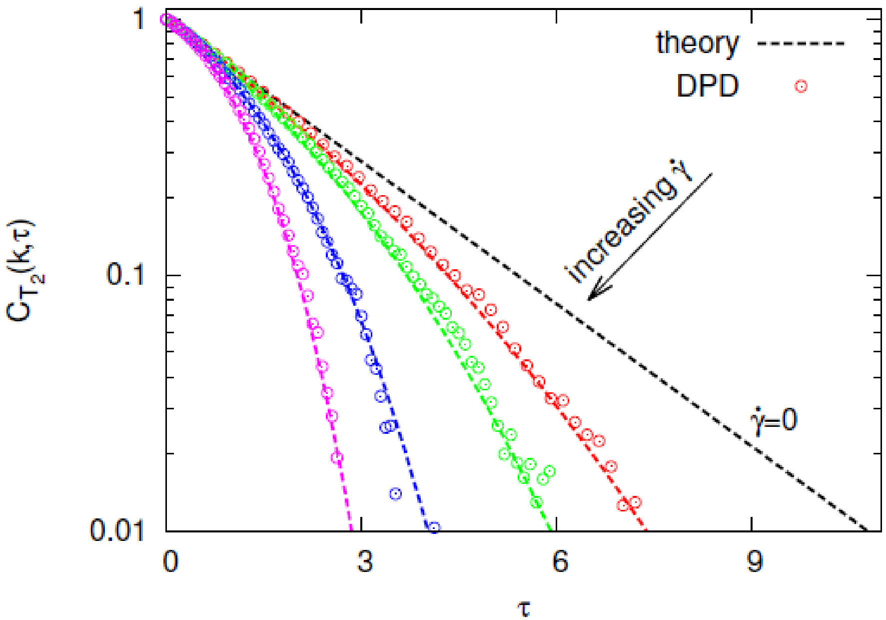
[11] Bian et al. 2016c, *J. Fluid Mech. submitted.*

# DPD simulation 3: transversal ACFs of fluctuations[12]

- $\mathbf{k}_1 = (2\pi/L_x, -2\pi/L_y, 0)$

$$\alpha(\mathbf{k}, t) = k_0^2 t - \dot{\gamma} k_x k_y t^2 + \frac{1}{3}\dot{\gamma}^2 k_x^2 t^3 \qquad (37)$$



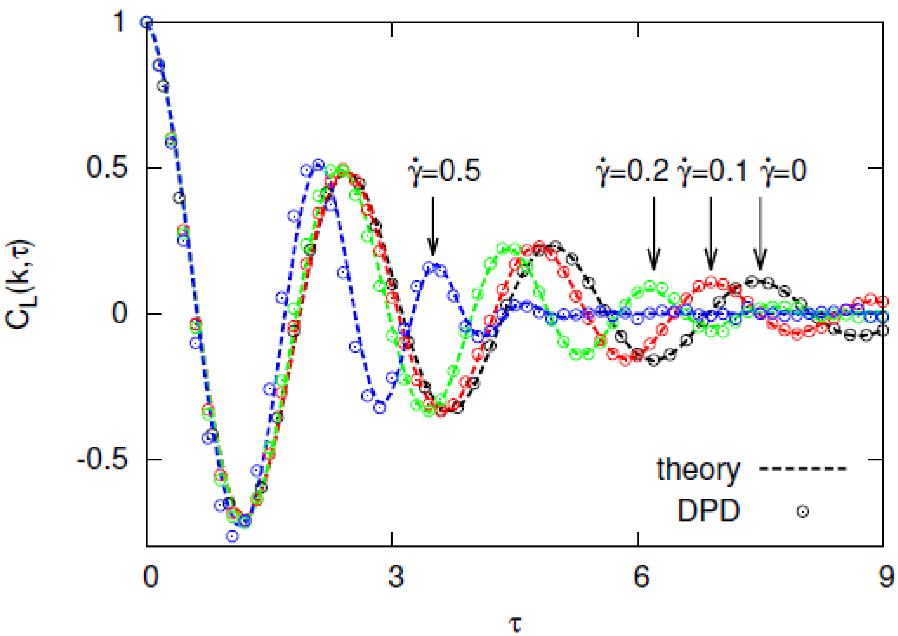

$\dot{\gamma} = 1.0, 0.5, 0.2, 0.1$ and 0 (at equilibrium)

[12] Bian et al. 2016c, *J. Fluid Mech. submitted.*

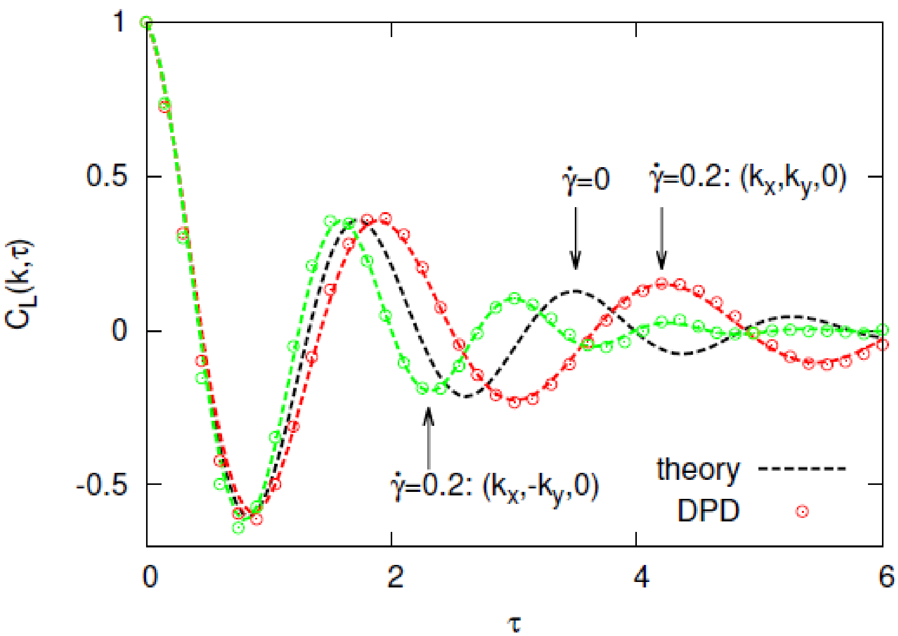
# DPD simulation 4: longitudinal ACFs of fluctuations[13]

- Doppler effects for $\dot{\gamma} > 0$

$$\beta(\mathbf{k}, t) = \frac{1}{2\dot{\gamma} k_x} \left\{ k_y k_0 - k_y(t) k(t) - k_\perp^2 \ln \left[ \frac{k_y(t) + k(t)}{k_y + k_0} \right] \right\} \quad (38)$$



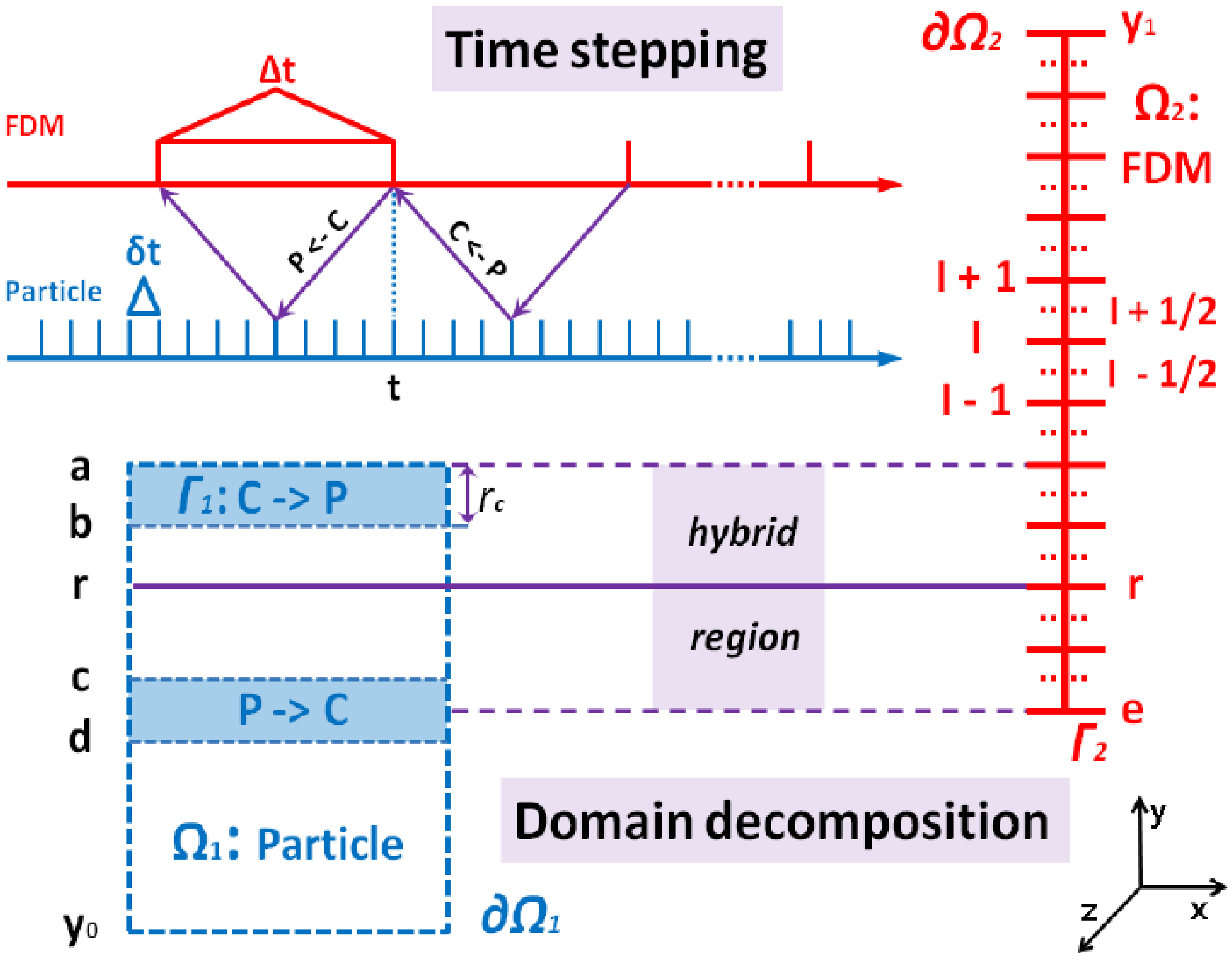

$\mathbf{k}_1 = (2\pi/L_x, 0, 0)$




$\mathbf{k}_1 = (2\pi/L_x, \pm 2\pi/L_y, 0)$

[13] Bian et al. 2016c, *J. Fluid Mech. submitted.*

# DDM: nonequilibrium coupling[14]




Sketch of coupling between particles and finite difference method: $\Delta t_{comm} = \Delta t$

[14] X. Bian et al. (2016a). "Analysis of hydrodynamic fluctuations in heterogeneous adjacent multidomains in shear flow". In: *Phys. Rev. E* 93 (3), p. 033312. DOI:

# DDM: artificial b.c. and constraint dynamics

- $P \rightarrow C$: simple spatial-temporal average

$$V_e = \frac{1}{N_t} \sum_{j=1}^{N_t} \frac{1}{N_{cd}} \sum_{i=1}^{N_{cd}} v_i \tag{39}$$

  - $N_{cd}$ is the instantaneous number of particles in cell $P \rightarrow C$
  - $N_t = \Delta t / \delta t$ (example latter $N_t = 180$, VACF is below 1.5% at $180\delta t$)

- at truncation line $a$:
  - mean pressure by integral function Lei et al. 2011, *J. Comput. Phys.*
  - specular reflection Bian et al. 2015b, *J. Comput. Phys.*

- $C \rightarrow P$: *non-holonomic constraint*

$$\frac{1}{N_{\Gamma_1}} \sum_{i=1}^{N_{\Gamma_1}} v_i = \overline{V}_{\Gamma_1}, \tag{40}$$

  - tends to be satisfied at every $\delta t$
  - leave thermal fluctuations unaffected as much as possible

# Constraint dynamics 1: relaxation dynamics

- idea: let the average of $\Gamma_1$ relax towards $\overline{V}_{\Gamma_1}$ over $\Delta t_{comm}$

$$\dot{v}_i = \frac{F_i}{m} + \frac{\epsilon}{\delta t}\left(\overline{V}_{\Gamma_1} - \frac{1}{N_{\Gamma_1}}\sum_{i=1}^{N_{\Gamma_1}} v_i\right), \tag{41}$$

