School of Mathematics, University of Birmingham

Stochastic Norton Dynamics: An Alternative Approach for the Computation of Transport Coefficients in Dissipative Particle Dynamics

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The Third Joint SIAM/CAIMS Annual Meetings (AN25)
1 August, 2025

Outline

Outline

Background

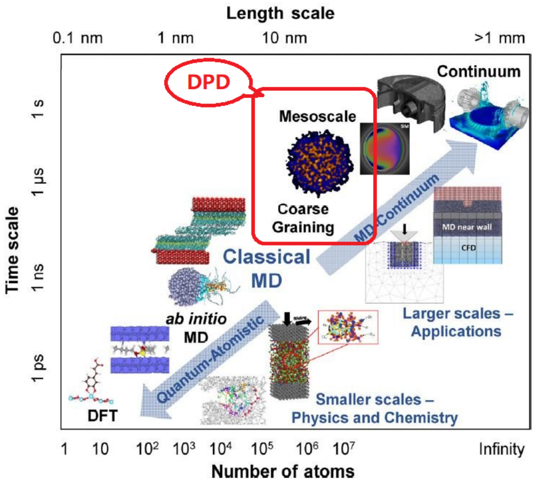
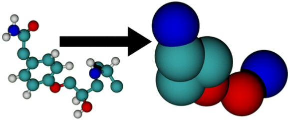


Figure: Different scales for dynamics simulations [Ewen et al., 2018]

Dissipative Particle Dynamics (DPD) method was proposed to simulate dynamical systems with the following characteristics [Hoogerbrugge and Koelman, 1992]:

- meshless
- coarse-grained
- momentum-conserving



Credit: [Graham et al., 2017]

Relevant fields: complex fluids (e.g. rheological properties of concrete), microbiology (e.g., liposome formation in biophysics), health data (e.g., heterogeneous multi-phase flows containing deformable objects), etc.

Breakthrough

DPD has been utilized in large-scale simulations of blood and cancer cell separation in complex microfluidic channels!

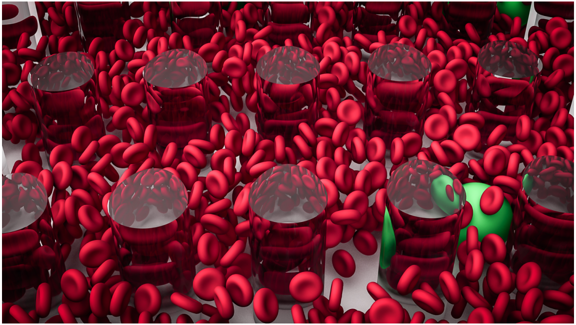


Figure: Simulation of a system with 200,000 red blood cells traveling through a cell-sorting micro channel [Rossinelli et al., 2015]

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Outline

Dissipative Particle Dynamics (DPD)

Formulation of DPD [Leimkuhler and Shang, 2016]

$$\mathrm{d}\mathbf{q} = \mathbf{M}^{-1}\mathbf{p}\mathrm{d}t\,,$$
$$\mathrm{d}\mathbf{p} = -\nabla U(\mathbf{q})\mathrm{d}t - \gamma\mathbf{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\mathrm{d}t + \sigma\mathbf{\Sigma}(\mathbf{q})\mathrm{d}\mathbf{W}\,.$$

Formulation of DPD [Leimkuhler and Shang, 2016]

$$
\begin{aligned}
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\end{aligned}
$$

The shifted Lennard-Jones potential

$$
U(\mathbf{q}) = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\varphi(r_{ij})\,,
$$

with the pair potential energy

$$
\varphi(r_{ij}) = \begin{cases} u(r_{ij}) - u(r_\mathrm{c}) - u'(r_\mathrm{c})(r_{ij} - r_\mathrm{c})\,, & r_{ij} < r_\mathrm{c}\,; \\ 0\,, & r_{ij} \geq r_\mathrm{c}\,, \end{cases}
$$

where

$$
u(r) = 4\varepsilon\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right]\,,
$$

Dissipative Particle Dynamics (DPD)

The symmetric matrix $\boldsymbol{\Gamma} \in \mathbb{R}^{dN\times dN}$ can be given by

$$\begin{pmatrix} \sum_{j\neq 1}\omega^{\mathrm{D}}(r_{1j})\mathbf{e}_{1j}\mathbf{e}_{1j}^{\mathrm{T}} & -\omega^{\mathrm{D}}(r_{12})\mathbf{e}_{12}\mathbf{e}_{12}^{\mathrm{T}} & \cdots & -\omega^{\mathrm{D}}(r_{1N})\mathbf{e}_{1N}\mathbf{e}_{1N}^{\mathrm{T}} \\ -\omega^{\mathrm{D}}(r_{21})\mathbf{e}_{21}\mathbf{e}_{21}^{\mathrm{T}} & \sum_{j\neq 2}\omega^{\mathrm{D}}(r_{2j})\mathbf{e}_{2j}\mathbf{e}_{2j}^{\mathrm{T}} & \cdots & -\omega^{\mathrm{D}}(r_{2N})\mathbf{e}_{1N}\mathbf{e}_{1N}^{\mathrm{T}} \\ \vdots & \vdots & \ddots & \vdots \\ -\omega^{\mathrm{D}}(r_{N1})\mathbf{e}_{N1}\mathbf{e}_{N1}^{\mathrm{T}} & -\omega^{\mathrm{D}}(r_{N2})\mathbf{e}_{N2}\mathbf{e}_{N2}^{\mathrm{T}} & \cdots & \sum_{j\neq N}\omega^{\mathrm{D}}(r_{Nj})\mathbf{e}_{Nj}\mathbf{e}_{Nj}^{\mathrm{T}} \end{pmatrix}$$

where

$$\mathbf{q}_{ij} = \mathbf{q}_i - \mathbf{q}_j \qquad \mathbf{v}_{ij} = \mathbf{p}_i/m_i - \mathbf{p}_j/m_j$$

$$r_{ij} = |\mathbf{q}_{ij}| \qquad \omega_{ij}^{\mathrm{D}}(r_{ij}) = [\omega_{ij}^{\mathrm{R}}(r_{ij})]^2 = \left(1 - \frac{r_{ij}}{r_{\mathrm{c}}}\right)^2 \mathbf{1}_{\{r_{ij}<r_{\mathrm{c}}\}}$$

$$\mathbf{e}_{ij} = \mathbf{q}_{ij}/r_{ij} \qquad \mathrm{d}\mathbf{W}_{ij} = \mathrm{d}\mathbf{W}_{ji} \sim \mathcal{N}(0, dt)$$

Dissipative Particle Dynamics (DPD)

Fluctuation Dissipation Relation (FDR)

$$\mathbf{\Gamma} = \mathbf{\Sigma}\mathbf{\Sigma}^{\mathrm{T}}\,, \quad \sigma = \sqrt{2\gamma k_{\mathrm{B}} T}\,,$$

where k_{B} is the Boltzmann constant and T is the equilibrium temperature.

Dissipative Particle Dynamics (DPD)

Fluctuation Dissipation Relation (FDR)

$$\mathbf{\Gamma} = \mathbf{\Sigma}\mathbf{\Sigma}^{\mathrm{T}}, \quad \sigma = \sqrt{2\gamma k_{\mathrm{B}} T},$$

where k_{B} is the Boltzmann constant and T is the equilibrium temperature.

The canonical ensemble is preserved with the density

$$\rho_{\beta}(\mathbf{q}, \mathbf{p}) = Z^{-1} e^{-\beta H(\mathbf{q}, \mathbf{p})} \times \prod_{b=x,y,z} \delta_b \left(\sum_i p_{bi} - \pi_b \right),$$

where $\beta = (k_{\mathrm{B}} T)^{-1}$, Z is the partition function, and H is the Hamiltonian $H(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^{\mathrm{T}} \mathbf{M}^{-1} \mathbf{p}}{2} + U(\mathbf{q})$.

