From Micro-physics to Stable Macro-models: Variational Learning for Non-Newtonian Fluids

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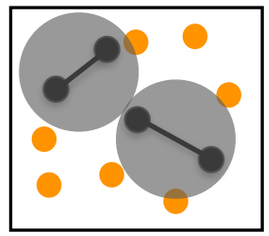
Outline

- Background
- DeePN^2: A variational-informed machine-learning model of non-Newtonian hydrodynamics
  - Macro-model energy stability
  - Frame-indifference and physical constraints
  - Micro-scale molecular fidelity and interpretation
- Numerical results and open problems

Hydrodynamics of non-Newtonian fluids

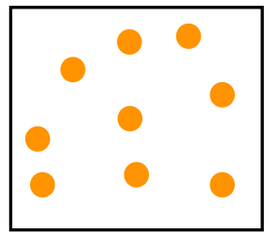
- Continuum hydrodynamic model of incompressible non-Newtonian fluids

$$\nabla \cdot \mathbf{u} = 0$$
$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} = -\nabla p + \nabla \cdot (\tau_\mathrm{s} + \tau_\mathrm{p}) + \mathbf{f}_\mathrm{ext}$$



- Newtonian model of solvent stress τ_s

$$\tau_\mathrm{s} = \eta_\mathrm{s}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top)$$