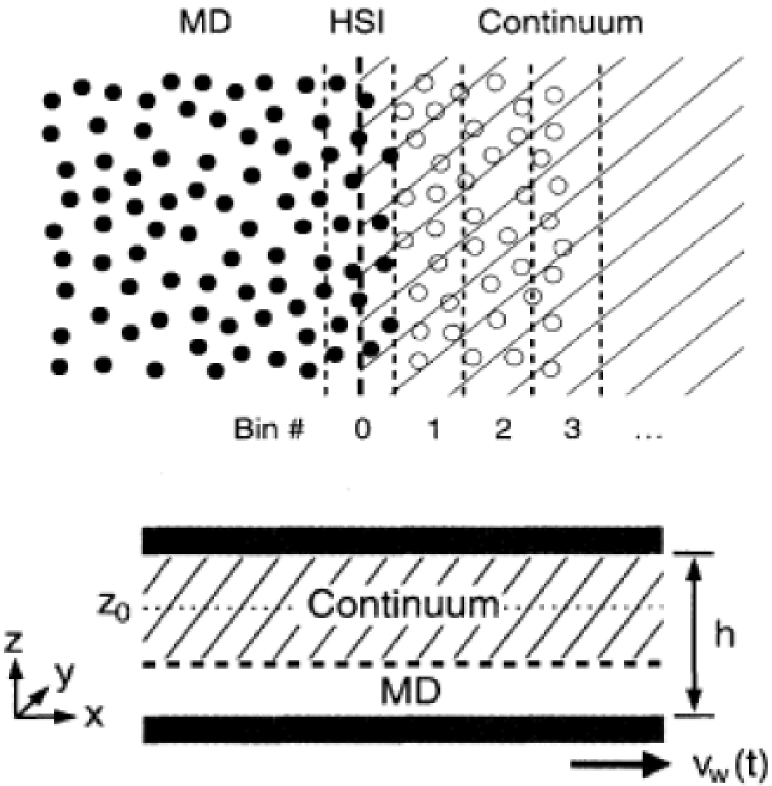
where $\mathbf{F}_i$ is the usual particle force and $\epsilon (= 0.01)$ is a tuning parameter

O'Connell et al. 1995, *Phys. Rev. E*

remark:

- little intrusion on fluctuations
- $\epsilon$ depends on both fluid properties and flow condition

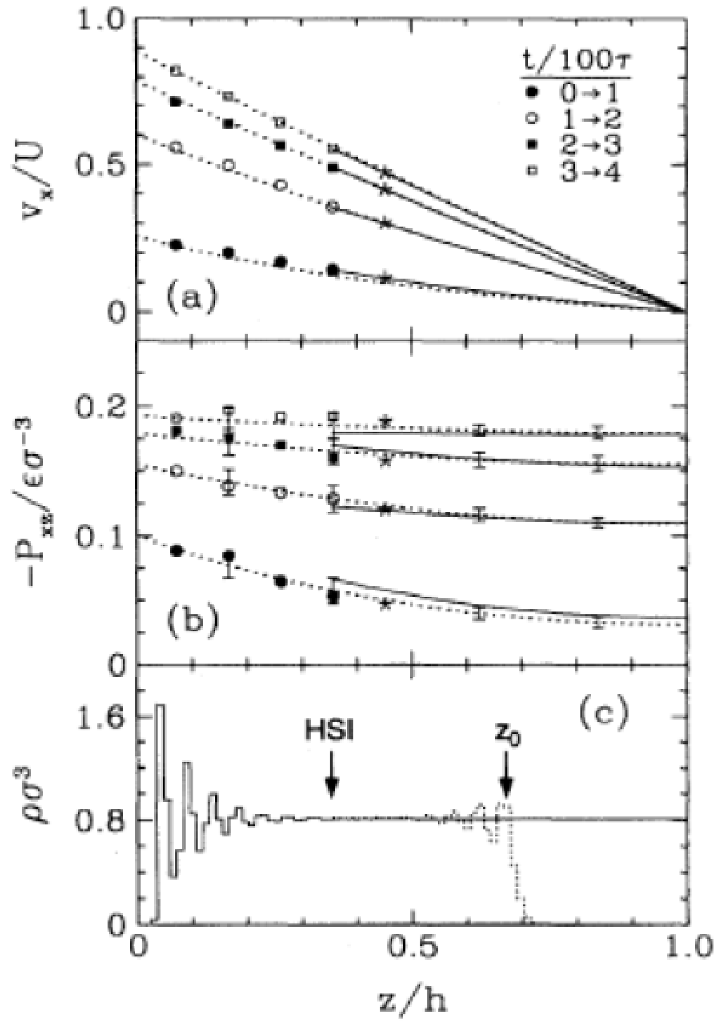
# Relaxation dynamics for Couette flow




Schematic for coupling MD-continuum and a setup for Couette flow

O'Connell et al. 1995, *Phys. Rev. E*

- velocity, shear stress and density



# Constraint dynamics 2: Maxwell buffer

- idea: equation of motion for particles in $\Gamma_1$ is shuffled at every $\delta t$
  - mean: interpolated from the continuum
  - fluctuation: drawn randomly

$$
\begin{aligned}
v_i &= V_i + \delta v_i, && (42)\\
V_i &= V_b + (V_a - V_b)(y_i - y_b)/\Delta y, && (43)\\
p(\delta v_i) &= \sqrt{\frac{m}{2\pi k_B T}} exp\left[\frac{-m(\delta v_i)^2}{2k_B T}\right], && (44)
\end{aligned}
$$

where $p$ is the Maxwell-Boltzmann distribution

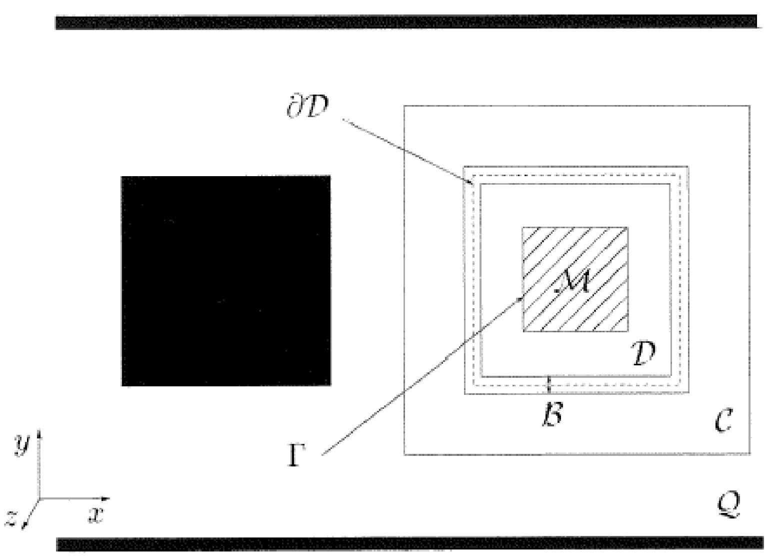
Hadjiconstantinou et al. 1997, *Int. J. Mod. Phys. C*

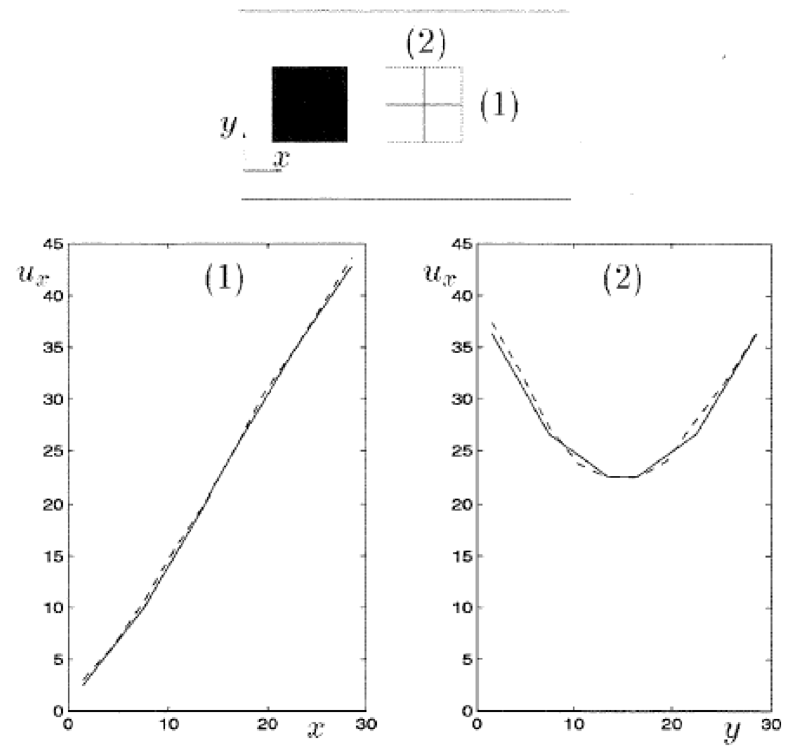
remark:

- very effective for the mean
- strong intervention: abrupt move on iso-surface ($T_c$) in phase-space

# Maxwell buffer for obstructed channel flow

- inflow: parabolic velocity
- outflow: no-stress




problem setup and velocity profiles at stead state

Hadjiconstantinou et al. 1997, *Int. J. Mod. Phys. C*

# Constraint dynamics 3: flux imposition

- idea: impose stress $\tau_a^{xy}$ on the interface

$$\dot{v}_i = \frac{F_i}{m} + F_i^{\mathcal{T}}, \quad (45)$$

$$F_i^{\mathcal{T}} = \tau_a^{xy} A \lambda(y_i), \quad (46)$$

where $A$ is the interface area and

$$\lambda(y_i) = g(y_i) / \sum_{i=1}^{N_{\Gamma_1}} g(y_i), \quad (47)$$

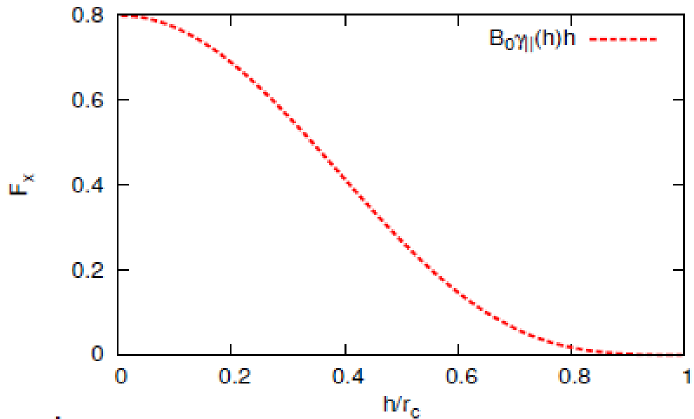
is an arbitrary but normalized function in the original work.

Flekkøy et al. 2000, *Europhys. Lett.*

- if assuming linear shear locally

Ren 2007, *J. Comput. Phys.*

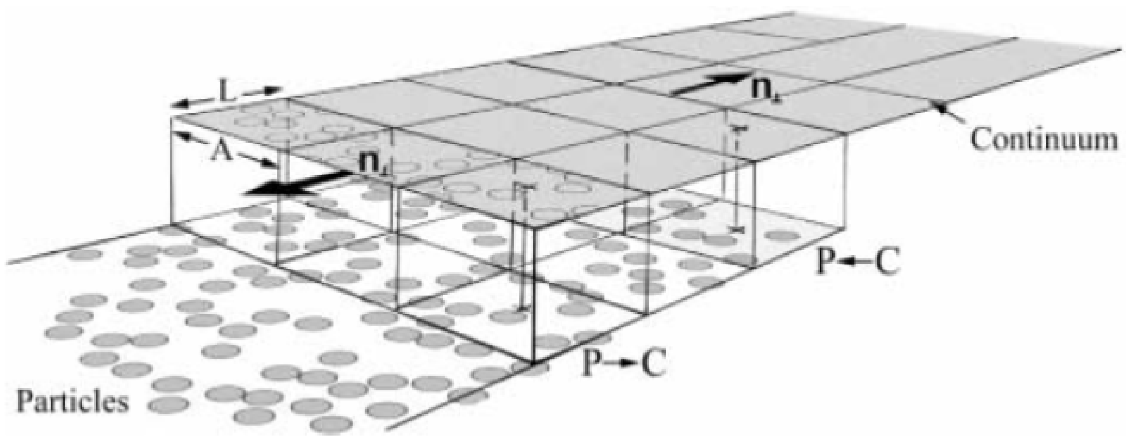
$$F_i^{\mathcal{T}} = B_0 \tau_a^{xy} \gamma_{||}^{D}(h) h, \quad (48)$$



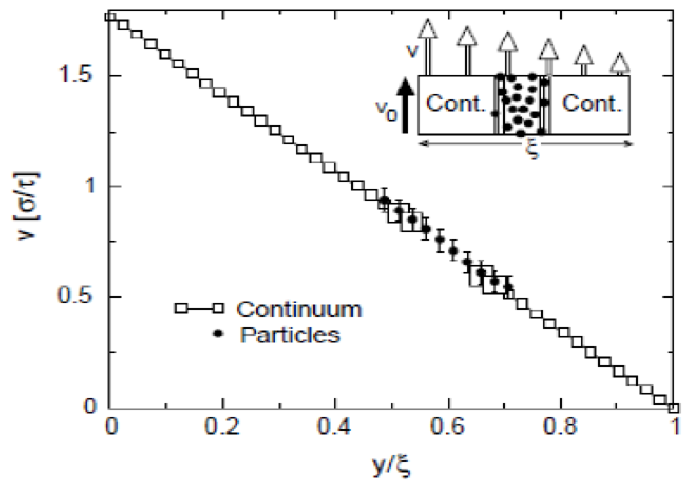

remark:

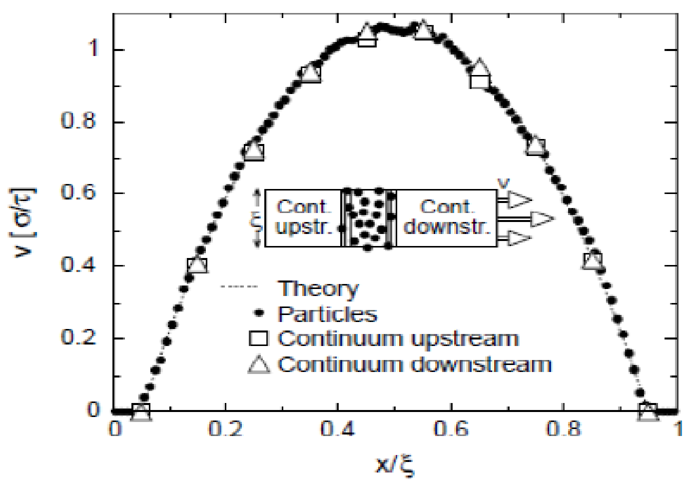
- more fundamental, two fluids may have different properties
- conservative? not really
- $B_0$ depends on fluids property and flow conditions

# Flux imposition for Couette and Poiseuille flows




Flux exchange in an overlapping region




Couette and Poiseuille flows at steady state

Flekkøy et al. 2000, *Europhys. Lett.*

# Constraint dynamics 4: least constraint dynamics

- idea: principle of least constraint (non-holonomic on $\overline{V}_{\Gamma_1}$)

$$\dot{v}_i = \frac{F_i}{m} - \frac{1}{N_{\Gamma_1}} \sum_{i=1}^{N_{\Gamma_1}} \frac{F_i}{m} + \frac{1}{\delta t} \left( \overline{V}_{\Gamma_1} - \frac{1}{N_{\Gamma_1}} \sum_{i=1}^{N_{\Gamma_1}} v_i \right), \quad (49)$$

where $\mathbf{F}_i$ is the usual particle force

Nie et al. 2004, *J. Fluid Mech.*

- alternative but equivalent idea: body force adjustment

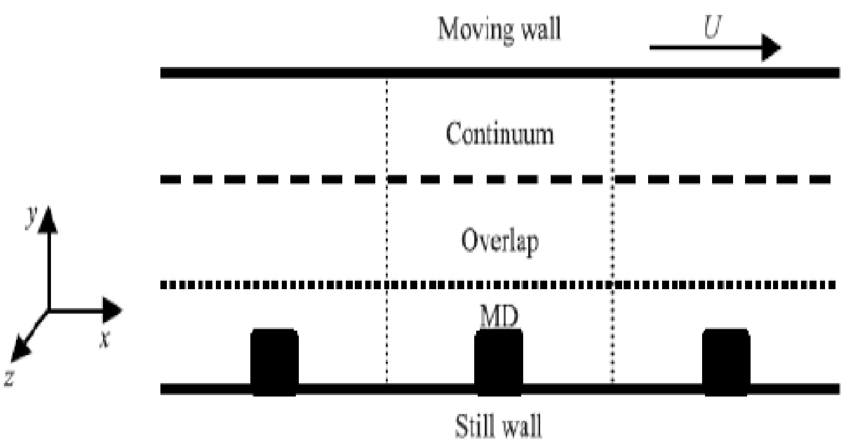
Werder et al. 2005, *J. Comput. Phys.*

remark:

- little intrusion on fluctuations
- non-holonomic constraint at every $\delta t$ too strong? $\epsilon$ again?

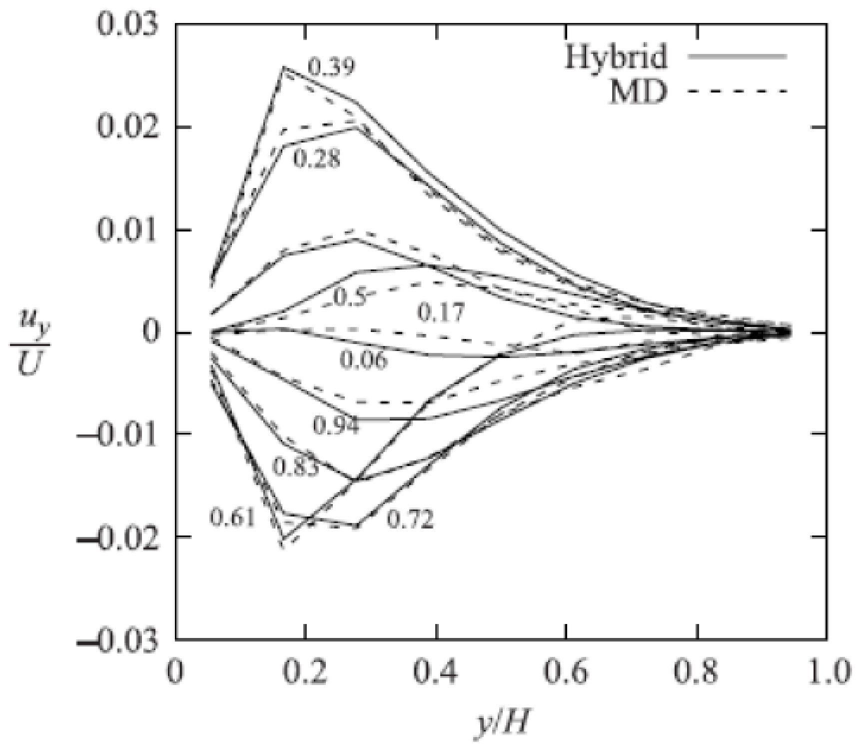
# Least constrain dynamics for channel flow