Formulation of DPD-NEMD

$$
\begin{aligned}
\mathrm{d}\mathbf{q} &= \mathbf{M}^{-1}\mathbf{p}\,\mathrm{d}t\,, \\
\mathrm{d}\mathbf{p} &= [-\nabla U(\mathbf{q}) + \eta\mathbf{F}(\mathbf{q})]\mathrm{d}t - \gamma\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\,\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q})\mathrm{d}\mathbf{W}\,.
\end{aligned}
$$

Formulation of DPD-NEMD

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- Based on **linear response theory**, the related transport coefficients can be given by [Hairer and Majda, 2010]

$$\alpha = \lim_{\eta\to 0}\frac{\mathbb{E}_\eta[R]}{\eta}\,.$$

Formulation of DPD-NEMD

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- We consider the response observable R has the form

$$R(\mathbf{q},\mathbf{p}) = \mathbf{G}(\mathbf{q}) \cdot \mathbf{p}\,.$$

Formulation of DPD-Norton

$$
\begin{aligned}
&\mathrm{d}\mathbf{q}_t = \mathbf{M}^{-1}\mathbf{p}_t\mathrm{d}t\,,\\
&\mathrm{d}\mathbf{p}_t = -\nabla U(\mathbf{q}_t)\mathrm{d}t - \gamma\mathbf{\Gamma}(\mathbf{q}_t)\mathbf{M}^{-1}\mathbf{p}_t\mathrm{d}t + \sigma\mathbf{\Sigma}(\mathbf{q}_t)\mathrm{d}\mathbf{W}_t + \mathbf{F}(\mathbf{q}_t)\mathrm{d}\Lambda_t\,,\\
&R(\mathbf{q}_t,\mathbf{p}_t) = R(\mathbf{q}_0,\mathbf{p}_0) = r\,,
\end{aligned}
$$

Formulation of DPD-Norton

$$\mathrm{d}\mathbf{q}_t = \mathbf{M}^{-1}\mathbf{p}_t \mathrm{d}t\,,$$
$$\mathrm{d}\mathbf{p}_t = -\nabla U(\mathbf{q}_t)\mathrm{d}t - \gamma\boldsymbol{\Gamma}(\mathbf{q}_t)\mathbf{M}^{-1}\mathbf{p}_t\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q}_t)\mathrm{d}\mathbf{W}_t + \mathbf{F}(\mathbf{q}_t)\mathrm{d}\Lambda_t\,,$$
$$R(\mathbf{q}_t, \mathbf{p}_t) = R(\mathbf{q}_0, \mathbf{p}_0) = r\,,$$

where

$$\Lambda_t = \Lambda_0 + \int_0^t \lambda(\mathbf{q}_s, \mathbf{p}_s)\,\mathrm{d}s + \widetilde{\Lambda}_t\,, \quad \widetilde{\Lambda}_t = \int_0^t \widetilde{\boldsymbol{\lambda}}(\mathbf{q}_s, \mathbf{p}_s)\,\mathrm{d}\mathbf{W}_s\,,$$

$$\lambda(\mathbf{q}, \mathbf{p}) = \frac{1}{\mathbf{F}(\mathbf{q}) \cdot \mathbf{G}(\mathbf{q})} \left(\mathbf{G}(\mathbf{q}) \cdot \left[\nabla U(\mathbf{q}) + \gamma\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} \right] - \nabla\mathbf{G}(\mathbf{q})\mathbf{p} \cdot \mathbf{M}^{-1}\mathbf{p} \right).$$

Stochastic Norton Dynamics

Formulation of DPD-Norton

$$
\begin{aligned}
\mathrm{d}\mathbf{q}_t &= \mathbf{M}^{-1}\mathbf{p}_t\mathrm{d}t\,,\\
\mathrm{d}\mathbf{p}_t &= -\nabla U(\mathbf{q}_t)\mathrm{d}t - \gamma\boldsymbol{\Gamma}(\mathbf{q}_t)\mathbf{M}^{-1}\mathbf{p}_t\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q}_t)\mathrm{d}\mathbf{W}_t + \mathbf{F}(\mathbf{q}_t)\mathrm{d}\Lambda_t\,,\\
R(\mathbf{q}_t,\mathbf{p}_t) &= R(\mathbf{q}_0,\mathbf{p}_0) = r\,,
\end{aligned}
$$

where

$$
\Lambda_t = \Lambda_0 + \int_0^t \lambda(\mathbf{q}_s,\mathbf{p}_s)\,\mathrm{d}s + \widetilde{\Lambda}_t\,, \quad \widetilde{\Lambda}_t = \int_0^t \widetilde{\boldsymbol{\lambda}}(\mathbf{q}_s,\mathbf{p}_s)\,\mathrm{d}\mathbf{W}_s\,,
$$

$$
\lambda(\mathbf{q},\mathbf{p}) = \frac{1}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}\left(\mathbf{G}(\mathbf{q})\cdot\left[\nabla U(\mathbf{q}) + \gamma\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\right] - \nabla\mathbf{G}(\mathbf{q})\mathbf{p}\cdot\mathbf{M}^{-1}\mathbf{p}\right)\,.
$$

The transport coefficient: $\alpha^* = \lim_{r\to 0}\frac{r}{\mathbb{E}_r^*[\lambda]}$

Outline

Overview of Previous Work

Existing methods for computing transport coefficients in DPD:

1. Equilibrium approaches:
   - The mean squared displacement method [Chaudhri and Lukes, 2010, Panoukidou et al., 2021]
   - The Green–Kubo integration of the stress autocorrelation function [Green, 1954, Kubo, 1957]
2. Nonequilibrium approaches:
   - The shear flow method (Lees-Edwards boundary conditions) [Pagonabarraga et al., 1998, Shang, 2021]
   - The periodic Poiseuille flow method [Backer et al., 2005]

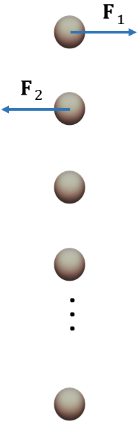
The List of Parameters

Parameters	Descriptions	Values
d	dimension	3
N	number of particles	500
m_i	mass of particle i	1
ρ	density of particles	0.85
r_c	cutoff radius	2.5
ε	energy parameter	1
r_0	length scales	1
γ	dissipative strength	4.5, 40.5
σ	random strength	3.0, 9.0
k_B	Boltzmann constant	1
T	equilibrium temperature	1
Δt	stepsize	0.01

Outline

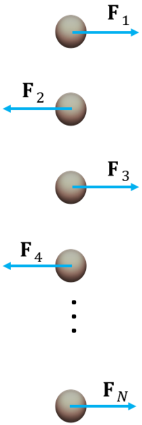
Two drifts

$$\mathbf{F}_1 = \frac{1}{\sqrt{2}}\mathbf{e}_x = -\mathbf{F}_2,\ \mathbf{F}_i = \mathbf{0}\ (i \geq 3)$$