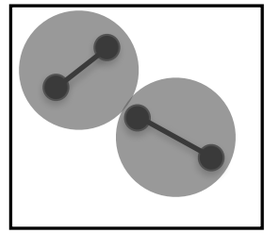


$t_s \ll t_c$

- Constitutive closure needed for polymer stress τ_p

t_p - relaxation time of liquid molecules

t_c - characteristic time of transport process

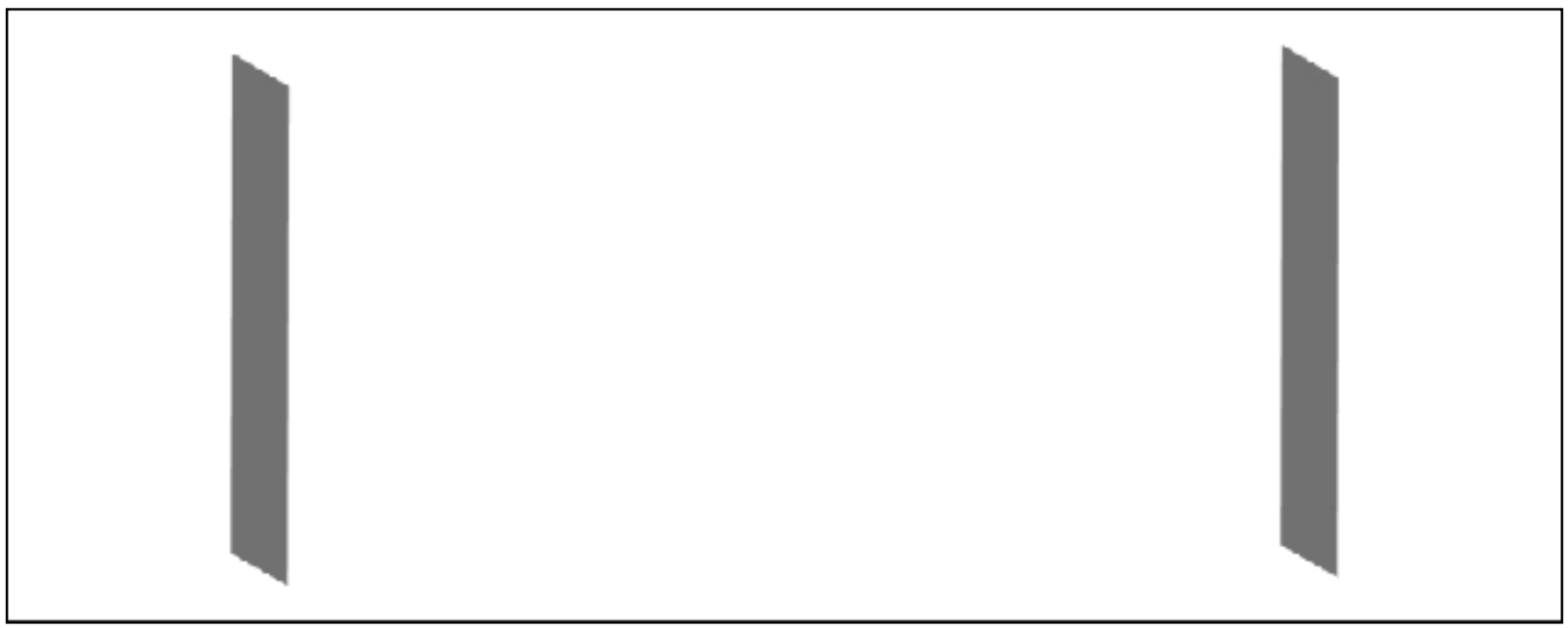


$t_p \not\ll t_c$

Why difficult? Micro-to-Macro: one-dimensional chain

- x

$$\ddot{x}_i = -k(2x_i - x_{i-1} - x_{i+1})$$



- X

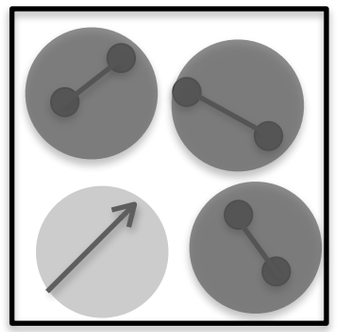
$$\ddot{X}_i = -K(2X_i - X_{i-1} - X_{i+1}) + \int_0^t \Gamma_{ij}(t-s)\dot{X}_j(s)\mathrm{d}s + R_i(t)$$

Lei-Baker-Li, *Proc. Natl. Acad. Sci.*, 2016

Why difficult?

- ***Full-model***: polymer stress τ_{p} determined by the micro-scale molecular interactions

$$\tau_{\mathrm{p}}(\boldsymbol{x}) = \sum_{j=1}^{N_b} \left\langle \mathbf{r}_j \otimes \nabla_{\mathbf{r}_j} V(\mathbf{r}) \right\rangle := \sum_{j=1}^{N_b} \int \mathbf{r}_j \otimes \nabla V_{\mathbf{r}_j}(\mathbf{r}) f(\mathbf{r}, \boldsymbol{x}) \mathrm{d}\mathbf{r}$$



$\mathbf{r} \in \mathbb{R}^{3N_b}$ - bond vector $\quad V : \mathbb{R}^{3N_b} \to \mathbb{R}$ - potential function $\quad \mathrm{r} \in \mathbb{R}^3, N_b = 1$

$f : \mathbb{R}^{3N_b} \times \mathbb{R}^3 \to \mathbb{R}_+$ - probability density function (PDF) of polymer configuration $\mathbf{r}$ at $\boldsymbol{x}$

- ***Computational challenges***
    - Multi-scale dynamics without scale separation
    - τ_{p} unclosed on the macro-scale
    - High-dimensional PDF estimation and calculation (e.g., Fokker-Planck equation)

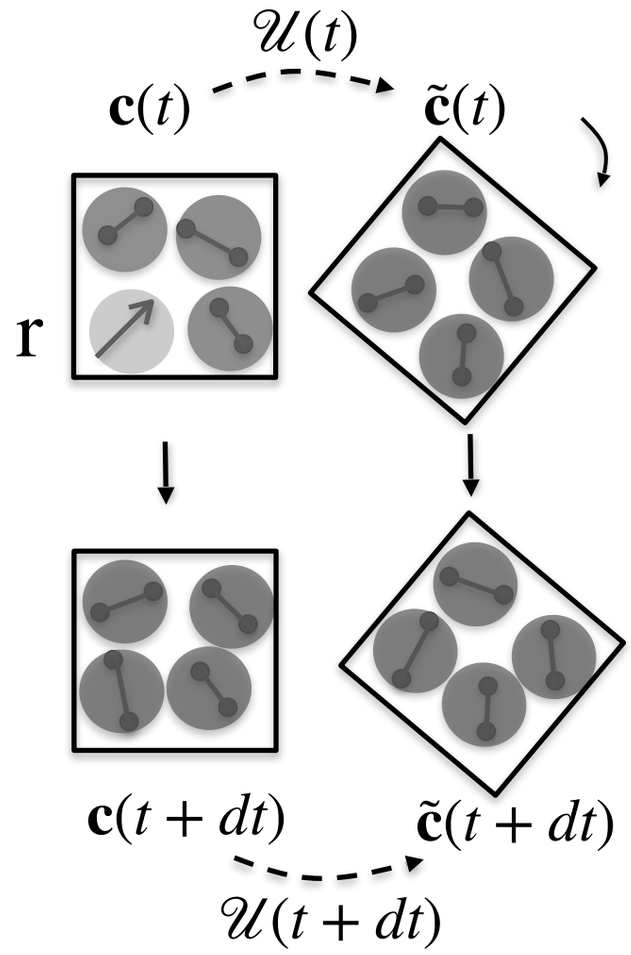
Existing approaches: empirical closures

- Macro-model empirical closures

$\tau_p = \mathbf{G}(\mathbf{c})$ $\quad \mathbf{c}(\boldsymbol{x}, t) = \left\langle \mathbf{r}\mathbf{r}^{\mathsf{T}} \right\rangle$ - orientation tensor