- nano-scale rough walls



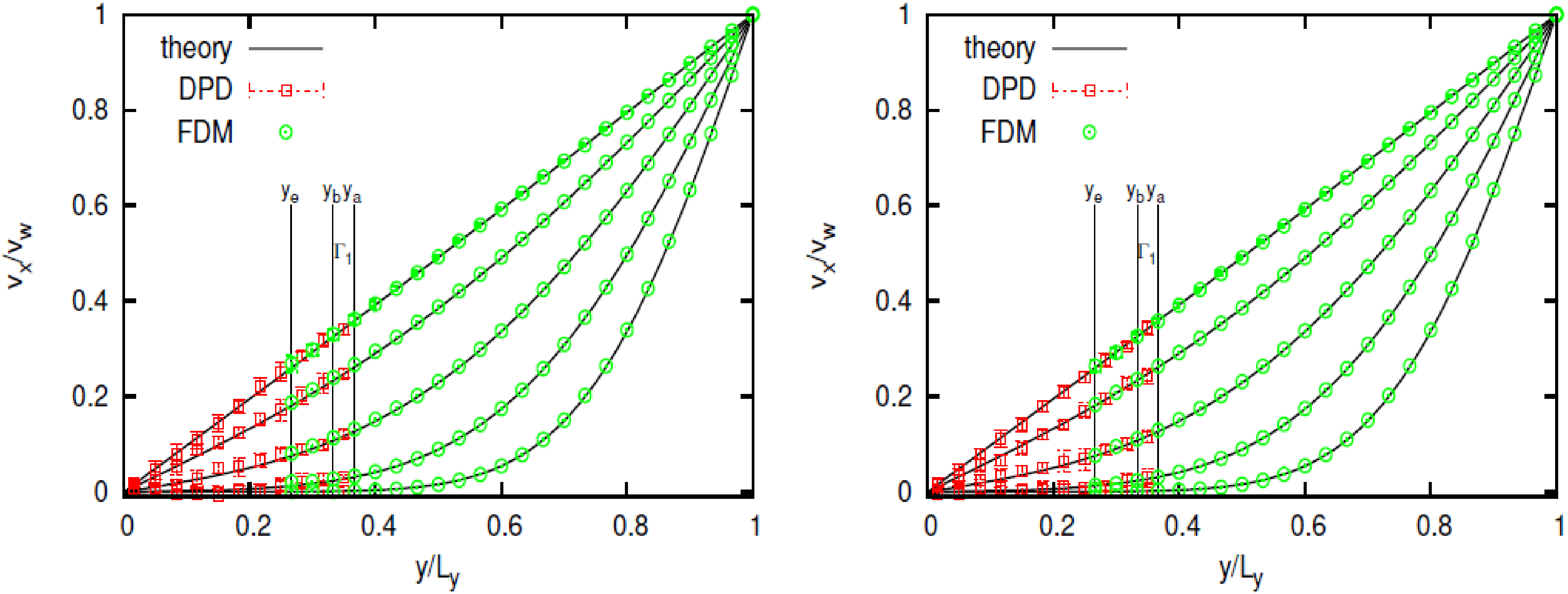

Nie et al. 2004, *J. Fluid Mech.*

- velocity profiles at various $x$



# Hybrid DPD+FDM simulations: transient mean profiles[15]

- $L_y^{FDM} = 2L_y^{DPD}$ and $\Delta t = 180\delta t$

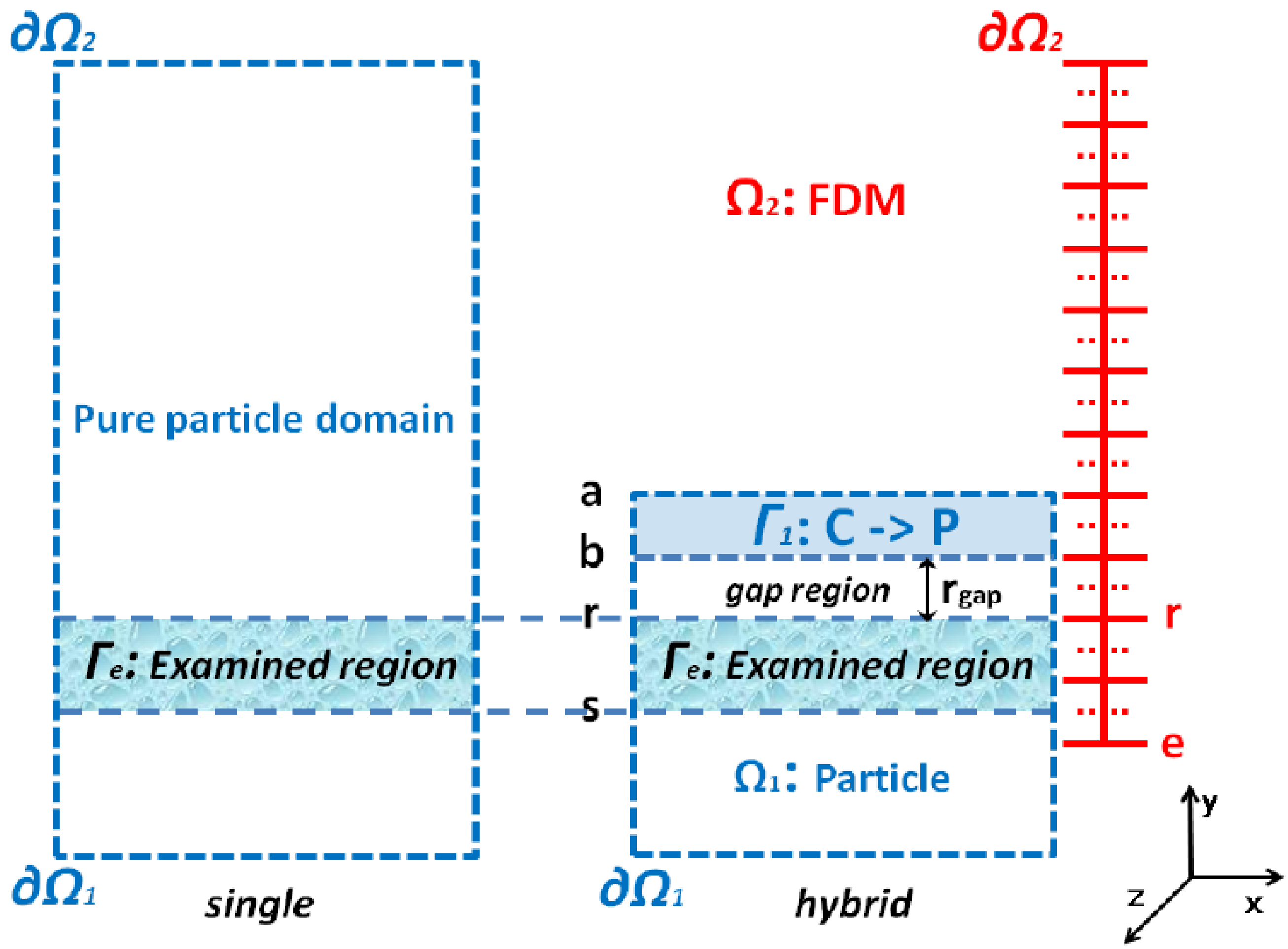



relaxation dynamics ($\epsilon = 0.02$) flux-imposition

- Maxwell buffer & least constraint: similar accuracy, not shown

[15] Bian et al. 2016a, *Phys. Rev. E.*

# Single particle simulations versus hybrid simulations[16]

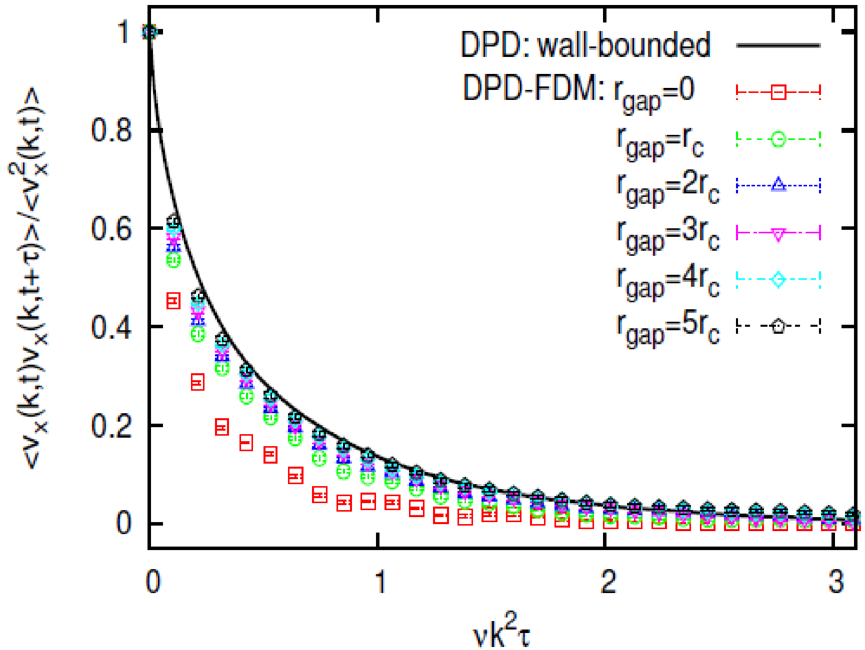



Sketch of examined region for fluctuations

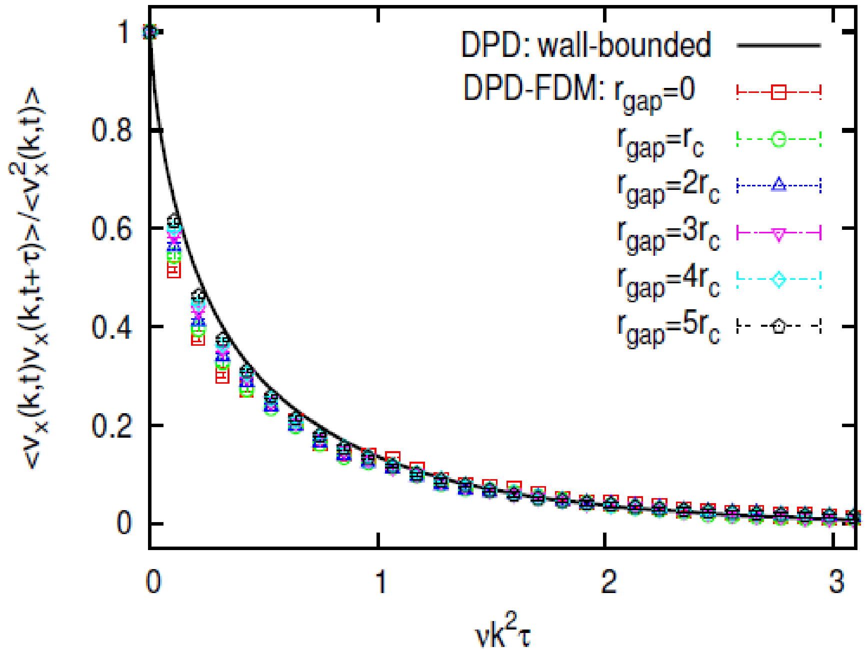
[16] Bian et al. 2016a, *Phys. Rev. E.*

# Hybrid simulations: fluctuations $\delta v_x$

- transversal ACF: $\mathbf{k}_1 = (0, 0, 2\pi/L_z)$



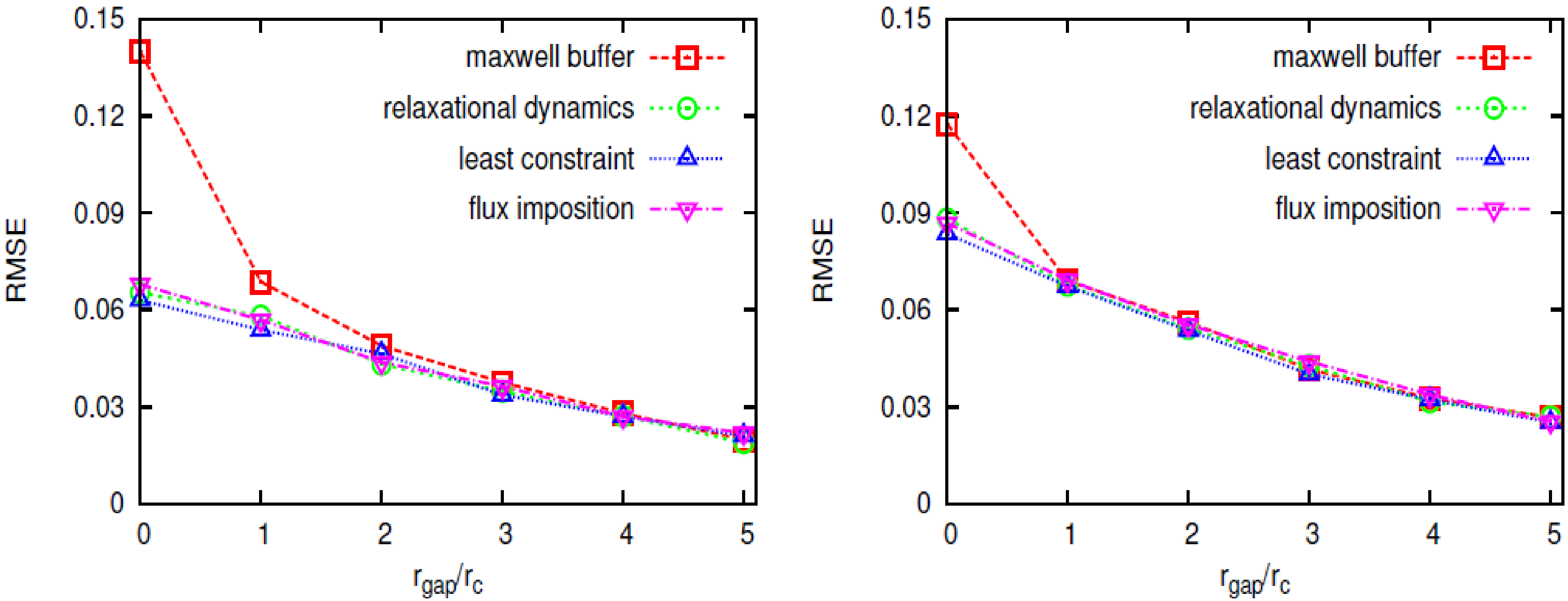

Maxwell buffer




least constraint dynamics

- $\mathbf{k}_2 = (0, 0, 4\pi/L_z)$: similar, not shown

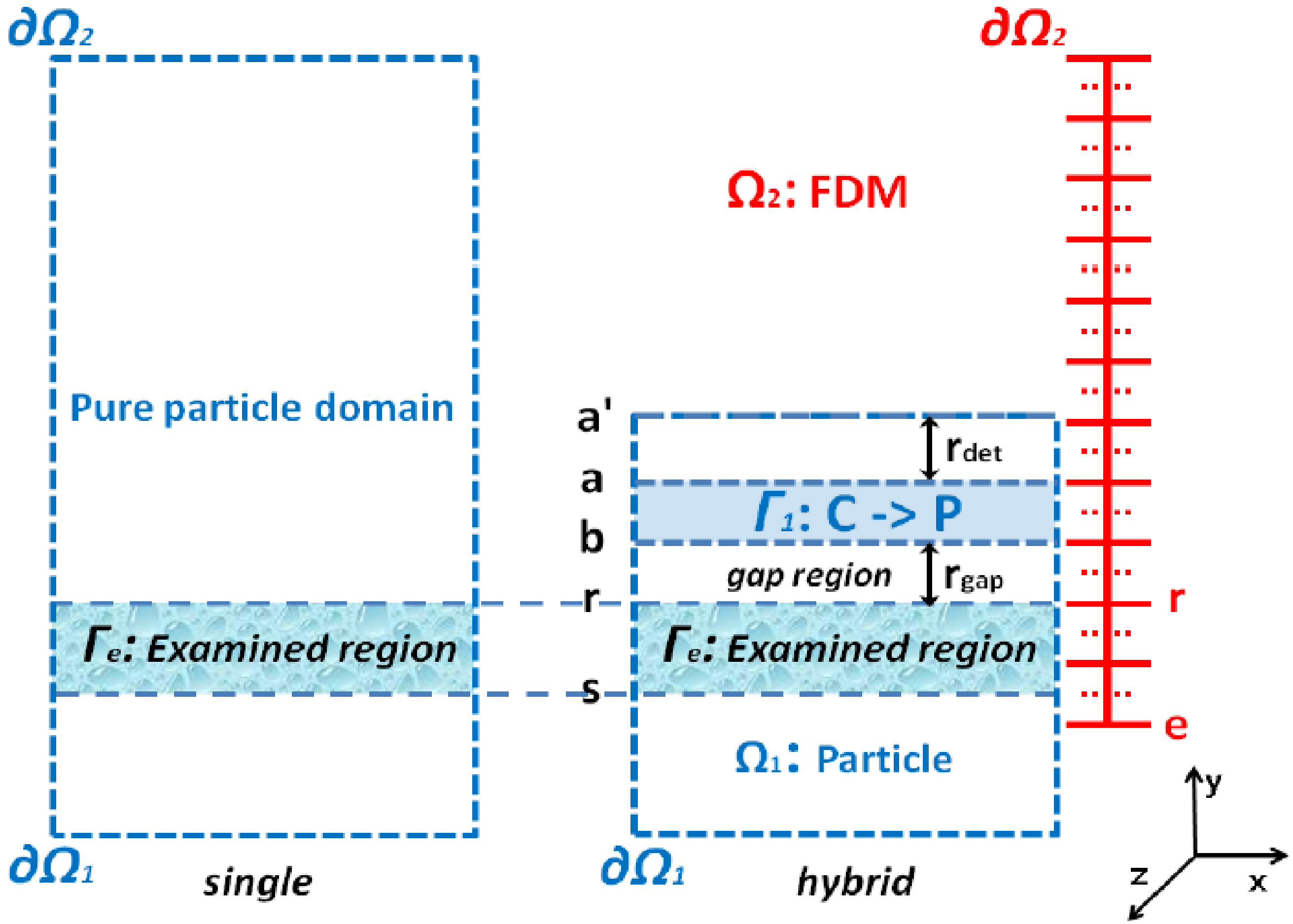
# Root mean squared errors on fluctuations $\delta v_x$[17]




$\mathbf{k}_1 = (0, 0, 2\pi/L_z)$ $\mathbf{k}_2 = (0, 0, 4\pi/L_z)$

- Maxwell-buffer: a strong intrusion
- with a sufficient gap, all are the same and error decays linearly

[17] Bian et al. 2016a, *Phys. Rev. E.*

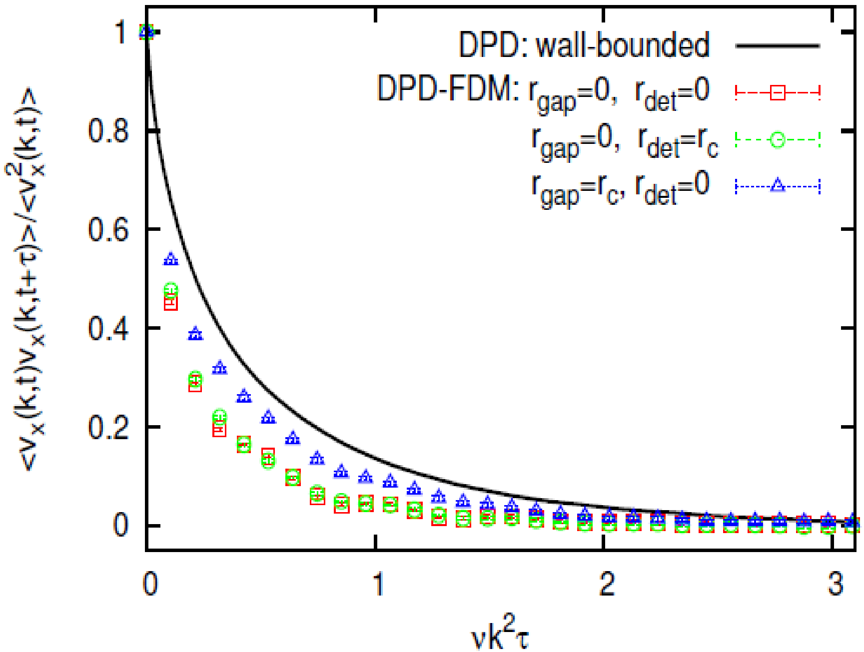



Sketch of two sources of contaminations

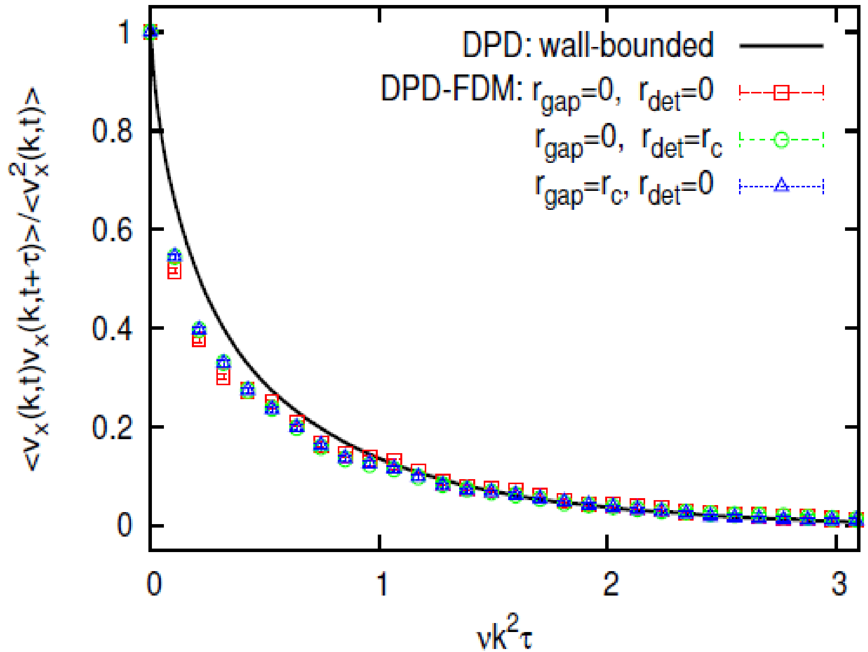
- truncation effects: mean pressure and specular reflection
- artifacts by constraint dynamics: four methods