Colour drifts

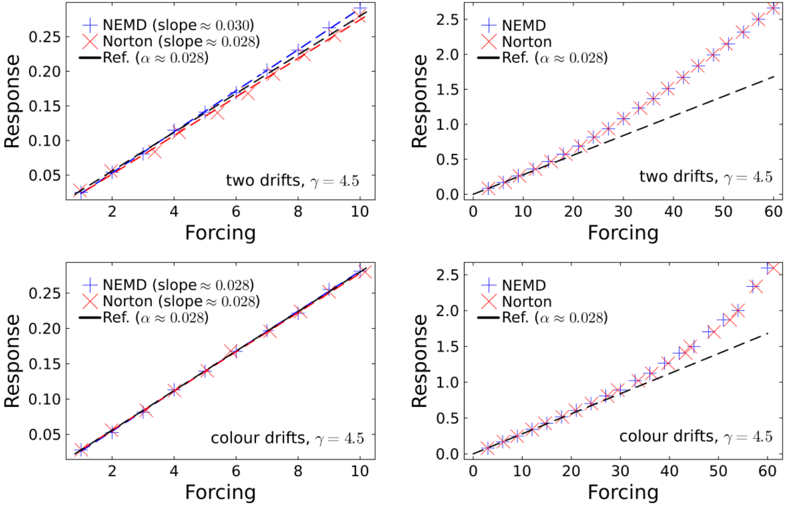
$$\mathbf{F}_i = \frac{(-1)^i}{\sqrt{N}}\mathbf{e}_x\ (i = 1, 2, ..., N)$$



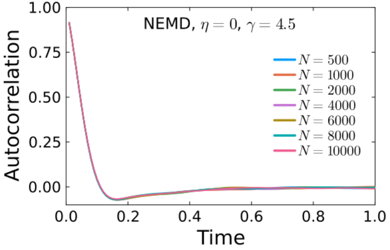
$$\mathbf{e}_x = (1, 0, 0)^{\mathrm{T}}$$

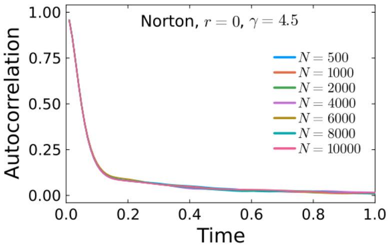
Response Profiles

$$R(\mathbf{q},\mathbf{p}) = \mathbf{G}(\mathbf{q}) \cdot \mathbf{p} = \mathbf{F} \cdot \mathbf{M}^{-1}\mathbf{p}\,.$$



Autocorrelation Functions in Equilibrium

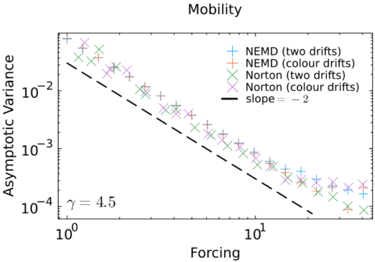


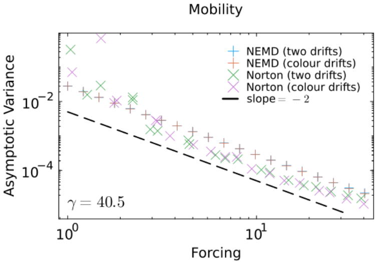


- DPD-NEMD: $\langle R(t+s)R(s)\rangle = \langle R(t)R(0)\rangle$
- DPD-Norton: $\langle \lambda(t+s)\lambda(s)\rangle = \langle \lambda(t)\lambda(0)\rangle$

Asymptotic Variance

Use the block average method [Flyvbjerg and Petersen, 1989]





- DPD-NEMD: $\sigma^2_{\alpha,\eta} = \frac{2}{\eta^2}\mathrm{Var}_\eta(R)\Theta_\eta(R)$
- DPD-Norton: $\sigma^2_{\alpha^*,r} = \frac{2r^2}{(\mathbb{E}^*_r[\lambda])^4}\mathrm{Var}^*_r(\lambda)\Theta^*_r(\lambda)$

Outline

External Forcing

A forcing is applied on the momenta in the longitudinal direction x, depending on the coordinate y:

$$\mathbf{F}(\mathbf{q}_j) = \begin{pmatrix} f(q_{j,y}) & 0 & 0 \end{pmatrix}^{\mathrm{T}}$$

- sinusoidal force: $f(y) = \sin\left(\frac{2\pi y}{L_y}\right), \quad 0 \leqslant y \leqslant L_y$
- linear force: $f(y) = \begin{cases} \frac{4}{L_y}\left(y - \frac{L_y}{4}\right), & 0 \leqslant y \leqslant \frac{L_y}{2}, \\ \frac{4}{L_y}\left(\frac{3L_y}{4} - y\right), & \frac{L_y}{2} < y \leqslant L_y \end{cases}$
- constant force: $f(y) = \begin{cases} 1, & 0 < y \leqslant \frac{L_y}{2}, \\ -1, & \frac{L_y}{2} < y \leqslant L_y \end{cases}$

Shear Viscosity Computation in DPD (1/3)

- The average longitudinal velocity:

$$U_x^\varepsilon(Y, \mathbf{q}, \mathbf{p}) = \frac{L_y}{Nm} \sum_{i=1}^{N} p_{xi} \chi_\varepsilon(q_{yi} - Y)$$

- The xy component of the stress tensor:

$$\Sigma_{xy}^\varepsilon(Y, \mathbf{q}, \mathbf{p}) = \frac{1}{L_x L_z} \left(\sum_{i=1}^{N} \frac{p_{xi} p_{yi}}{m} \chi_\varepsilon(q_{yi} - Y) + \sum_{1 \leq i < j \leq N} F_{ij}^x(r_{ij}) \int_{q_{yj}}^{q_{yi}} \chi_\varepsilon(s - Y) \, \mathrm{d}s \right)$$

where χ_ε is the Dirac delta function on $[0, L_y]$ with $0 < \varepsilon \leq 1$, and the intermolecular force:

$$F_{ij}^x(r_{ij}) = -U'(r_{ij}) e_{ij}^x - \gamma \omega^{\mathrm{D}}(r_{ij})(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) e_{ij}^x$$

Shear Viscosity Computation in DPD (2/3)

Proposition

Suppose that the limits

$$u_x(Y) = \lim_{\varepsilon\to 0}\lim_{\eta\to 0} \frac{\langle U_x^{\varepsilon}(Y,\mathbf{q},\mathbf{p})\rangle_\eta}{\eta},$$

$$\sigma_{xy}(Y) = \lim_{\varepsilon\to 0}\lim_{\eta\to 0} \frac{\langle \Sigma_{xy}^{\varepsilon}(Y,\mathbf{q},\mathbf{p})\rangle_\eta}{\eta}$$

exist and are smooth with respect to $Y \in [0, L_y]$, where $\langle\cdot\rangle_\eta$ denotes the average associated with the measure of the dynamics, then

$$\frac{\partial \sigma_{xy}(Y)}{\partial Y} = \rho F(Y),$$

where $\rho = \frac{N}{L_x L_y L_z}$ is the density and $F(Y)$ is the external force.

Shear Viscosity Computation in DPD (3/3)

- Consider a bulk homogeneous system and assume that the external force is sufficiently small:

$$\sigma_{xy}(Y) = -\nu \frac{\mathrm{d}u_x(Y)}{\mathrm{d}Y} \, .$$

Shear Viscosity Computation in DPD (3/3)

- Consider a bulk homogeneous system and assume that the external force is sufficiently small:

$$\sigma_{xy}(Y) = -\nu \frac{\mathrm{d}u_x(Y)}{\mathrm{d}Y} .$$

- The shear viscosity can be computed by the related Fourier coefficients as follows:

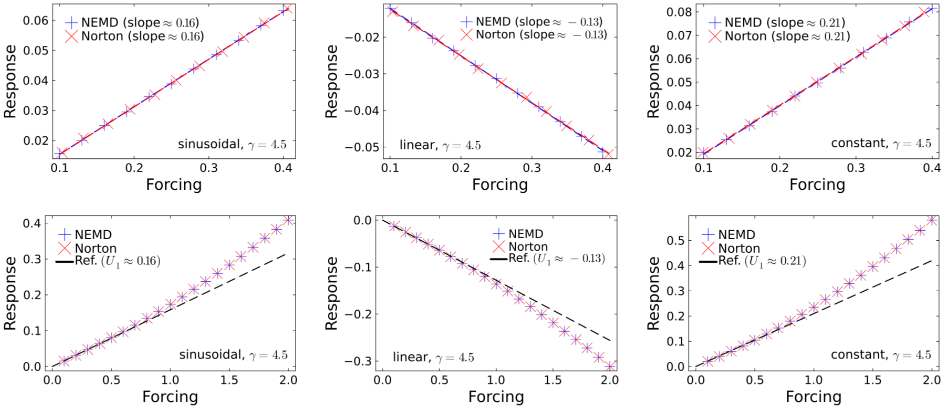
$$\nu = \frac{\rho F_1}{U_1} \left(\frac{L_y}{2\pi} \right)^2 ,$$

where the Fourier coefficients of the forcing F_1 is analytically known, and the Fourier coefficients of the longitudinal velocity U_1 is given by

$$U_1 = \lim_{\eta \to 0} \frac{1}{\eta N} \mathbb{E}_\eta \left[\sum_{j=1}^{N} (\mathbf{M}^{-1}\mathbf{p})_{j,x} \exp\left(\frac{2i\pi q_{j,y}}{L_y} \right) \right]$$

Response Profiles (U_1)

$$R(\mathbf{q},\mathbf{p}) = \frac{1}{N}\sum_{j=1}^{N}(\mathbf{M}^{-1}\mathbf{p})_{j,x}\exp\left(\frac{2i\pi q_{j,y}}{L_y}\right)$$



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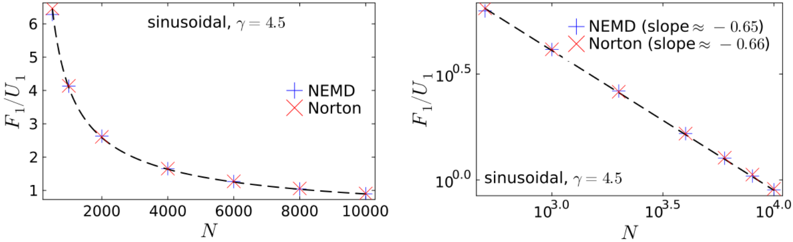
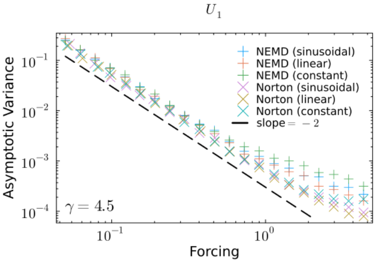
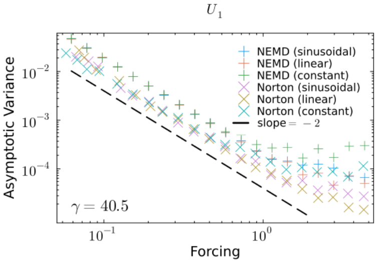


Asymptotic Variance

Use the block average method [Flyvbjerg and Petersen, 1989]





- DPD-NEMD: $\sigma^2_{U_1,\eta} = \frac{2}{\eta^2}\mathrm{Var}_\eta(R)\Theta_\eta(R)$
- DPD-Norton: $\sigma^2_{U_1^*,r} = \frac{2r^2}{(\mathbb{E}_r^*[\lambda])^4}\mathrm{Var}_r^*(\lambda)\Theta_r^*(\lambda)$

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Main Contribution

- Study a novel alternative approach for the computation of transport coefficients at mesoscale: the DPD-Norton dynamics.

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Main Contribution

- Study a novel alternative approach for the computation of transport coefficients at mesoscale: the DPD-Norton dynamics.
- Derive a closed-form expression for the shear viscosity computation.
- Conduct various numerical experiments on the computation of the mobility and the shear viscosity, respectively, using different types of external forces for each case.
- The numerical Experiments demonstrate that the DPD-Norton approach outperforms the DPD-NEMD in controlling the asymptotic variance.

Future Work

- Explore how the DPD-Norton dynamics performs with more complicated potential energies (for instance, in polymer melts);
- Employ machine learning methods in DPD to address real-world problems;
- Enhance the numerical efficiency;
- ......

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Acknowledgement

- Registration and travel support for this presentation was provided by the Society for Industrial and Applied Mathematics;
- Research was funded by University of Birmingham – China Scholarship Council.

The paper is available at

https://arxiv.org/abs/2504.14479

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Thank you for your listening!

Question?

Mean Squared Displacement

- The diffusion coefficient:

$$D = \frac{1}{2d} \lim_{t \to \infty} \frac{\mathrm{MSD}(t)}{t} \,,$$

where the mean squared displacement (MSD) is given by

$$\mathrm{MSD}(t) = \left\langle |\mathbf{q}(t) - \mathbf{q}(0)|^2 \right\rangle = \frac{1}{N} \sum_{i=1}^{N} |\mathbf{q}_i(t) - \mathbf{q}_i(0)|^2 \,.$$

- The Einstein relation:

$$\alpha = \beta D \,.$$

DPD-NEMD

$$
\mathrm{d}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = \underbrace{\begin{bmatrix}\mathbf{M}^{-1}\mathbf{p}\\ \mathbf{0}\end{bmatrix}\mathrm{d}t}_{\text{A}} + \underbrace{\begin{bmatrix}\mathbf{0}\\ -\nabla U(\mathbf{q}) + \eta\mathbf{F}(\mathbf{q})\end{bmatrix}\mathrm{d}t}_{\text{B}}
$$

$$
+ \underbrace{\begin{bmatrix}\mathbf{0}\\ -\gamma\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q})\mathrm{d}\mathbf{W}\end{bmatrix}}_{\text{O}}
$$

DPD-NEMD

$$\mathrm{d}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = \underbrace{\begin{bmatrix}\mathbf{M}^{-1}\mathbf{p}\\ \mathbf{0}\end{bmatrix}\mathrm{d}t}_{\mathrm{A}} + \underbrace{\begin{bmatrix}\mathbf{0}\\ -\nabla U(\mathbf{q}) + \eta\mathbf{F}(\mathbf{q})\end{bmatrix}\mathrm{d}t}_{\mathrm{B}}$$

$$+ \underbrace{\begin{bmatrix}\mathbf{0}\\ -\gamma\mathbf{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\mathrm{d}t + \sigma\mathbf{\Sigma}(\mathbf{q})\mathrm{d}\mathbf{W}\end{bmatrix}}_{\mathrm{O}}$$

$$\begin{aligned}
\mathcal{L}_{\mathrm{A}} &= \mathbf{M}^{-1}\mathbf{p}\cdot\nabla_{\mathbf{q}}\,,\\
\mathcal{L}_{\mathrm{B}} &= -\nabla U(\mathbf{q})\cdot\nabla_{\mathbf{p}} + \eta\mathbf{F}(\mathbf{q})\cdot\nabla_{\mathbf{p}}\,,\\
\mathcal{L}_{\mathrm{O}} &= -\gamma\mathbf{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\cdot\nabla_{\mathbf{p}} + \frac{\sigma^2}{2}\mathbf{\Sigma}(\mathbf{q})(\mathbf{\Sigma}(\mathbf{q}))^T : \nabla_{\mathbf{p}}^2\,.
\end{aligned}$$

DPD-NEMD

- The generator of the DPD-NEMD system:

$$\mathcal{L} = \mathcal{L}_{\mathrm{A}} + \mathcal{L}_{\mathrm{B}} + \mathcal{L}_{\mathrm{O}}\,.$$

DPD-NEMD

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- The flow map of the DPD-NEMD system:

$$\mathcal{F}_t = \exp\left(t\mathcal{L}\right) \,.$$

DPD-NEMD

- The generator of the DPD-NEMD system:

$$\mathcal{L} = \mathcal{L}_{\mathrm{A}} + \mathcal{L}_{\mathrm{B}} + \mathcal{L}_{\mathrm{O}} \,.$$