$\dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t} = \mathbf{H}(\mathbf{c})$ $\quad \dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}$ - objective tensor derivative

frame-indifference constraint: $\quad \widetilde{\dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}} = \mathscr{U}\dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}\mathscr{U}^T, \;\; \mathscr{U}\mathscr{U}^T = \mathbf{I}$



- Non-unique choices of the objective tensor derivative $\dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}$
  - Upper convected: $\quad \overset{\triangledown}{\mathbf{c}} = \dfrac{\mathrm{d}\mathbf{c}}{\mathrm{dt}} - \nabla\mathbf{u}^{\mathsf{T}}\mathbf{c} - \mathbf{c}\nabla\mathbf{u}$
  - Lower convected: $\quad \overset{\triangle}{\mathbf{c}} = \dfrac{\mathrm{d}\mathbf{c}}{\mathrm{dt}} + \nabla\mathbf{u}\mathbf{c} + \mathbf{c}\nabla\mathbf{u}^{\mathsf{T}}$
  - Corotational: $\quad \mathring{\mathbf{c}} = \dfrac{1}{2}(\overset{\triangledown}{\mathbf{c}} + \overset{\triangle}{\mathbf{c}})$
  - .....

Bird-Curtiss-Armstrong-Hassager, *Dynamics of Polymeric Liquids,* 1987; Laso-Öttinger, *JNNFM*, 1993; Hulsen-Heel-Brule, *JNNFM,* 1997; Lielens-Keunings-Legat, *JNNFM*, 1999; Ren-E, *J. Comput. Phys*, 2005; Hyon-Du-Liu, *SIAM MMS, 2008; etc.*

Limitations of empirical models

- **Example:** Hookean model with $\mathbf{c} = \left\langle \mathbf{r}\mathbf{r}^{\mathsf{T}} \right\rangle$ and $V(\mathbf{r}) \propto \frac{1}{2}|\mathbf{r}|^2$

$$\tau_{\mathrm{p}} = \left\langle \mathbf{r} \otimes \nabla_{\mathbf{r}} V(\mathbf{r}) \right\rangle \propto \underbrace{\left\langle \mathbf{r}\mathbf{r}^{\mathsf{T}} \right\rangle = \mathbf{c}}_{\mathbf{G}(\mathbf{c})}$$

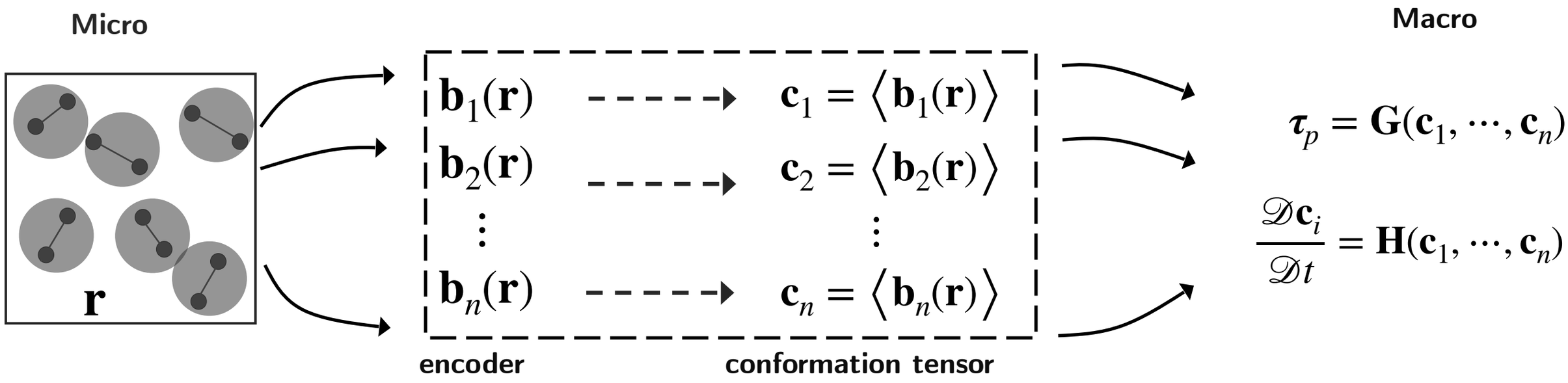
$$\underbrace{\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}t} - \nabla\mathbf{u}^{\mathsf{T}}\mathbf{c} - \mathbf{c}\nabla\mathbf{u}}_{\frac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}} = \underbrace{\frac{1}{\lambda}(\mathbf{I} - \mathbf{c})}_{\mathbf{H}(\mathbf{c})}$$

- **Challenges for real applications**
  - τ_{p} unclosed for nonlinear $V(\mathbf{r})$ and complex molecule structures
  - Multiple $\mathbf{c}$ are needed
  - Each $\mathbf{c}$ needs its own objective tensor derivative $\dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}$