# Two sources of contaminations on fluctuations $\delta v_x$

- transversal ACF: $\mathbf{k}_1 = (0, 0, 2\pi/L_z)$




Maxwell buffer

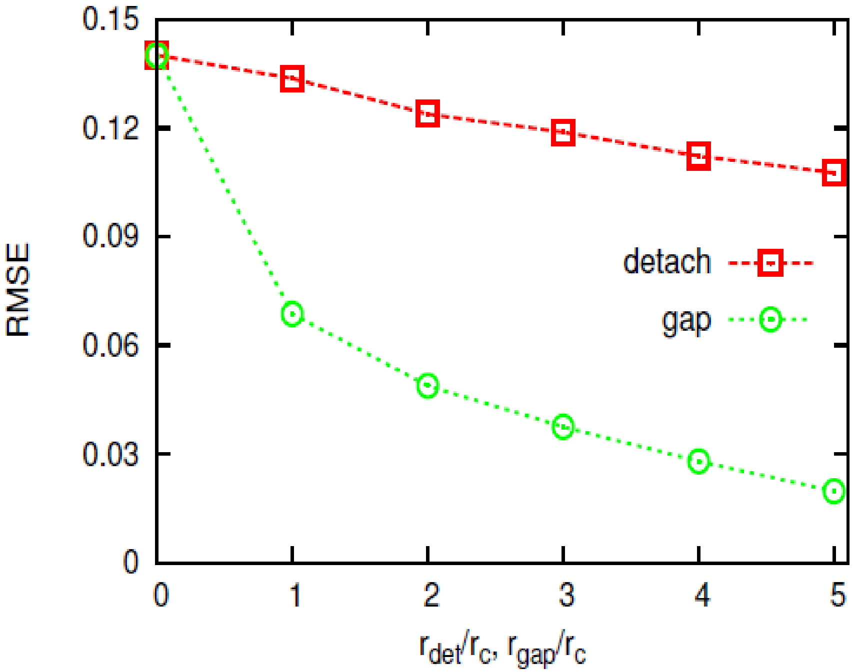



least constraint dynamics

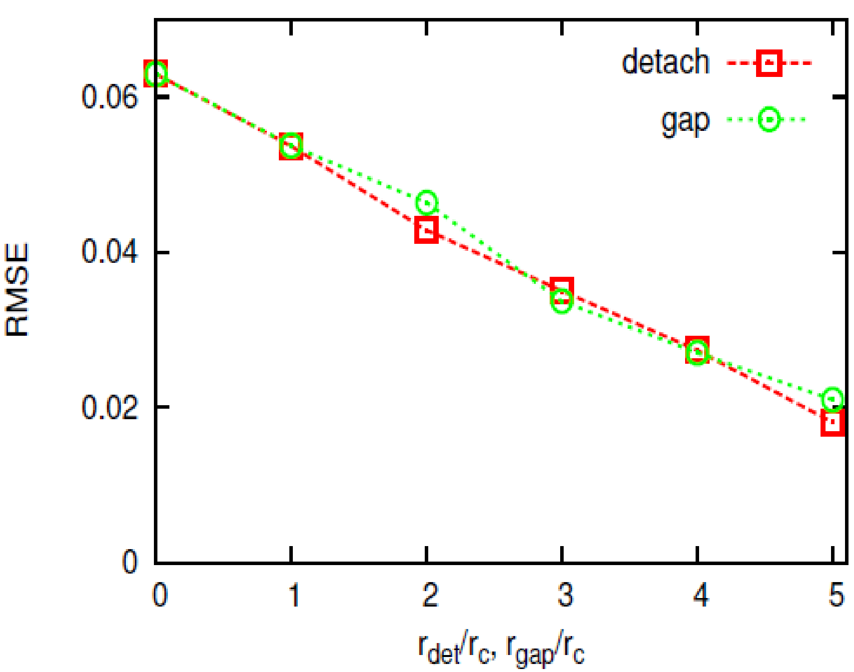
- relaxation dynamics: similar to least constraint dynamics, not shown
- flux imposition: two sources can not be separated
- $\mathbf{k}_2 = (0, 0, 4\pi/L_z)$: similar, not shown

# Two errors on fluctuations $\delta v_x$[18]

- $\mathbf{k}_1 = (0, 0, 2\pi/L_z)$




Maxwell buffer



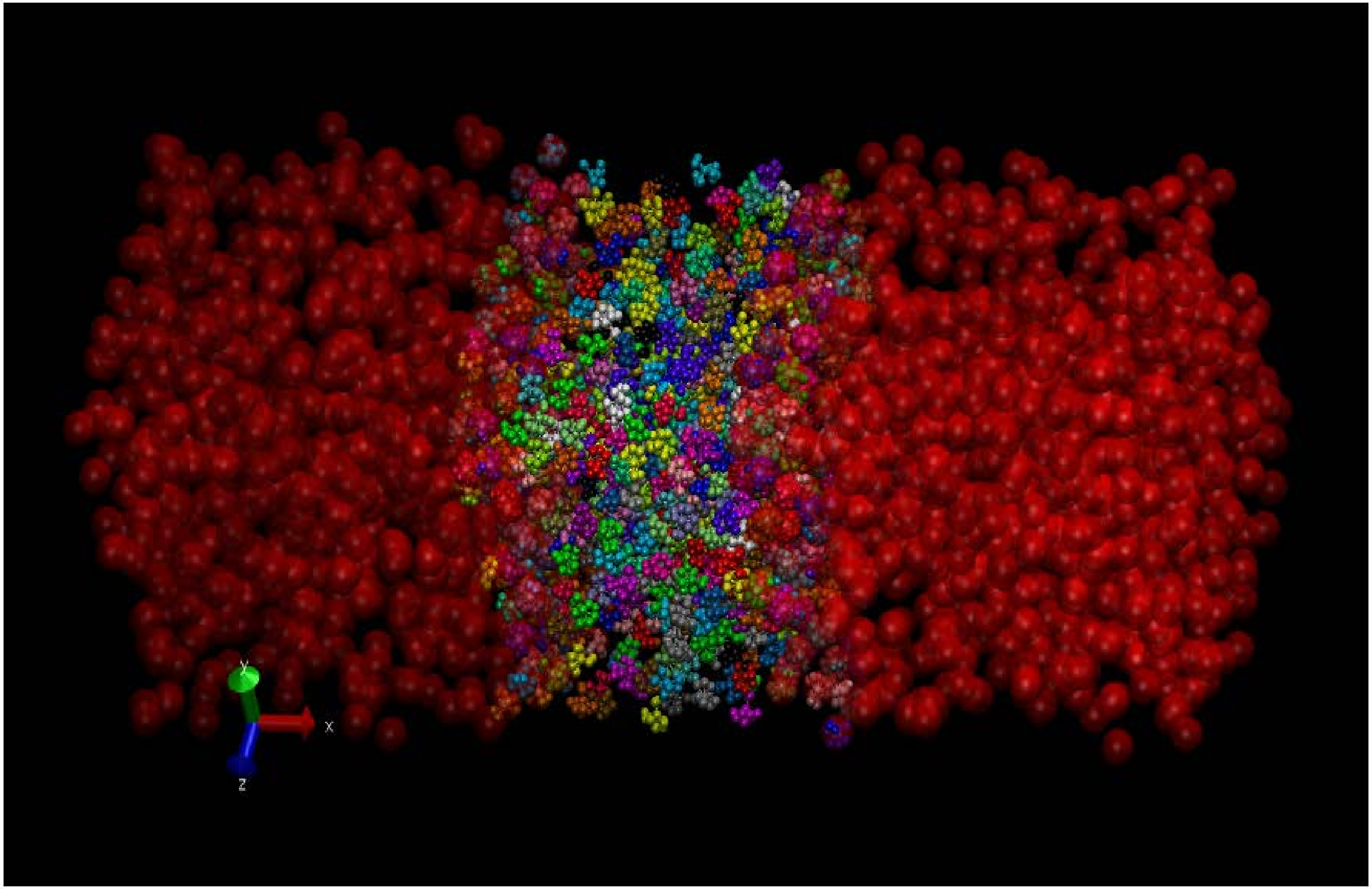

least constraint dynamics

- relaxation dynamics: similar to least constraint dynamics, not shown
- flux imposition: two sources can not be separated
- $\mathbf{k}_2 = (0, 0, 4\pi/L_z)$: similar, not shown

[18] Bian et al. 2016a, *Phys. Rev. E.*

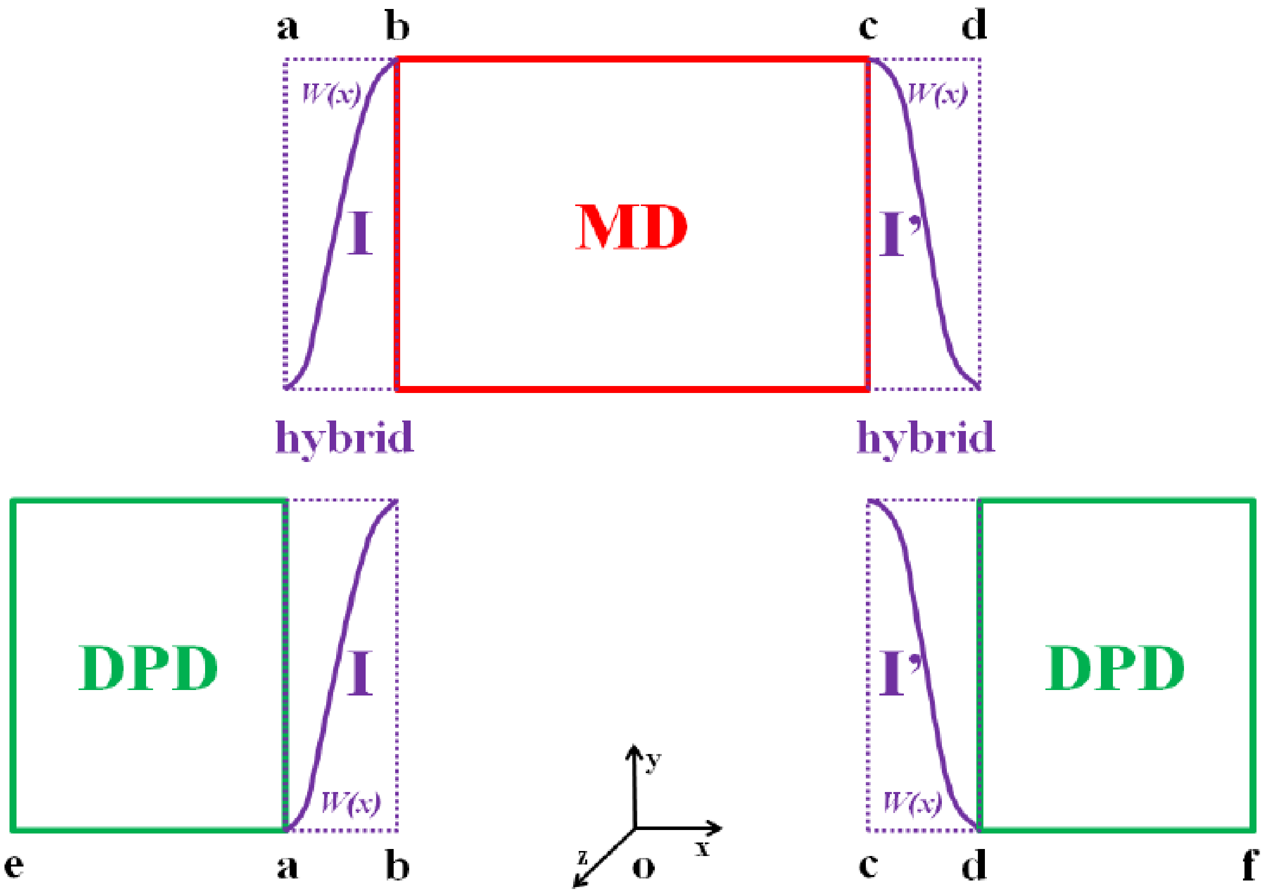
# Outline

# Adaptive resolution scheme (AdResS)




changing degrees of freedom on the fly

# AdResS: force coupling




- hybrid force between MD and DPD Praprotnik et al. 2005, *J. Chem. Phys.*

$$\mathbf{F}^{H}_{\alpha\beta} = \lambda(X_\alpha, X_\beta)\mathbf{F}^{MD}_{\alpha\beta} + [1 - \lambda(X_\alpha, X_\beta)]\,\mathbf{F}^{C}_{\alpha\beta}, \quad (50)$$

$$\mathbf{F}^{MD}_{\alpha\beta} = \sum_{i}^{N_\alpha}\sum_{j}^{N_\beta} F^{LJ}_{ij}. \quad (51)$$