- The flow map of the DPD-NEMD system:

$$\mathcal{F}_t = \exp\left(t\mathcal{L}\right) \,.$$

- The phase space propagation for the ABOBA method:

$$e^{\Delta t \mathcal{L}_{\mathrm{ABOBA}}} = e^{\frac{\Delta t}{2}\mathcal{L}_{\mathrm{A}}} e^{\frac{\Delta t}{2}\mathcal{L}_{\mathrm{B}}} e^{\Delta t \widehat{\mathcal{L}}_{\mathrm{O}}} e^{\frac{\Delta t}{2}\mathcal{L}_{\mathrm{B}}} e^{\frac{\Delta t}{2}\mathcal{L}_{\mathrm{A}}} \,,$$

  where the propagation of the O part is defined by

$$e^{\Delta t \widehat{\mathcal{L}}_{\mathrm{O}}} = e^{\Delta t \widehat{\mathcal{L}}_{\mathrm{O}_{N-1,N}}} \ldots e^{\Delta t \widehat{\mathcal{L}}_{\mathrm{O}_{1,3}}} e^{\Delta t \widehat{\mathcal{L}}_{\mathrm{O}_{1,2}}} \,.$$

The ABOBA Method: O part

Pairwise interaction between the *i*-th and the *j*-th particles:

$$\mathbf{p}_i^{n+2/3} = \mathbf{p}_i^{n+1/3} + m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+1/3}) + \Delta v_{ij}^{\mathrm{R}}(\mathbf{q}^{n+1/2})\right]\mathbf{e}_{ij}^{n+1/2},$$
$$\mathbf{p}_j^{n+2/3} = \mathbf{p}_j^{n+1/3} - m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+1/3}) + \Delta v_{ij}^{\mathrm{R}}(\mathbf{q}^{n+1/2})\right]\mathbf{e}_{ij}^{n+1/2},$$

where the relative velocity is given by

$$\Delta v_{ij}^{\mathrm{D}}(\mathbf{q}, \mathbf{p}) = \left[\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}\right]\left(e^{-\tau \Delta t} - 1\right), \; \Delta v_{ij}^{\mathrm{R}}(\mathbf{q}) = \frac{\sigma \omega^{\mathrm{R}}(r_{ij})}{m_{ij}} \sqrt{\frac{1 - e^{-2\tau \Delta t}}{2\tau}} \mathrm{R}_{ij}^n,$$

with $m_{ij} = m_i m_j / (m_i + m_j)$, $\tau(r_{ij}) = \gamma \omega^{\mathrm{D}}(r_{ij}) / m_{ij}$, $\mathrm{R}_{ij} \sim \mathcal{N}(0, 1)$.

The ABOBA Method (DPD-NEMD)

Step 1: for all particles,

$$\mathbf{q}^{n+1/2} = \mathbf{q}^n + (\Delta t/2)\mathbf{M}^{-1}\mathbf{p}^n \,,$$
$$\mathbf{p}^{n+1/3} = \mathbf{p}^n - (\Delta t/2)\nabla U(\mathbf{q}^{n+1/2}) + (\Delta t/2)\eta\mathbf{F}(\mathbf{q}^{n+1/2}) \,.$$

Step 2: for each interacting pair within cutoff radius ($r_{ij} < r_\mathrm{c}$),

$$\mathbf{p}_i^{n+2/3} = \mathbf{p}_i^{n+1/3} + m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+1/3}) + \Delta v_{ij}^{\mathrm{R}}(\mathbf{q}^{n+1/2})\right]\mathbf{e}_{ij}^{n+1/2} \,,$$
$$\mathbf{p}_j^{n+2/3} = \mathbf{p}_j^{n+1/3} - m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+1/3}) + \Delta v_{ij}^{\mathrm{R}}(\mathbf{q}^{n+1/2})\right]\mathbf{e}_{ij}^{n+1/2} \,,$$

Step 3: for all particles,

$$\mathbf{p}^{n+1} = \mathbf{p}^{n+2/3} - (\Delta t/2)\nabla U(\mathbf{q}^{n+1/2}) + (\Delta t/2)\eta\mathbf{F}(\mathbf{q}^{n+1/2}) \,,$$
$$\mathbf{q}^{n+1} = \mathbf{q}^{n+1/2} + (\Delta t/2)\mathbf{M}^{-1}\mathbf{p}^{n+1} \,.$$

Outline

DPD-Norton

$$
\mathrm{d}\begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{M}^{-1}\mathbf{p}\,\mathrm{d}t \\ \mathbf{F}(\mathbf{q})\,\mathrm{d}\Lambda^{\mathrm{A}} \end{bmatrix}}_{\mathrm{A}} + \underbrace{\begin{bmatrix} \mathbf{0} \\ -\nabla U(\mathbf{q})\,\mathrm{d}t + \mathbf{F}(\mathbf{q})\,\mathrm{d}\Lambda^{\mathrm{B}} \end{bmatrix}}_{\mathrm{B}}
$$

$$
+ \underbrace{\begin{bmatrix} \mathbf{0} \\ -\gamma\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\,\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q})\,\mathrm{d}\mathbf{W} + \mathbf{F}(\mathbf{q})\,\mathrm{d}\Lambda^{\mathrm{O}} \end{bmatrix}}_{\mathrm{O}},
$$

DPD-Norton

$$
\mathrm{d}\begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{M}^{-1}\mathbf{p}\,\mathrm{d}t \\ \mathbf{F}(\mathbf{q})\,\mathrm{d}\Lambda^{\mathrm{A}} \end{bmatrix}}_{\mathrm{A}} + \underbrace{\begin{bmatrix} \mathbf{0} \\ -\nabla U(\mathbf{q})\,\mathrm{d}t + \mathbf{F}(\mathbf{q})\,\mathrm{d}\Lambda^{\mathrm{B}} \end{bmatrix}}_{\mathrm{B}}
$$

$$
+ \underbrace{\begin{bmatrix} \mathbf{0} \\ -\gamma\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\,\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q})\,\mathrm{d}\mathbf{W} + \mathbf{F}(\mathbf{q})\,\mathrm{d}\Lambda^{\mathrm{O}} \end{bmatrix}}_{\mathrm{O}},
$$

- The generator of the DPD-Norton system:

$$
\mathfrak{L} = \mathfrak{L}_{\mathrm{A}} + \mathfrak{L}_{\mathrm{B}} + \mathfrak{L}_{\mathrm{O}}\,.
$$

DPD-Norton

$$
\begin{aligned}
\mathfrak{L}_{\mathrm{A}} &= \mathbf{M}^{-1}\mathbf{p} \cdot \nabla_{\mathbf{q}} - \frac{\nabla \mathbf{G}(\mathbf{q})\mathbf{p} \cdot \mathbf{M}^{-1}\mathbf{p}}{\mathbf{F}(\mathbf{q}) \cdot \mathbf{G}(\mathbf{q})} \mathbf{F}(\mathbf{q}) \cdot \nabla_{\mathbf{p}} \,, \\
\mathfrak{L}_{\mathrm{B}} &= -\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q}) \nabla U(\mathbf{q}) \cdot \nabla_{\mathbf{p}} \,, \\
\mathfrak{L}_{\mathrm{O}} &= -\gamma \overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q}) \boldsymbol{\Gamma}(\mathbf{q}) \mathbf{M}^{-1}\mathbf{p} \cdot \nabla_{\mathbf{p}} \\
&\quad + \frac{\sigma^2}{2} \overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q}) \boldsymbol{\Sigma}(\mathbf{q}) (\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q}) \boldsymbol{\Sigma}(\mathbf{q}))^T : \nabla_{\mathbf{p}}^2 \,,
\end{aligned}
$$