Machine-learning based model beyond empirical closures

Proposition: seek a set of explicit micro-macro encoder functions

$$\langle \mathbf{b}_i(\mathbf{r}) \rangle := \int f(\mathbf{r}, \boldsymbol{x}) \mathbf{b}_i(\mathbf{r}) \mathrm{d}\mathbf{r} \qquad f(\mathbf{r}, \boldsymbol{x}) \text{ - PDF of polymer configuration } \mathbf{r}$$

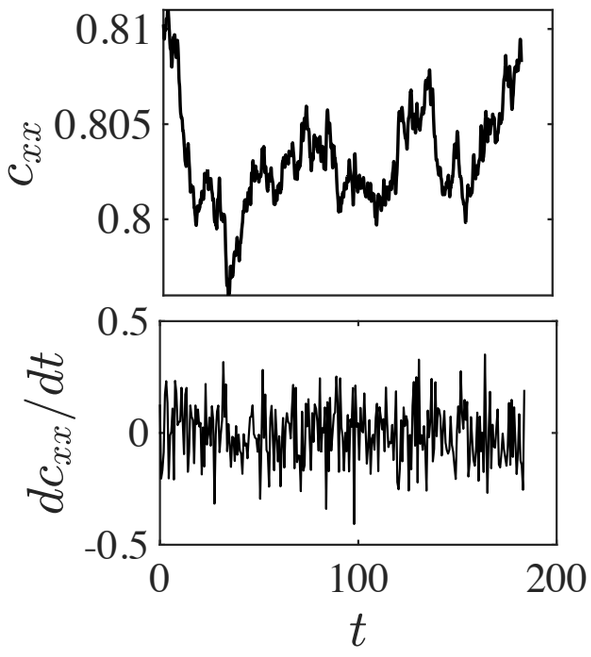


Machine-learning based model beyond empirical closures

Caution & criticism : A set of "black-box" tricks without fundamental principle .....

1. Pass physical laws across scales: discover or re-discover?

   - Time-series $\left\{\mathbf{c}(t_i)\right\}_{i=1}^{N}$ may not be feasible to learn $\frac{\mathscr{D}\mathbf{c}}{\mathscr{D}t} = \mathbf{H}(\mathbf{c})$



2. Retain physical interpretation and symmetry constraints

   - Frame-indifference operators $\frac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}$

upper convected

covariant

corotational

.....

3. Numerical stability and generalization ability

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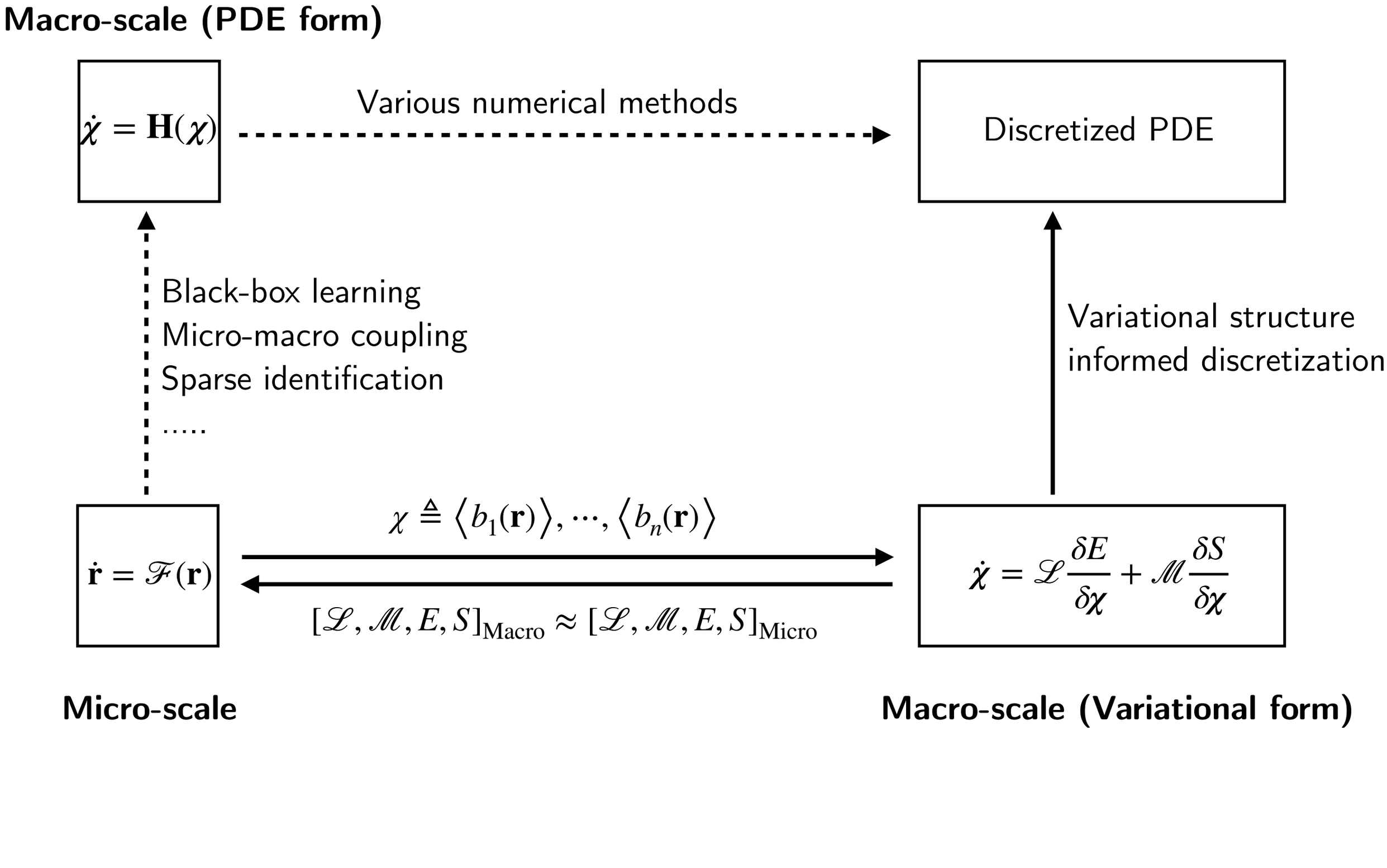
A variational-informed machine-learning modeling framework