# AdResS: weight function

The weighting function is $\lambda(X_\alpha, X_\beta) = w(X_\alpha)w(X_\beta)$ and

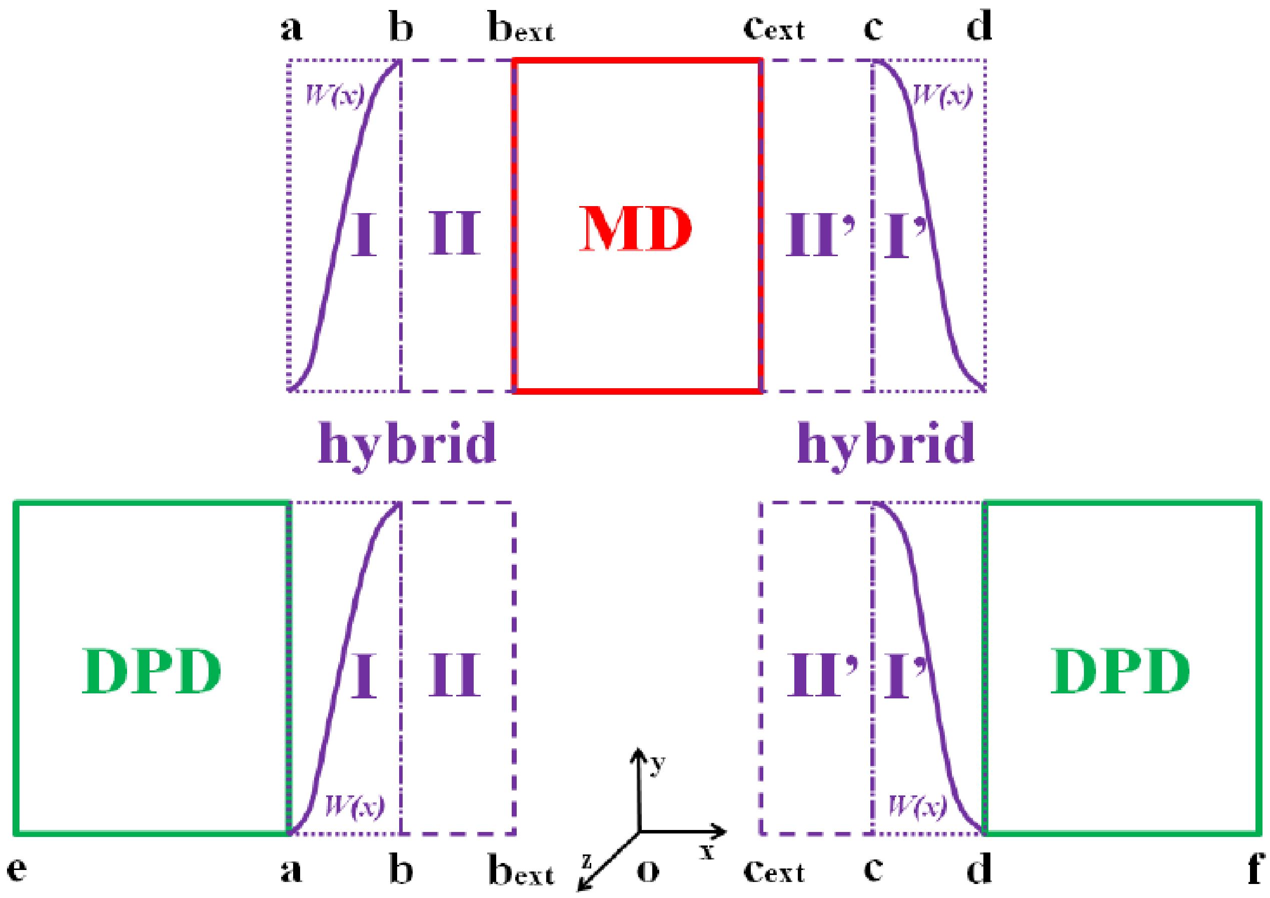
$$w(X) = \begin{cases} 0, & x_e \leq X < x_a \\ \cos^2\left[\frac{\pi}{2}\left(\frac{X - x_b}{x_a - x_b}\right)\right], & x_a \leq X < x_b \\ 1, & x_b \leq X < x_c \\ \cos^2\left[\frac{\pi}{2}\left(\frac{X - x_c}{x_d - x_c}\right)\right], & x_c \leq X < x_d \\ 0, & x_d \leq X < x_f \end{cases} \tag{52}$$

- weight function and its first derivative are continuous.

Praprotnik et al. 2005, *J. Chem. Phys.*

# AdResS: the actual hybrid regions

- Due to weighting function: $\lambda(X_\alpha, X_\beta) = w(X_\alpha)w(X_\beta)$




Hybrid molecules exist not only in I and I', but also in II and II'.

# AdReS: the actual interactions

- interactions between molecules $\alpha$ and $\beta$ in different regions

| molecules $\alpha \backslash \beta$ | DPD | hybrid I | hybrid II | MD |
|---|---|---|---|---|
| DPD | $\mathbf{F}^{C}_{\alpha\beta}$ | $\mathbf{F}^{C}_{\alpha\beta}$ | $\times$ | $\times$ |
| hybrid I | $\mathbf{F}^{C}_{\alpha\beta}$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\times$ |
| hybrid II | $\times$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\mathbf{F}^{MD}_{\alpha\beta}$ | $\mathbf{F}^{MD}_{\alpha\beta}$ |
| MD | $\times$ | $\times$ | $\mathbf{F}^{MD}_{\alpha\beta}$ | $\mathbf{F}^{MD}_{\alpha\beta}$ |

# Hamiltonian-AdResS: energy coupling $\longrightarrow$ force coupling

- A Hamiltonian $H$ for "mixed resolution" reads Potestio et al. 2013, *Phys. Rev. Lett.*

$$H = \sum_{\alpha i} \frac{P_{\alpha i}^2}{2m_{\alpha i}} + \sum_{\alpha} \left\{ w(X_\alpha) V_\alpha^{MD} + [1 - w(X_\alpha)] V_\alpha^C \right\} + V^{int}. \qquad (53)$$

- Force derived from $H$ on *atom level* reads

$$\mathbf{F}_{\alpha i}^H = \sum_{\beta, \beta \neq \alpha} \left\{ \lambda(X_\alpha, X_\beta) \sum_{j=1}^{N_c} \mathbf{F}_{\alpha i|\beta j}^{MD} + [1 - \lambda(X_\alpha, X_\beta)] \mathbf{F}_{\alpha i|\beta}^C \right\} + \mathbf{F}_{\alpha i}^{int} - \left( V_\alpha^{MD} - V_\alpha^C \right) \nabla_{\alpha i} w(X_\alpha). \qquad (54)$$

where $\lambda(X_\alpha, X_\beta) = \frac{w(X_\alpha) + w(X_\beta)}{2}$

- Force derived from $H$ between two *molecules* reads

$$\mathbf{F}_{\alpha\beta}^H = \lambda(X_\alpha, X_\beta) \mathbf{F}_{\alpha\beta}^{MD} + [1 - \lambda(X_\alpha, X_\beta)] \mathbf{F}_{\alpha\beta}^C \qquad (55)$$

$$- \left( V_{\alpha\beta}^{MD} - V_{\alpha\beta}^C \right) \nabla_\alpha w(X_\alpha) \qquad (56)$$

# Hamiltonian-AdResS: if drift force vanishes

- extra drift force from the H-AdResS:

$$\mathbf{F}^{dr} = -\left(V^{MD}_{\alpha\beta} - V^{C}_{\alpha\beta}\right)\nabla_\alpha w(X_\alpha) \tag{57}$$

- for $V^{MD}_{\alpha\beta} \approx V^{C}_{\alpha\beta}$ which is true for
  - force-matching coarse graining Izvekov et al. 2005, *J. Chem. Phys.*
  - Mori-Zwanzig coarse graining Li et al. 2014, *Soft Matter*

  we have from H-AdResS

$$\mathbf{F}^{H}_{\alpha\beta} = \lambda(X_\alpha, X_\beta)\mathbf{F}^{MD}_{\alpha\beta} + [1-\lambda(X_\alpha, X_\beta)]\,\mathbf{F}^{C}_{\alpha\beta} \tag{58}$$

- then the difference between force-coupling and energy-coupling is

$$\lambda(X_\alpha, X_\beta) = w(X_\alpha)w(X_\beta) \quad vs. \quad \lambda(X_\alpha, X_\beta) = \frac{w(X_\alpha) + w(X_\beta)}{2} \tag{59}$$

# AdResS: force coupling formula is non-symmetric[19]

Recall the force coupling in AdResS:

$$\mathbf{F}^{H}_{\alpha\beta} = \lambda(X_\alpha, X_\beta)\mathbf{F}^{MD}_{\alpha\beta} + [1 - \lambda(X_\alpha, X_\beta)]\,\mathbf{F}^{C}_{\alpha\beta}, \tag{60}$$

$$\lambda(X_\alpha, X_\beta) = w(X_\alpha)w(X_\beta). \tag{61}$$

This setup is *not symmetric*

- either by swapping MD and DPD regions
- or by changing the monotonic direction of the weight function $w$

For example, $X_\alpha$ and $X_\beta$ are both in the middle of the hybrid region $w(X_\alpha) = w(X_\beta) = 0.5$. Therefore, $\mathbf{F}^{H}_{\alpha\beta} = 0.25\mathbf{F}^{MD}_{\alpha\beta} + 0.75\mathbf{F}^{C}_{\alpha\beta}$

If swapping MD and DPD regions, or reversing monotonic direction of $w$, we get $\mathbf{F}^{H}_{\alpha\beta} = 0.75\mathbf{F}^{MD}_{\alpha\beta} + 0.25\mathbf{F}^{C}_{\alpha\beta}$.

A completely different physical system!

[19] X. Bian et al. (2016b). "Compatibility and symmetry of the adaptive resolution scheme". In: *J. Chem. Theo. Comput. in preparation*.

# A reconciliation of AdResS and H-AdResS: symmetry[20]

The simplest modification on the force-coupling formula in AdResS is:

$$\begin{aligned}\mathbf{F}^H_{\alpha\beta} &= \frac{1}{2}w(X_\alpha)w(X_\beta)\mathbf{F}^{MD}_{\alpha\beta} + \frac{1}{2}\left[1 - w(X_\alpha)w(X_\beta)\right]\mathbf{F}^C_{\alpha\beta} \\ &+ \frac{1}{2}\left[1 - w'(X_\alpha)w'(X_\beta)\right]\mathbf{F}^{MD}_{\alpha\beta} + \frac{1}{2}w'(X_\alpha)w'(X_\beta)\mathbf{F}^C_{\alpha\beta} \quad (62)\end{aligned}$$

If we take $w'(X)$ to be symmetric with $w(X)$, $\mathbf{F}^H_{\alpha\beta}$ is *symmetric*

- by either swapping MD and DPD regions
- or changing the direction of the weight function $w(x)$.