DPD-Norton

$$
\begin{aligned}
\mathfrak{L}_{\mathrm{A}} &= \mathbf{M}^{-1}\mathbf{p}\cdot\nabla_{\mathbf{q}} - \frac{\nabla\mathbf{G}(\mathbf{q})\mathbf{p}\cdot\mathbf{M}^{-1}\mathbf{p}}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}\mathbf{F}(\mathbf{q})\cdot\nabla_{\mathbf{p}}\,,\\
\mathfrak{L}_{\mathrm{B}} &= -\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q})\nabla U(\mathbf{q})\cdot\nabla_{\mathbf{p}}\,,\\
\mathfrak{L}_{\mathrm{O}} &= -\gamma\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q})\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\cdot\nabla_{\mathbf{p}}\\
&\quad+\frac{\sigma^2}{2}\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q})\boldsymbol{\Sigma}(\mathbf{q})\left(\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q})\boldsymbol{\Sigma}(\mathbf{q})\right)^T:\nabla_{\mathbf{p}}^2\,,
\end{aligned}
$$

- The nonorthogonal projector-valued map

$$
\overline{\mathbf{P}}_{\mathbf{F},\mathbf{G}}(\mathbf{q}) = \mathbf{I} - \frac{\mathbf{F}(\mathbf{q})\otimes\mathbf{G}(\mathbf{q})}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}\,,
$$

with the condition $(\mathbf{F}\cdot\mathbf{G})(\mathbf{q})\neq 0$ for any $\mathbf{q}\in\mathbb{R}^{dN}$, where $\otimes$ represents the Kronecker product and $\mathbf{I}$ is an identity matrix.

DPD-Norton (A-dynamics)

Discrete Flow of A-dynamics

$$\Phi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q}\,,\ \mathbf{p}\,,\ \ell) =$$

$$\Big(\mathbf{q} + \Delta t \mathbf{M}^{-1}\mathbf{p},\ \mathbf{p} + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}),\ \ell + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\Big)\ ,$$

where $\xi^{\mathrm{A}}_{\Delta t,r} \in \mathbb{R}$ is a Lagrange multiplier and $\ell \in \mathbb{R}$ is an auxiliary variable.

DPD-Norton (A-dynamics)

Discrete Flow of A-dynamics

$$\Phi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q}\,,\ \mathbf{p}\,,\ \ell) =$$

$$\Big(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p},\ \mathbf{p} + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}),\ \ell + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\Big)\ ,$$

where $\xi^{\mathrm{A}}_{\Delta t,r} \in \mathbb{R}$ is a Lagrange multiplier and $\ell \in \mathbb{R}$ is an auxiliary variable.

$$\mathbf{G}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}) \cdot \Big(\mathbf{p} + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p})\Big) = r$$

DPD-Norton (A-dynamics)

Discrete Flow of A-dynamics

$$\Phi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q}\,,\ \mathbf{p}\,,\ \ell) =$$

$$\Big(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p},\ \mathbf{p} + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}),\ \ell + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\Big)\ ,$$

where $\xi^{\mathrm{A}}_{\Delta t,r} \in \mathbb{R}$ is a Lagrange multiplier and $\ell \in \mathbb{R}$ is an auxiliary variable.

$$\mathbf{G}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}) \cdot \Big(\mathbf{p} + \xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p})\Big) = r$$

$$\Downarrow$$

$$\xi^{\mathrm{A}}_{\Delta t,r}(\mathbf{q},\mathbf{p}) = \frac{r - \mathbf{G}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}) \cdot \mathbf{p}}{\mathbf{F}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p}) \cdot \mathbf{G}(\mathbf{q} + \Delta t\mathbf{M}^{-1}\mathbf{p})}\ .$$

DPD-Norton (B-dynamics)

Discrete Flow of B-dynamics

$$\Phi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q}\,,\ \mathbf{p}\,,\ \ell) =$$

$$\Big(\mathbf{q}\,,\ \mathbf{p} - \Delta t \nabla U(\mathbf{q}) + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\,,\ \ell + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\Big)$$

DPD-Norton (B-dynamics)

Discrete Flow of B-dynamics

$$\Phi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q}\,,\ \mathbf{p}\,,\ \ell) =$$

$$\Big(\mathbf{q}\,,\ \mathbf{p} - \Delta t \nabla U(\mathbf{q}) + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\,,\ \ell + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\Big)$$

$$\mathbf{G}(\mathbf{q}) \cdot \Big(\mathbf{p} - \Delta t \nabla U(\mathbf{q}) + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\Big) = r$$

DPD-Norton (B-dynamics)

Discrete Flow of B-dynamics

$$\Phi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q}\,,\ \mathbf{p}\,,\ \ell) =$$

$$\Big(\mathbf{q}\,,\ \mathbf{p} - \Delta t \nabla U(\mathbf{q}) + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\,,\ \ell + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\Big)$$

$$\mathbf{G}(\mathbf{q}) \cdot \Big(\mathbf{p} - \Delta t \nabla U(\mathbf{q}) + \xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\Big) = r$$

$$\Downarrow$$

$$\xi^{\mathrm{B}}_{\Delta t,r}(\mathbf{q},\mathbf{p}) = \frac{r - \mathbf{G}(\mathbf{q}) \cdot (\mathbf{p} - \Delta t \nabla U(\mathbf{q}))}{\mathbf{F}(\mathbf{q}) \cdot \mathbf{G}(\mathbf{q})}\,.$$

DPD-Norton (O-dynamics) (1/3)

Discrete Flow of O-dynamics

$$\widehat{\Phi}^{\mathrm{O}}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell) = \widehat{\Phi}^{\mathrm{O}_\xi}_{\Delta t,r} \circ \widehat{\Phi}^{\mathrm{O}_{N-1,N}}_{\Delta t,r} \circ \cdots \circ \widehat{\Phi}^{\mathrm{O}_{1,3}}_{\Delta t,r} \circ \widehat{\Phi}^{\mathrm{O}_{1,2}}_{\Delta t,r}(\mathbf{q},\mathbf{p},\mathbf{0},0)\,,$$

where

- $\widehat{\Phi}^{\mathrm{O}_{i,j}}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell|R_{ij}) =$
  $\left(\mathbf{q},\mathbf{p}+m_{ij}\left[\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})+\Delta v^{\mathrm{R}}_{ij}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij},\Delta\mathbf{p}+m_{ij}\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})\widehat{\mathbf{e}}_{ij},\ell\right)$
- $\widehat{\Phi}^{\mathrm{O}_\xi}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell|R_{ij}) = \left(\mathbf{q},\mathbf{p}+\widehat{\xi}^{\mathrm{O}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q}),\Delta\mathbf{p},\ell-\frac{\mathbf{G}(\mathbf{q})\cdot\Delta\mathbf{p}}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}\right)$

(1) The propagator for each interacting pair

$$\widehat{\Phi}^{\mathrm{O}_{i,j}}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell|R_{ij}) =$$
$$\left(\mathbf{q}, \mathbf{p} + m_{ij}\left[\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p}) + \Delta v^{\mathrm{R}}_{ij}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij}, \Delta\mathbf{p} + m_{ij}\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})\widehat{\mathbf{e}}_{ij}, \ell\right),$$

DPD-Norton (O-dynamics) (2/3)