Variational structure of the macro-scale hydrodynamic model

- Macro-scale hydrodynamics governed by the coupling of a reversible and an irreversible process

$$\dot{\chi} = \mathscr{L}\frac{\delta E}{\delta \chi} + \mathscr{M}\frac{\delta S}{\delta \chi} \tag{1a}$$

$$\mathscr{L}\frac{\delta S}{\delta \chi} = \mathscr{M}\frac{\delta E}{\delta \chi} \equiv 0 \tag{1b}$$

$\chi : \Omega \to \mathbb{R}^d$ - field variables $\quad E[\chi] = \int_\Omega \hat{E}(\chi)\mathrm{d}\boldsymbol{x}$ - energy $\quad S[\chi] = \int_\Omega \hat{S}(\chi)\mathrm{d}\boldsymbol{x}$ - entropy

$\mathscr{L} = -\mathscr{L}^*$ - poisson matrix $\quad \mathscr{M} + \mathscr{M}^T \succ 0$, $\mathscr{M}$ - friction matrix

- The degeneracy condition (1b) ensures the energy conservation $\dot{E} \equiv 0$, the entropy production $\dot{S} \geq 0$ and therefore the free energy stability

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Onsager, *Physical review*, 1931; Morrison., *Physica D*, 1986; Grmela-Öttinger, *Phys. Rev. E*, 1997; Lin-Liu-Zhang, *Commun. Pure Appl. Math.*, 2005

Variational structure of the Hookean model

- **Example:** the PDE form of the incompressible Hookean non-Newtonian model

$$\nabla \cdot \mathbf{u} = 0 \qquad \rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} = -\nabla p + \nabla \cdot (\tau_{\mathrm{newton}} + \tau_{\mathrm{p}})$$

$$\overset{\nabla}{\mathbf{c}} = \frac{1}{\lambda}(\mathbf{I} - \mathbf{c}) \qquad \tau_{\mathrm{newton}} = \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T), \quad \tau_{\mathrm{p}} = \mathbf{c}$$

is governed by the variational structure

$$\chi = (\mathbf{u}, \mathbf{c}) \qquad E = \frac{1}{2}\int \|\mathbf{u}\|^2 \mathrm{d}\boldsymbol{x} \qquad \mathscr{L} = \begin{pmatrix} \mathscr{L}_{\mathrm{Newton}} & \mathscr{L}^{u^*}_{\mathbf{c}} \\ \mathscr{L}^{u}_{\mathbf{c}} & \end{pmatrix}$$

$$S = \frac{1}{2}\int \left[\mathrm{Tr}(\mathbf{I} - \mathbf{c}) + \ln(\det \mathbf{c})\right] \mathrm{d}\boldsymbol{x} \qquad \mathscr{M} = \begin{pmatrix} \mathscr{M}_{\mathrm{Newton}} & \\ & 1/\lambda \end{pmatrix}$$

$\mathscr{L}_{\mathrm{Newton}}$, $\mathscr{M}_{\mathrm{Newton}}$ - poisson and friction operators of incompressible Newtonian fluid

$\mathscr{L}^{u}_{\mathbf{c}}$ - poisson operator of the upper-convected derivative

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Grmela-Öttinger, *Phys. Rev. E*, 1997; Lin-Liu-Zhang, *Commun. Pure Appl. Math.*, 2005