Note that $w'(X_\alpha) = 1 - w(X_\alpha)$ and $w'(X_\beta) = 1 - w(X_\beta)$, we get

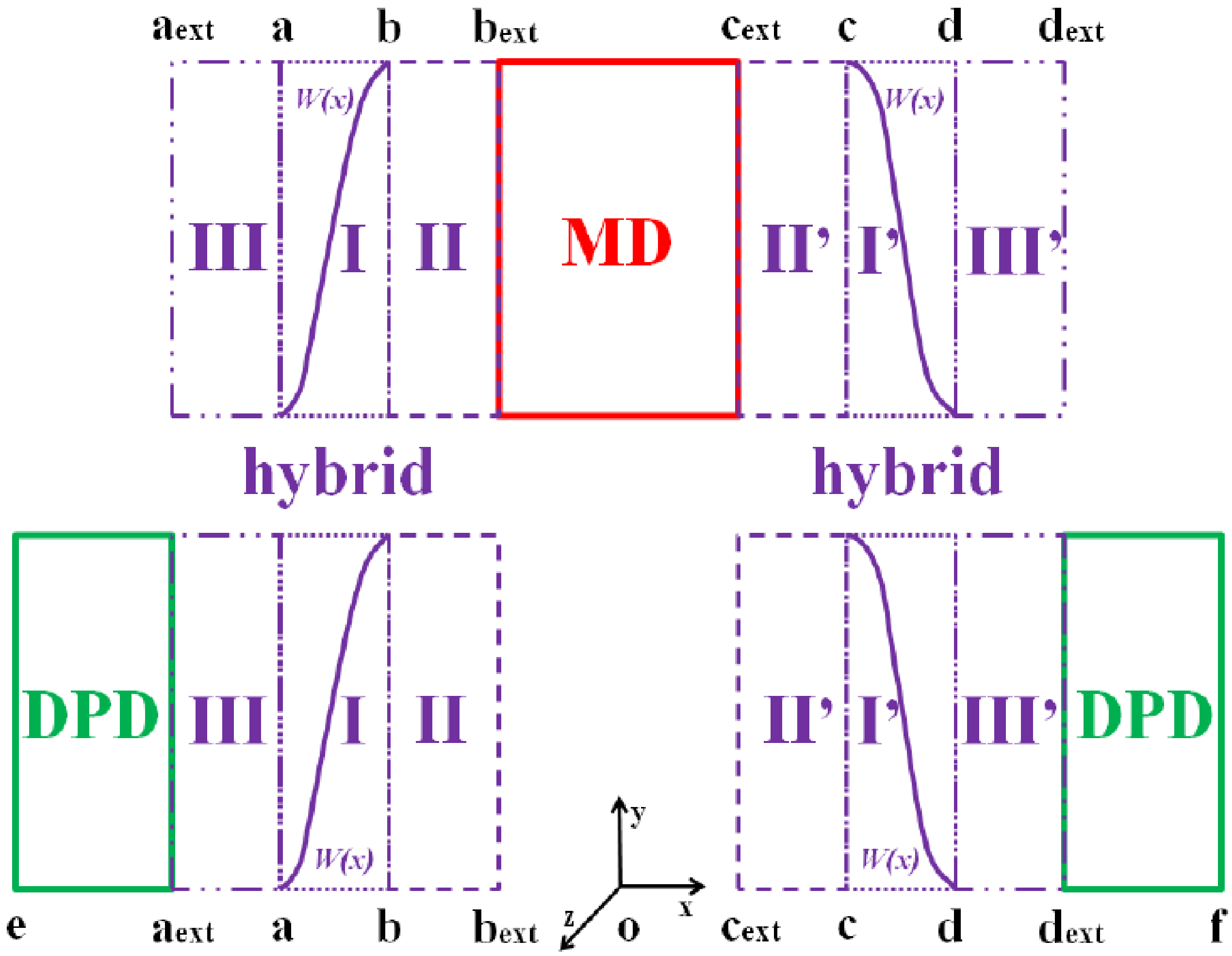
$$\mathbf{F}^H_{\alpha\beta} = \frac{w(X_\alpha) + w(X_\beta)}{2}\mathbf{F}^{MD}_{\alpha\beta} + \left[1 - \frac{w(X_\alpha) + w(X_\beta)}{2}\right]\mathbf{F}^C_{\alpha\beta}, \quad (63)$$

which coincides with the H-AdResS!

[20] Bian et al. 2016b, *J. Chem. Theo. Comput. in preparation.*

# Symmetric AdResS or H-AdResS: hybrid regions[21]

- Due to the weighting function: $\lambda(X_\alpha, X_\beta) = \frac{w(X_\alpha)+w(X_\beta)}{2}$




[21] Bian et al. 2016b, *J. Chem. Theo. Comput. in preparation.*

# Symmetric AdResS or H-AdResS: interactions[22]

Recall

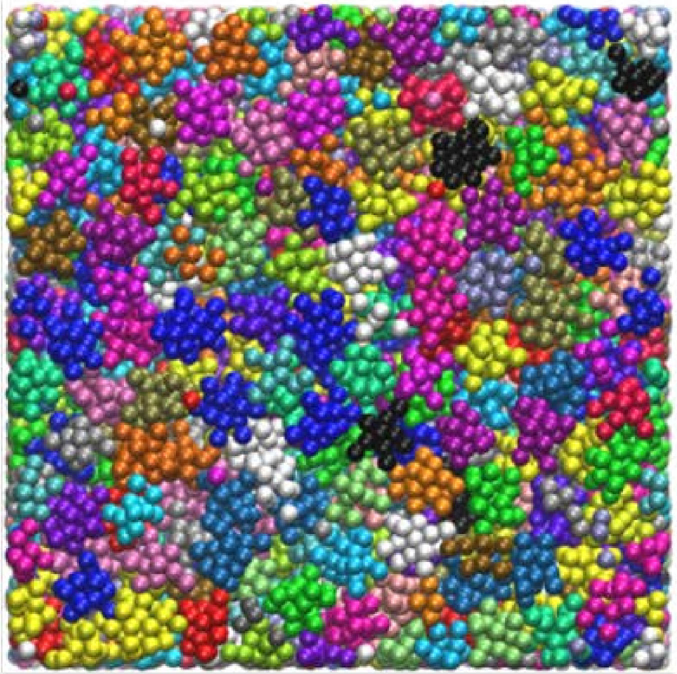
$$\mathbf{F}^{H}_{\alpha\beta} = \frac{w(X_\alpha)+w(X_\beta)}{2}\mathbf{F}^{MD}_{\alpha\beta} + \left[1 - \frac{w(X_\alpha)+w(X_\beta)}{2}\right]\mathbf{F}^{DPD}_{\alpha\beta}. \quad (64)$$

Interactions between molecules $\alpha$ and $\beta$ in different regions: conservative part

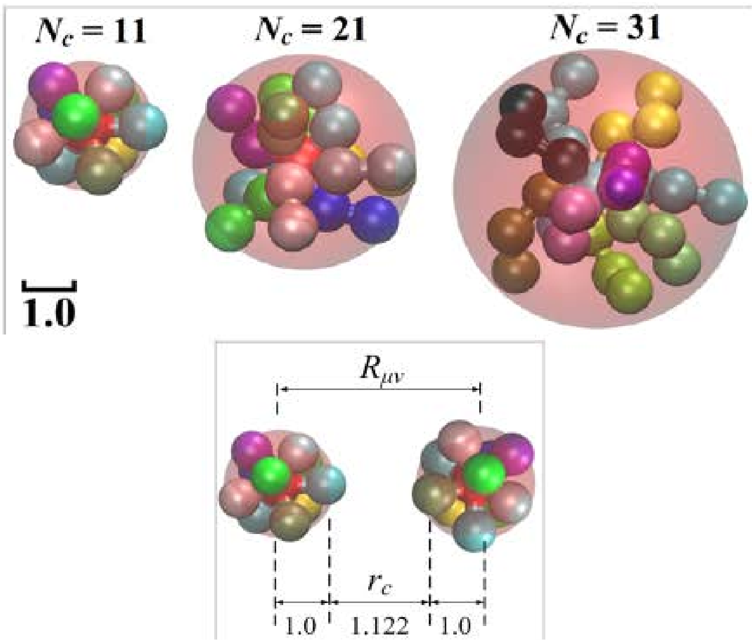
| molecules $\alpha \setminus \beta$ | DPD | hybrid III | hybrid I | hybrid II | MD |
|---|---|---|---|---|---|
| DPD | $\mathbf{F}^{C}_{\alpha\beta}$ | $\mathbf{F}^{C}_{\alpha\beta}$ | $\times$ | $\times$ | $\times$ |
| hybrid III | $\mathbf{F}^{C}_{\alpha\beta}$ | $\mathbf{F}^{C}_{\alpha\beta}$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\times$ | $\times$ |
| hybrid I | $\times$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\times$ |
| hybrid II | $\times$ | $\times$ | $\mathbf{F}^{H}_{\alpha\beta}$ | $\mathbf{F}^{MD}_{\alpha\beta}$ | $\mathbf{F}^{MD}_{\alpha\beta}$ |
| MD | $\times$ | $\times$ | $\times$ | $\mathbf{F}^{MD}_{\alpha\beta}$ | $\mathbf{F}^{MD}_{\alpha\beta}$ |

[22] Bian et al. 2016b, *J. Chem. Theo. Comput. in preparation.*

# A microscopic system by molecular dynamics[23]



polymeric melts




individual molecule

- Hamiltonian

$$H = \sum_{i=1}^{n} \frac{\mathbf{P}_i}{2m_i} + \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_{ij}) \quad (65)$$

- potentials

$$V(r_{ij}) = V_{WCA}(r_{ij}) + V_{FENE}(r_{ij}) \quad (66)$$

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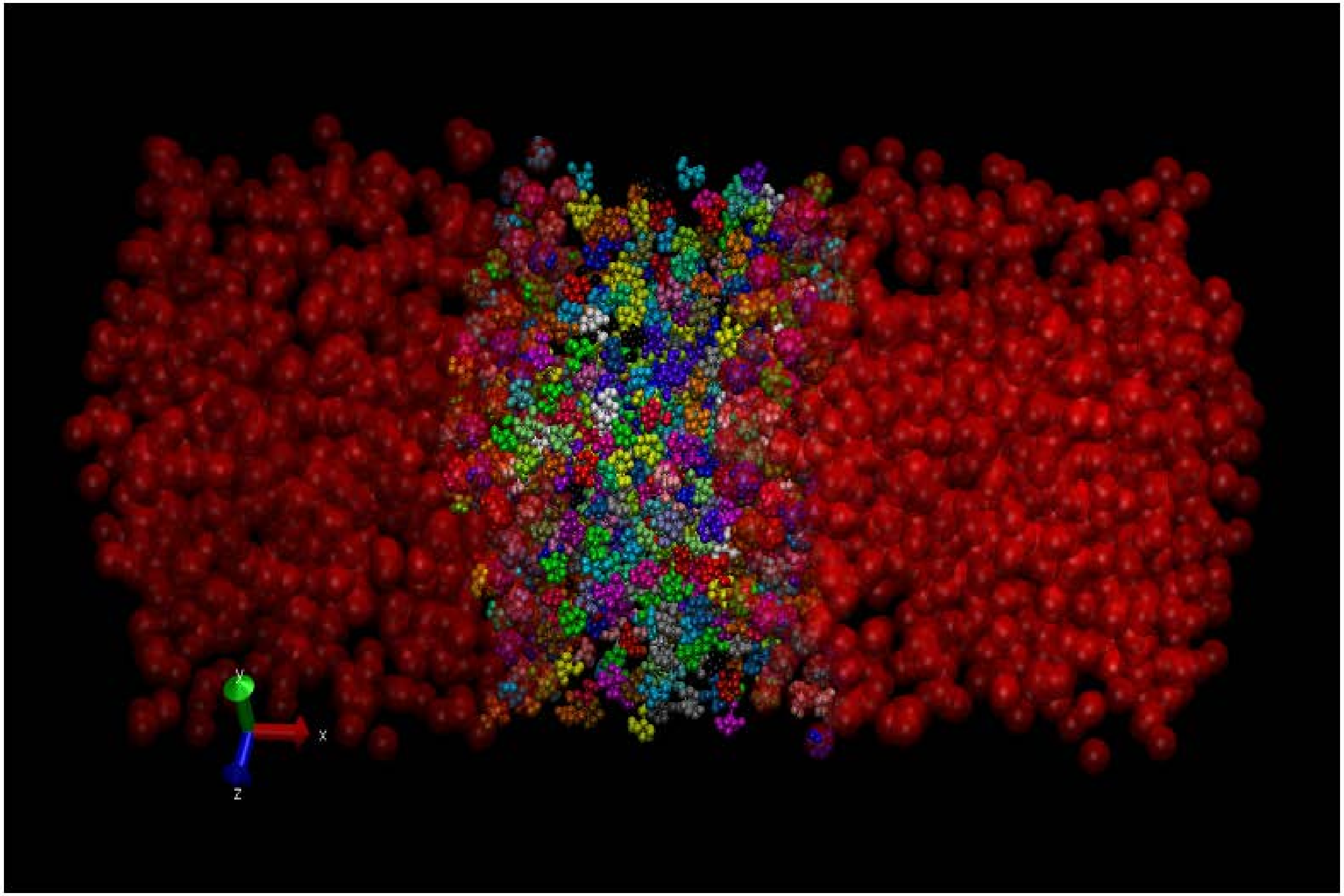
[23] Z. Li et al. (2014). "Construction of dissipative particle dynamics models for complex fluids via the Mori-Zwanzig formulation". In: *Soft Matter* 10 (43), pp. 8659–8672. DOI: 10.1039/C4SM01387E.