(1) The propagator for each interacting pair

$$\widehat{\Phi}^{\mathrm{O}_{i,j}}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell|R_{ij}) =$$
$$\left(\mathbf{q},\mathbf{p}+m_{ij}\left[\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})+\Delta v^{\mathrm{R}}_{ij}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij},\Delta\mathbf{p}+m_{ij}\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})\widehat{\mathbf{e}}_{ij},\ell\right),$$

where

$$\widehat{\mathbf{e}}_{ij} = \left(\mathbf{0},\ldots,\mathbf{0},\underbrace{\mathbf{e}_{ij}^{\mathrm{T}}}_{d(i-1)+1,\ldots,di},\mathbf{0},\ldots,\mathbf{0},\underbrace{-\mathbf{e}_{ij}^{\mathrm{T}}}_{d(j-1)+1,\ldots,dj},\mathbf{0},\ldots,0\right)^{\mathrm{T}} \in \mathbb{R}^{dN}.$$

DPD-Norton (O-dynamics) (2/3)

(1) The propagator for each interacting pair

$$\widehat{\Phi}^{\mathrm{O}_{i,j}}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell|R_{ij}) =$$
$$\left(\mathbf{q},\mathbf{p}+m_{ij}\left[\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})+\Delta v^{\mathrm{R}}_{ij}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij},\Delta\mathbf{p}+m_{ij}\Delta v^{\mathrm{D}}_{ij}(\mathbf{q},\mathbf{p})\widehat{\mathbf{e}}_{ij},\ell\right),$$

where

$$\widehat{\mathbf{e}}_{ij} = \left(\mathbf{0},\dots,\mathbf{0},\underbrace{\mathbf{e}_{ij}^{\mathrm{T}}}_{d(i-1)+1,\dots,di},\mathbf{0},\dots,\mathbf{0},\underbrace{-\mathbf{e}_{ij}^{\mathrm{T}}}_{d(j-1)+1,\dots,dj},\mathbf{0},\dots,0\right)^{\mathrm{T}} \in \mathbb{R}^{dN}.$$

(2) The propagator related to forcing observable

$$\widehat{\Phi}^{\mathrm{O}_\xi}_{\Delta t,r}(\mathbf{q},\mathbf{p},\Delta\mathbf{p},\ell|R_{ij}) = \left(\mathbf{q},\mathbf{p}+\widehat{\xi}^{\mathrm{O}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q}),\Delta\mathbf{p},\ell-\frac{\mathbf{G}(\mathbf{q})\cdot\Delta\mathbf{p}}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}\right)$$

DPD-Norton (O-dynamics) (3/3)

$$\mathbf{G}(\mathbf{q})\cdot\left(\mathbf{p} + \sum_{1\le i<j\le N} m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q},\mathbf{p}) + \Delta v_{ij}^{\mathrm{R}}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij} + \widehat{\xi}^{\mathrm{O}}_{\Delta t,r}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\right) = r$$

DPD-Norton (O-dynamics) (3/3)

$$\mathbf{G}(\mathbf{q})\cdot\left(\mathbf{p}+\sum_{1\le i<j\le N} m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q},\mathbf{p})+\Delta v_{ij}^{\mathrm{R}}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij}+\widehat{\xi}_{\Delta t,r}^{\mathrm{O}}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\right)=r$$

$$\Downarrow$$

$$\widehat{\xi}_{\Delta t,r}^{\mathrm{O}}(\mathbf{q},\mathbf{p})=\frac{r-\mathbf{G}(\mathbf{q})\cdot\left(\mathbf{p}+\sum_{1\le i<j\le N} m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q},\mathbf{p})+\Delta v_{ij}^{\mathrm{R}}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij}\right)}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}$$

DPD-Norton (O-dynamics) (3/3)

$$\mathbf{G}(\mathbf{q})\cdot\left(\mathbf{p}+\sum_{1\le i<j\le N} m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q},\mathbf{p})+\Delta v_{ij}^{\mathrm{R}}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij}+\widehat{\xi}_{\Delta t,r}^{\mathrm{O}}(\mathbf{q},\mathbf{p})\mathbf{F}(\mathbf{q})\right)=r$$

$$\Downarrow$$

$$\widehat{\xi}_{\Delta t,r}^{\mathrm{O}}(\mathbf{q},\mathbf{p})=\frac{r-\mathbf{G}(\mathbf{q})\cdot\left(\mathbf{p}+\sum_{1\le i<j\le N} m_{ij}\left[\Delta v_{ij}^{\mathrm{D}}(\mathbf{q},\mathbf{p})+\Delta v_{ij}^{\mathrm{R}}(\mathbf{q})\right]\widehat{\mathbf{e}}_{ij}\right)}{\mathbf{F}(\mathbf{q})\cdot\mathbf{G}(\mathbf{q})}$$

The phase space propagation for the ABOBA method

$$(\mathbf{q}^{n+1},\mathbf{p}^{n+1},\ell^{n+1})=$$
$$\Phi_{\Delta t/2,r}^{\mathrm{A}}\circ\Phi_{\Delta t/2,r}^{\mathrm{B}}\circ\widehat{\Phi}_{\Delta t,r}^{\mathrm{O}}(\cdot|R_{ij})\circ\Phi_{\Delta t/2,r}^{\mathrm{B}}\circ\Phi_{\Delta t/2,r}^{\mathrm{A}}(\mathbf{q}^{n},\mathbf{p}^{n},\ell^{n})$$

DPD-Norton (1/3)

Starting from $\ell^n = 0$, for all particles,

$$
\begin{aligned}
\mathbf{q}^{n+1/2} &= \mathbf{q}^n + (\Delta t/2)\mathbf{M}^{-1}\mathbf{p}^n \,, \\
\mathbf{p}^{n+1/5} &= \mathbf{p}^n + \xi^{\mathrm{A}}_{\Delta t/2,r}(\mathbf{q}^n, \mathbf{p}^n)\mathbf{F}(\mathbf{q}^{n+1/2}) \,, \\
\ell^{n+1/5} &= \ell^n + \xi^{\mathrm{A}}_{\Delta t/2,r}(\mathbf{q}^n, \mathbf{p}^n) \,, \\
\widetilde{\mathbf{p}}^{n+2/5} &= \mathbf{p}^{n+1/5} - (\Delta t/2)\nabla U(\mathbf{q}^{n+1/2}) \,, \\
\mathbf{p}^{n+2/5} &= \widetilde{\mathbf{p}}^{n+2/5} + \xi^{\mathrm{B}}_{\Delta t/2,r}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+1/5})\mathbf{F}(\mathbf{q}^{n+1/2}) \,, \\
\ell^{n+2/5} &= \ell^{n+1/5} + \xi^{\mathrm{B}}_{\Delta t/2,r}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+1/5}) \,.
\end{aligned}
$$

DPD-Norton (2/3)

Starting from $\Delta\mathbf{p}^n = \mathbf{0}$, for each interacting pair within cutoff radius ($r_{ij} < r_\mathrm{c}$), in a successive manner,

$$\widetilde{\mathbf{p}}_i^{n+3/5} = \mathbf{p}_i^{n+2/5} + m_{ij}\left[\Delta v_{ij}^\mathrm{D}(\mathbf{q}^{n+1/2},\mathbf{p}^{n+2/5}) + \Delta v_{ij}^\mathrm{R}(\mathbf{q}^{n+1/2})\right]\mathbf{e}_{ij}^{n+1/2},$$
$$\widetilde{\mathbf{p}}_j^{n+3/5} = \mathbf{p}_j^{n+2/5} - m_{ij}\left[\Delta v_{ij}^\mathrm{D}(\mathbf{q}^{n+1/2},\mathbf{p}^{n+2/5}) + \Delta v_{ij}^\mathrm{R}(\mathbf{q}^{n+1/2})\right]\mathbf{e}_{ij}^{n+1/2},$$
$$\Delta\mathbf{p}_i^{n+1} = \Delta\mathbf{p}_i^n + m_{ij}\Delta v_{ij}^\mathrm{D}(\mathbf{q}^{n+1/2},\mathbf{p}^{n+2/5})\mathbf{e}_{ij}^{n+1/2},$$
$$\Delta\mathbf{p}_j^{n+1} = \Delta\mathbf{p}_j^n - m_{ij}\Delta v_{ij}^\mathrm{D}(\mathbf{q}^{n+1/2},\mathbf{p}^{n+2/5})\mathbf{e}_{ij}^{n+1/2},$$

for all particles,

$$\mathbf{p}^{n+3/5} = \widetilde{\mathbf{p}}^{n+3/5} + \widehat{\xi}_{\Delta t,r}^\mathrm{O}(\mathbf{q}^{n+1/2},\mathbf{p}^{n+2/5})\mathbf{F}(\mathbf{q}^{n+1/2}),$$
$$\ell^{n+3/5} = \ell^{n+2/5} - \frac{\mathbf{G}(\mathbf{q}^{n+1/2})\cdot\Delta\mathbf{p}^{n+1}}{\mathbf{F}(\mathbf{q}^{n+1/2})\cdot\mathbf{G}(\mathbf{q}^{n+1/2})}.$$