A generalized extendable variational structure

- **Key observation:** the variational structure can be violated if constructed in the PDE form

  model construction: $\dot{\chi} = H[\chi]$ vs $\{E, S, \mathscr{L}, \mathscr{M}\}$

- **Main idea I**: seek an extendable energy variational form $\dot{\chi} = \mathscr{L}\dfrac{\delta E}{\delta \chi} + \mathscr{M}\dfrac{\delta S}{\delta \chi}$

$$\chi = (\mathbf{u}, \mathbf{c}_1, \cdots, \mathbf{c}_n) \qquad E = \frac{1}{2}\int \|\mathbf{u}\|^2 \mathrm{d}\boldsymbol{x} \qquad S = \frac{1}{2}\int \hat{S}(\mathbf{c}_1, \cdots, \mathbf{c}_n)\mathrm{d}\boldsymbol{x}$$

$$\mathscr{L} = \begin{pmatrix} \mathscr{L}_{\text{Newton}} & \mathscr{L}_c^{u^*}\cdots \\ \mathscr{L}_c^u & \\ \vdots & \end{pmatrix} \qquad \mathscr{M} = \begin{pmatrix} \mathscr{M}_{\text{Newton}} & \\ & \boxed{\begin{matrix} \mathscr{M}_{44} & \cdots \\ \vdots & \ddots \end{matrix}}_{\mathscr{M}^S \in \mathbb{R}^{3n\times 3n}} \end{pmatrix} + \begin{pmatrix} & \\ & \boxed{\begin{matrix} \widetilde{\mathscr{M}}_{42} & \widetilde{\mathscr{M}}_{43} \\ \vdots & \vdots \end{matrix}}_{\mathscr{M}^A \in [\mathbb{R}^{3n\times 3\times 3}\ \mathbb{R}^{3n\times 3}]} \end{pmatrix} \begin{bmatrix} & \\ & \mathscr{M}^A \end{bmatrix}^*$$

$\mathscr{M}^s$ - constitutive dynamics of $\{\mathbf{c}_i\}_{i=1}^n$ $\mathscr{M}^A$ - objective tensor derivative $\left\{\dfrac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}\right\}_{i=1}^n$

- Jointly learn $\{\mathbf{c}_i\}_{i=1}^n$ and the variational structure $\{S, \mathscr{M}\}$ rather than the PDE form

Constitutive dynamics of the generalized variational structure

$$\chi = (\mathbf{u}, \mathbf{c}_1, \cdots, \mathbf{c}_n) \qquad E = \frac{1}{2}\int \|\mathbf{u}\|^2 \mathrm{d}\boldsymbol{x} \qquad S = \frac{1}{2}\int \hat{S}(\mathbf{c}_1, \cdots, \mathbf{c}_n)\mathrm{d}\boldsymbol{x}$$

$$\mathscr{L} = \begin{pmatrix} \mathscr{L}_{\text{Newton}} & \mathscr{L}_c^{u*}\cdots \\ \mathscr{L}_c^u & \\ \vdots & \end{pmatrix} \qquad \mathscr{M} = \begin{pmatrix} \mathscr{M}_{\text{Newton}} & \boxed{\begin{matrix} \mathscr{M}_{44} & \cdots \\ \vdots & \ddots \end{matrix}}_{\mathscr{M}^S \in \mathbb{R}^{3n\times 3n}} \end{pmatrix} + \begin{pmatrix} & \left[\mathscr{M}^A\right]^* \\ \boxed{\begin{matrix} \widetilde{\mathscr{M}}_{42} & \widetilde{\mathscr{M}}_{43} \\ \vdots & \vdots \end{matrix}}_{\mathscr{M}^A \in [\mathbb{R}^{3n\times 3\times 3}\ \mathbb{R}^{3n\times 3}]} & \end{pmatrix}$$

- ***Proposition***: The following structures satisfy the degeneracy condition $\mathscr{M}\dfrac{\delta E}{\delta \chi} \equiv 0$

$$[\widetilde{\mathscr{M}}_{42}]_{jkl}\mathbf{u}_l + [\widetilde{\mathscr{M}}_{43}]_{jk} \equiv 0, \qquad [\widetilde{\mathscr{M}}_{42}]_{jkl} = (\frac{\partial}{\partial \boldsymbol{x}} \cdot \widehat{\mathscr{E}}_i)_{jkl} \qquad \widehat{\mathscr{E}}_i : \mathbb{R}^{3\times 3\times n} \to \mathbb{R}^{3\times 3\times 3\times 3}$$