# A hybrid simulation by AdResS: MD sandwiched by DPD[26]

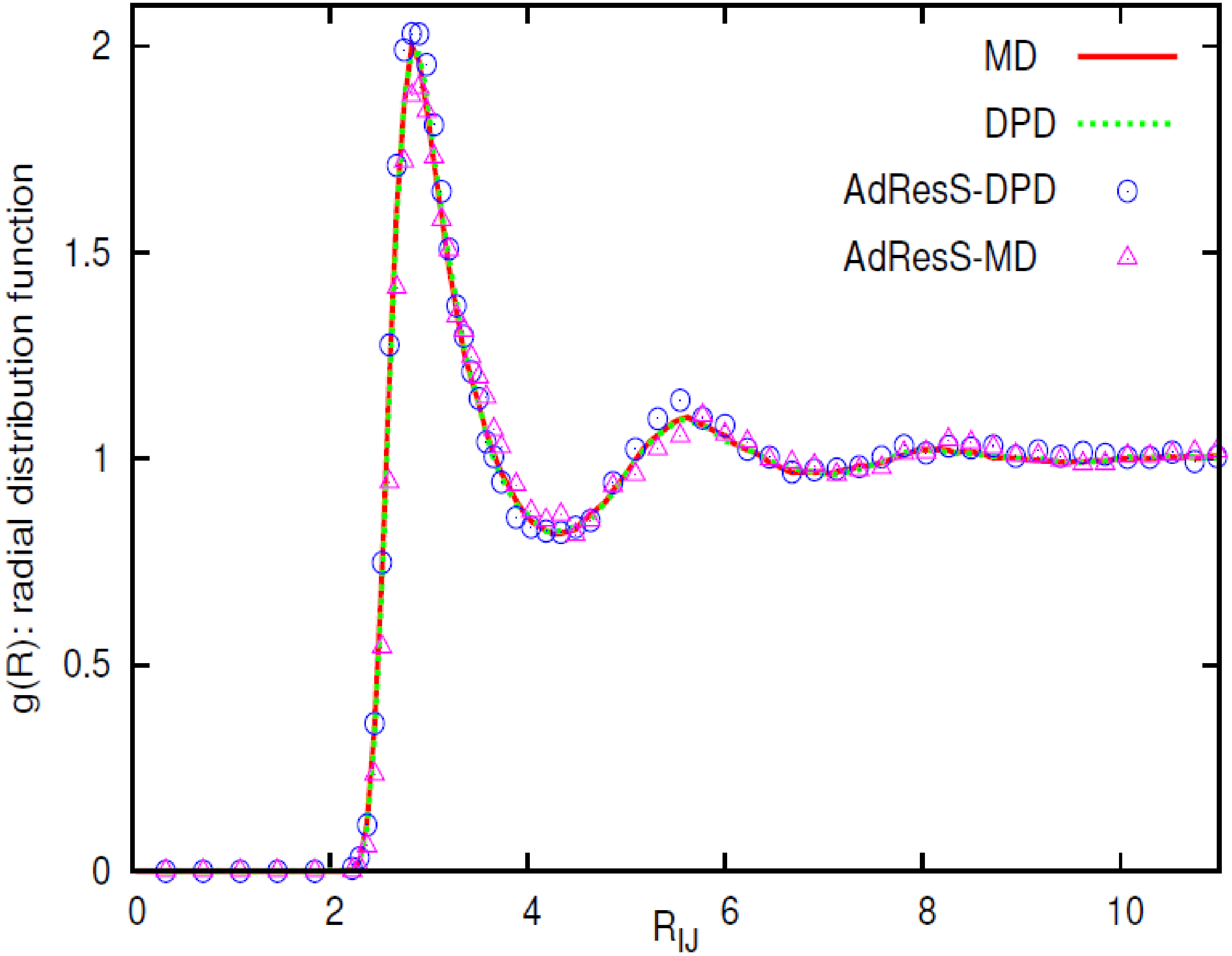



changing degrees of freedom on the fly

- temperature: $T = T_0(1 \pm 1\%)$
- pressure: $P = P_0(1 \pm 5\%)$

[26] Bian et al. 2016b, *J. Chem. Theo. Comput. in preparation.*

# Structure of the hybrid simulation[27]




Radial distribution function of CoMs of molecules

- RDF is reproduced well

[27] Bian et al. 2016b, *J. Chem. Theo. Comput. in preparation.*

# Outline

1. Introduction
   - particle methods at various scales
2. Deterministic-deterministic coupling
   - Schwartz alternating method
   - multi-resolution SPH
3. Deterministic-stochastic coupling
   - fluctuations at equilibrium
     - periodic domain
     - truncated domain
   - fluctuations at nonequilibrium
     - periodic domain
     - heterogeneous adjacent multi-domains
4. Stochastic-stochastic coupling
   - the adaptive resolution scheme
     - force-force coupling
     - energy-energy coupling
5. Summary and some perspectives

# Summary

- deterministic-deterministic coupling: classical DDM
  - extension to multi-resolution particle simulations
- deterministic-stochastic coupling:
  - often focus on the mean quantites, such as, velocity.
  - fluctuations in the stochastic sub-domain need to be preserved well
- stochastic-stochastic coupling: for complex fluid melts
  - reproducibility of MD via corase-grained (Mori-Zwanzig) DPD
  - compatibility and symmetry of MD and MZ-DPD within AdResS

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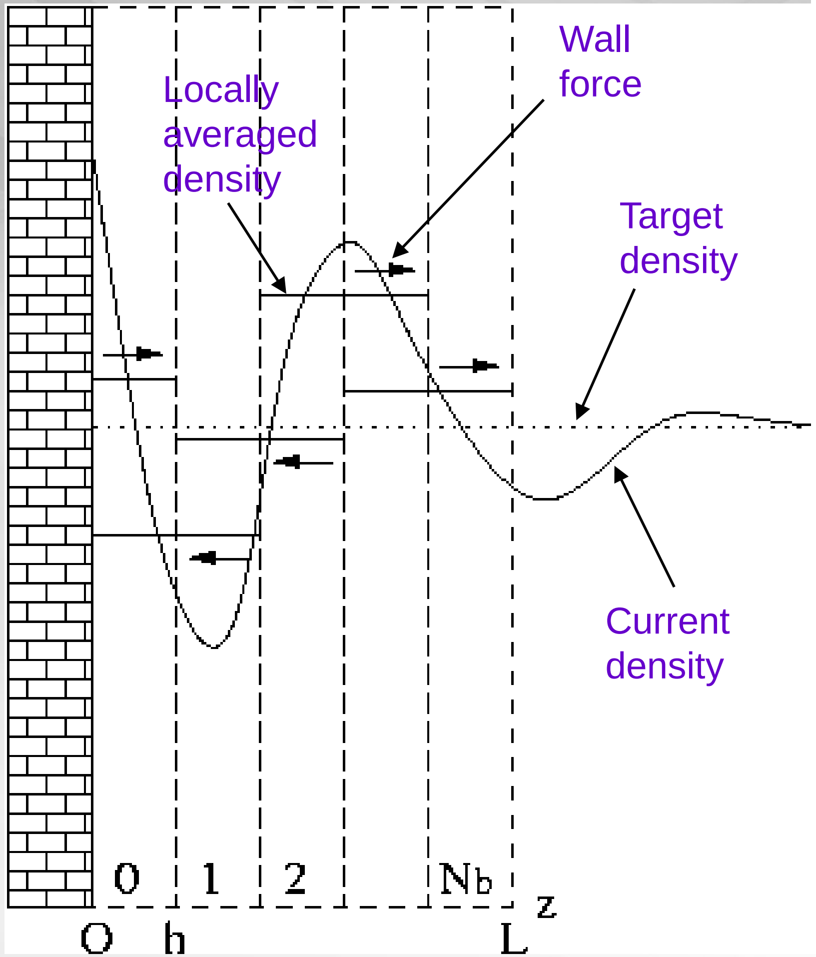
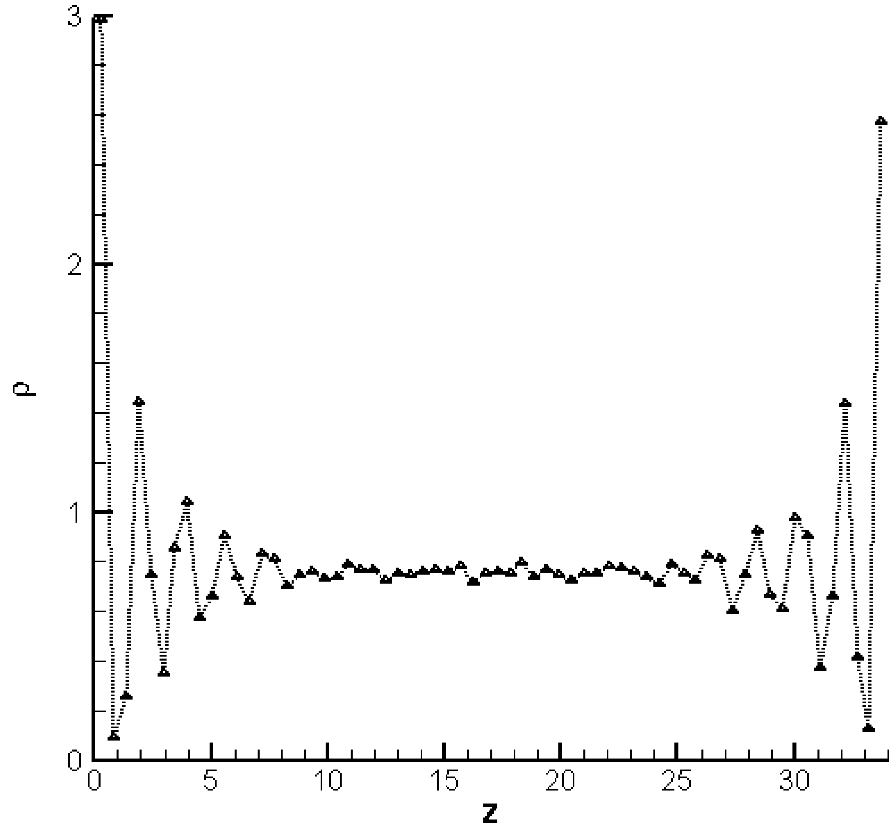
# Adaptive Boundary Conditions




Adaptive BC:

- layers of particles
- bounce back reflection
- adaptive wall force

Iteratively adjust the wall repulsion force in each bin based on the averaged density values.

**I.V. Pivkin and G.E. Karniadakis, PRL, vol.96, 206001, 2006**

# Navier-Stokes: continuum



$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \vec{u}$$

$$\nabla \cdot \vec{u} = 0$$

- Incompressible Navier-Stokes equations
- Spectral element method discretization
- Dirichlet boundary conditions

# Dissipative Particle Dynamics*

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Force is the sum of three pair-wise additive terms:

$$\vec{\mathbf{F}}_i dt = \vec{\mathbf{F}}_i^C dt + \vec{\mathbf{F}}_i^R \sqrt{dt} + \vec{\mathbf{F}}_i^D dt$$

1) Conservative force:

$$\vec{F}_i^C = \sum_{i \neq j} F_{ij}^C (r_{ij}) \vec{e}_{ij}$$

$$\mathbf{F}_{ij}^C (r_{ij}) = a_{ij} (1 - \frac{r_{ij}}{r_c}) \quad \text{for} \quad r_{ij} \leq r_c$$

2) Random force:

$$\vec{F}_i^R = \sigma \sum_{i \neq j} w^R (r_{ij}) \xi_{ij} \vec{e}_{ij}$$

$$w^R (r_{ij}) = \left( 1 - \frac{r_{ij}}{r_c} \right)^p \quad \text{for} \quad r_{ij} \leq r_c$$

3) Dissipative force:

$$\vec{F}_i^D = -\gamma \sum_{i \neq j} w^D (r_{ij}) (\vec{v}_{ij} \cdot \vec{e}_{ij}) \vec{e}_{ij}$$

$$w^D (r_{ij}) = \left( w^R (r_{ij}) \right)^2$$

$$\sigma^2 = 2 \gamma k_B T$$

- (Espanol & Warren, *Europhys Lett*, 30:191, 1995)

* Hoogerbrugge & Koelman, *Europhys Lett*, 19:155, 1992

# Molecular Dynamics: microscopic



- Lennard-Jones particle interactions

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- System is kept at equilibrium temperature through the DPD thermostat
- The particles evolve according to Newton's second law of motion

# DPD and MD boundary conditions

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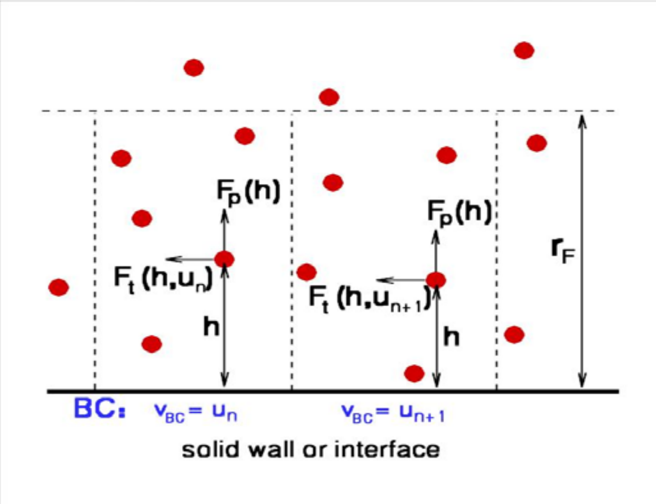
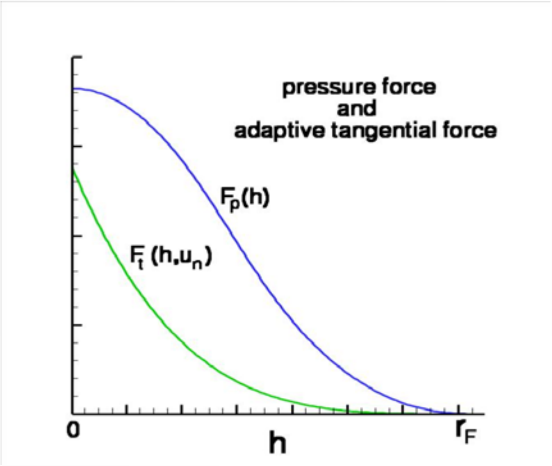
## 1) Imposition of normal velocity component

- Specular reflection at the interface in the system of coordinates at the moving boundary #
- Deletion of particles leaving the computational domain and insertion of particles according to BC flux $N = nAv_n\Delta t$

## 2) Imposition of tangential velocity component




$$F_t(h) = C(v_t - v_{BC}) * w(h) \qquad C_{n+1} = C_n + \alpha(v_t - v_{BC})$$

# Werder et al., *J Comp Phys*, 205:373-390, 2005