DPD-Norton (3/3)

For all particles,

$$
\begin{aligned}
\widetilde{\mathbf{p}}^{n+4/5} &= \mathbf{p}^{n+3/5} - (\Delta t/2)\nabla U(\mathbf{q}^{n+1/2}) \, , \\
\mathbf{p}^{n+4/5} &= \widetilde{\mathbf{p}}^{n+4/5} + \xi^{\mathrm{B}}_{\Delta t/2,r}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+3/5})\mathbf{F}(\mathbf{q}^{n+1/2}) \, , \\
\ell^{n+4/5} &= \ell^{n+3/5} + \xi^{\mathrm{B}}_{\Delta t/2,r}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+3/5}) \, , \\
\mathbf{q}^{n+1} &= \mathbf{q}^{n+1/2} + (\Delta t/2)\mathbf{M}^{-1}\mathbf{p}^{n+4/5} \, , \\
\mathbf{p}^{n+1} &= \mathbf{p}^{n+4/5} + \xi^{\mathrm{A}}_{\Delta t/2,r}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+4/5})\mathbf{F}(\mathbf{q}^{n+1}) \, , \\
\ell^{n+1} &= \ell^{n+4/5} + \xi^{\mathrm{A}}_{\Delta t/2,r}(\mathbf{q}^{n+1/2}, \mathbf{p}^{n+4/5}) \, .
\end{aligned}
$$

The average of forcing variable can be estimated by

$$
\mathbb{E}^*_r[\lambda] = \frac{1}{N_{\mathrm{iter}}} \sum_{n=1}^{N_{\mathrm{iter}}} \lambda^n \, , \qquad \lambda^n = \Delta t^{-1} \ell^n \, .
$$

Proof of Proposition (1/3)

Re-decompose the generator for the perturbed DPD system:

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_\eta \,,$$

where

$$\begin{aligned}
\mathcal{L}_0 &= \mathcal{L}_{\mathrm{ham}} + \mathcal{L}_{\mathrm{thm}} \,, \\
\mathcal{L}_{\mathrm{ham}} &= \mathbf{M}^{-1}\mathbf{p} \cdot \nabla_{\mathbf{q}} - \nabla U(\mathbf{q}) \cdot \nabla_{\mathbf{p}} \,, \\
\mathcal{L}_{\mathrm{thm}} &= -\gamma \boldsymbol{\Gamma}(\mathbf{q}) \mathbf{M}^{-1}\mathbf{p} \cdot \nabla_{\mathbf{p}} + \frac{\sigma^2}{2} \boldsymbol{\Sigma}(\mathbf{q}) [\boldsymbol{\Sigma}(\mathbf{q}))]^T : \nabla_{\mathbf{p}}^2 \,, \\
\mathcal{L}_\eta &= \eta \sum_{i=1}^{N} F(q_{yi}) \partial_{p_{xi}} \,.
\end{aligned}$$

The corresponding adjoint operator:

$$\mathcal{L}^* = \mathcal{L}_0^* + \mathcal{L}_\eta^* \,,$$

where

$$\begin{aligned}
\mathcal{L}_0^* &= -\mathcal{L}_{\mathrm{ham}} + \mathcal{L}_{\mathrm{thm}} \,, \\
\mathcal{L}_\eta^* &= -\eta \sum_{i=1}^{N} \left(F(q_{yi}) \partial_{p_{xi}} - \frac{\beta}{m} p_{xi} F(q_{yi}) \right) \,.
\end{aligned}$$

Proof of Proposition (2/3)

The proof of equations (1) below in the context of DPD is similar to the proof of Corollary 1 in [Joubaud and Stoltz, 2012] in Langevin dynamics:

$$\lim_{\eta\to 0}\frac{\langle \mathcal{L}_0 U_x^{\varepsilon}(Y,\mathbf{q},\mathbf{p})\rangle_{\eta}}{\eta} = -\frac{\beta}{m}\left\langle U_x^{\varepsilon}(Y,\mathbf{q},\mathbf{p}), \sum_{i=1}^{N} p_{xi}F(q_{yi})\right\rangle_{L^2(\rho_\beta)}, \qquad (1)$$

where $\langle\cdot\rangle_{L^2(\rho_\beta)}$ denotes the average associated with the measure of DPD. Therefore, we have

$$\lim_{\varepsilon\to 0}\lim_{\eta\to 0}\frac{\langle \mathcal{L}_0 U_x^{\varepsilon}(Y,\mathbf{q},\mathbf{p})\rangle_{\eta}}{\eta} = -\frac{1}{m}F(Y)\,.$$

Proof of Proposition (3/3)

Meanwhile, splitting $\mathcal{L}_0 U_x^\varepsilon(Y, \mathbf{q}, \mathbf{p})$ into Hamiltonian and thermostat parts, we have

$$\mathcal{L}_{\text{ham}} U_x^\varepsilon(Y, \mathbf{q}, \mathbf{p}) = -\frac{L_y}{Nm} \frac{\mathrm{d}}{\mathrm{d}Y} \left(\sum_{i=1}^{N} \frac{p_{xi} p_{yi}}{m} \chi_\varepsilon(q_{yi} - Y) - \sum_{1 \le i < j \le N} U'(r_{ij}) e_{ij}^x \int_{q_{yj}}^{q_{yi}} \chi_\varepsilon(s - Y) \, \mathrm{d}s \right) ,$$

$$\begin{aligned} \mathcal{L}_{\text{thm}} U_x^\varepsilon(Y, \mathbf{q}, \mathbf{p}) &= -\frac{\gamma L_y}{Nm} \sum_{1 \le i < j \le N} \omega^{\mathrm{D}}(r_{ij}) (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) e_{ij}^x \left[\chi_\varepsilon(q_{yi} - Y) - \chi_\varepsilon(q_{yj} - Y) \right] \\ &= \frac{\gamma L_y}{Nm} \frac{\mathrm{d}}{\mathrm{d}Y} \left(\sum_{1 \le i < j \le N} \omega^{\mathrm{D}}(r_{ij}) (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) e_{ij}^x \int_{q_{yj}}^{q_{yi}} \chi_\varepsilon(s - Y) \, \mathrm{d}s \right) . \end{aligned}$$

Recalling the definition of the xy component of stress tensor, we have

$$-\rho m \mathcal{L}_0 U_x^\varepsilon(Y, \mathbf{q}, \mathbf{p}) = \frac{\partial \Sigma_{xy}^\varepsilon(Y, \mathbf{q}, \mathbf{p})}{\partial Y} .$$

Therefore, passing to the limits $\varepsilon \to 0$ and $\eta \to 0$, we have

$$\rho F(Y) = \frac{\partial \sigma_{xy}(Y)}{\partial Y} .$$