- ***Corollary***: The constitutive dynamics takes the PDE form

$$\underbrace{\dot{\mathbf{c}}_i - \nabla \mathbf{u}^\top : \mathscr{E}_i}_{\dfrac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}} = \underbrace{[\mathscr{M}^S]_{ij}\frac{\partial \hat{S}}{\partial c_j}}_{\mathbf{H}_i(\,\cdot\,)} \qquad \boldsymbol{\tau}_p = \underbrace{\mathscr{E}_j : \frac{\partial \hat{S}}{\partial \mathbf{c}_j}}_{\mathbf{G}(\,\cdot\,)} \qquad \mathscr{E}_i = \mathscr{L}_c^u + \widehat{\mathscr{E}}_i$$

- ***Q***: how to learn $\hat{S}, \mathscr{M}^s,\ \left\{\mathbf{c}_i, \mathscr{E}_i\right\}_{i=1}^n$ preserving the **physical constraints** and **micro-model fidelity**?

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Neural network representation with physical constraints

- Recall the macro-model

$$\frac{\mathrm{d}\mathbf{c}_i}{\mathrm{dt}} - \nabla \mathbf{u}^\top : \mathscr{E}_i = [\mathscr{M}^S]_{ij} \frac{\partial \hat{S}}{\partial \mathbf{c}_j}, \quad i = 1, \cdots, n$$

- **Q**: What constraints should $\hat{S}, \mathscr{E}, \mathscr{M}^s$ follow?

  - Frame-indifference

  - $\mathscr{M}^s$ - positive definite

  - $\hat{S}$ - concave with specific maximum point

  - If $\mathbf{c}(0) \succ 0$, $\mathbf{c}(t) \succ 0 \ \forall t > 0$

DeePN^2: Entropy

- Entropy $\hat{S}$ is concave and frame-indifferent

$$\nabla^2 \hat{S} \preccurlyeq 0$$

$$\hat{S}(\widetilde{\mathbf{c}}_1, \cdots, \widetilde{\mathbf{c}}_n) = \hat{S}(\mathbf{c}_1, \cdots, \mathbf{c}_n) \qquad \widetilde{\mathbf{c}_i} = \mathcal{U}\mathbf{c}_i\mathcal{U}^T$$

- Frame-indifference inputs: $\mathbf{x}_c = \{\mathrm{Tr}(\mathbf{c}_i), -\log(\det(\mathbf{c}_i)), \mathrm{Tr}(\mathbf{c}_i^2)\} \in \mathbb{R}^{3n\times 1}$

- Convex neural network representation

$$\mathbf{z}_0 = g_0(W_0^x \mathbf{x}_c + \mathbf{b}_0)$$
$$\mathbf{z}_{l+1} = g_{l+1}(W_{l+1}^z \mathbf{z}_{l+1} + W_{l+1}^x \mathbf{x}_c + \mathbf{b}_{l+1})$$
$$\widetilde{S}(\mathbf{x}) = W_L^z \mathbf{z}_L + W_L^x \mathbf{x}_c + \mathbf{b}_L \qquad l = 0, \cdots, L-1$$

$W_l^z \geq 0, \quad W_l^x \geq 0, \quad g_l$ - convex and non-decreasing activation functions

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Amos-Xu-Kolter, *International Conference on Machine Learning*, 2017

DeePN^2: Entropy

- The equilibrium state without external force is given by

$$\mathbf{c}_{\text{eq}} = \arg\max \hat{S}(\mathbf{c})$$

$$\frac{\mathrm{d}\hat{\mathrm{S}}(\mathbf{c})}{\mathrm{d}\mathbf{c}}\Big|_{\mathbf{c}_{\text{eq}}} = 0$$

- $\mathbf{c}_{\text{eq}}$ corresponds to the micro-scale Boltzmann distribution $f_{\text{eq}}(\mathbf{r}) \propto \exp\left[-V(\mathbf{r})/k_B T\right]$

- Concave and frame-indifference entropy

$$\hat{S}(\mathbf{c}) = -\left(\tilde{S}(\mathbf{x}_c) - \frac{\mathrm{d}\tilde{\mathrm{S}}(\mathbf{c})}{\mathrm{d}\mathbf{c}}\Big|_{\mathbf{c}_{\text{eq}}} : \mathbf{c}\right)$$

DeePN^2: Friction matrix

- Friction matrix $\mathscr{M}^s$ needs to be SPD, frame-indifference and commutable with $\left\{\mathbf{c}_i\right\}_{i=1}^n$

$$\mathscr{M}^s \succ 0 \qquad \mathscr{M}^s \frac{\partial \hat{S}}{\partial \mathbf{c}_i} = \frac{\partial \hat{S}}{\partial \mathbf{c}_i} \mathscr{M}^s \qquad (\text{i.e., } \mathbf{H}_i = \mathbf{H}_i^\top)$$

$$\mathscr{M}^s(\widetilde{\mathbf{c}}_1, \cdots, \widetilde{\mathbf{c}}_n) = \mathscr{M}^s(\mathbf{c}_1, \cdots, \mathbf{c}_n) \qquad \widetilde{\mathbf{c}_i} = \mathcal{U}\mathbf{c}_i\mathcal{U}^\top$$

- **Proposition**: Represent $\mathscr{M}^s$ by the polynomial bases $\left\{\mathbf{c}_i\right\}_{i=1}^n$

- **Key observation**: Let $\mathbf{A} \in \mathbb{R}^{3\times 3}$, the Cayley–Hamilton theorem yields

$$\mathbf{A}^{p+1} = \mathrm{Tr}(\mathbf{A})\mathbf{A}^p - \frac{1}{2}\left(\mathrm{Tr}(\mathbf{A}) - \mathrm{Tr}(\mathbf{A}^2)\right)\mathbf{A}^{p-1} + \det(\mathbf{A})\mathbf{A}^{p-2}$$

Therefore, higher-order polynomials can be represented by

$$\mathbf{c}^p = \xi_1(x_c)\mathbf{I} + \xi_2(x_c)\mathbf{c} + \xi_3(x_c)\mathbf{c}^2 \qquad x_c = (\mathrm{Tr}(\mathbf{c}), \mathrm{Tr}(\mathbf{c}^2), \det(\mathbf{c})) \quad p > 2$$

DeePN^2: Friction matrix

- Representation by polynomial basis functions

$$\mathbf{W}(\mathbf{c}) = \left\{ \mathbf{I}, \mathbf{c}_i, \mathbf{c}_i^2, \mathbf{I} + (\mathbf{c}_i - \mathbf{c}_j)^2, \left(\mathbf{I} + (\mathbf{c}_i - \mathbf{c}_j)^2 \right)^2 \right\} \in \mathbb{R}^{m \times 3 \times 3} \qquad 1 \le i < j \le n$$

- Neural network representation of $\mathscr{M}^s = \mathrm{diag}\left(\mathscr{M}^s_1, \mathscr{M}^s_2, \cdots, \mathscr{M}^s_n\right)$

$$\mathscr{M}^s_i = \mathbf{W}(\mathbf{c})^\top \cdot \left(\Gamma_i(\mathbf{x}_c) \Gamma_i(\mathbf{x}_c)^\top \right) \cdot \mathbf{W}(\mathbf{c}) \in \mathbb{R}^{3\times3\times3\times3}$$

$\Gamma_i : \mathbb{R}^{3n} \to \mathbb{R}^{m \times m}$ $\qquad$ $\mathbf{x}_c \in \mathbb{R}^{3n}$ - invariants of $\left\{\mathbf{c}_i\right\}_{i=1}^n$

$$\mathscr{M}^s_i \frac{\partial \hat{S}}{\partial \mathbf{c}_i} \triangleq \left[\mathscr{M}^s_i\right] : \left[\frac{\partial \hat{S}}{\partial \mathbf{c}_i}\right] \in \mathbb{R}^{3\times3} \qquad 1 \le i \le n$$

satisfies the SPD, frame-indifference constraints and is commutable with $\left\{\mathbf{c}_i\right\}_{i=1}^n$

DeePN²: Objective tensor derivative

- Representation by polynomial basis functions

$$\mathbf{W}(\mathbf{c}) = \left\{ \mathbf{I}, \mathbf{c}_i, \mathbf{c}_i^2, \mathbf{I} + (\mathbf{c}_i - \mathbf{c}_j)^2, \left(\mathbf{I} + (\mathbf{c}_i - \mathbf{c}_j)^2 \right)^2 \right\} \in \mathbb{R}^{m \times 3 \times 3} \qquad 1 \le i < j \le n$$

- Neural network representation of the source term $\widehat{\mathscr{E}}_i = \sum_{s=1}^{N_s} \mathbf{E}_{1,i}^{(s)}(\mathbf{c}) \otimes \mathbf{E}_{2,i}^{(s)}(\mathbf{c})$

$$\widehat{\mathscr{E}}_i = \mathbf{W}(\mathbf{c})^\top \cdot \left(\Lambda_i(\mathbf{x}_c) \right) \cdot \mathbf{W}(\mathbf{c}) \in \mathbb{R}^{3 \times 3 \times 3 \times 3}$$

$\Lambda_i : \mathbb{R}^{3n} \to \mathbb{R}^{m \times m}$ $\qquad$ $\mathbf{x}_c \in \mathbb{R}^{3n}$ - invariants of $\left\{ \mathbf{c}_i \right\}_{i=1}^n$

satisfies the frame-indifference constraints for the objective tensor derivative

$$\frac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t} = \overset{\triangledown}{\mathbf{c}}_i - \nabla \mathbf{u}^\top : \widehat{\mathscr{E}}_i \qquad \widetilde{\frac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}} = \mathscr{U} \frac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t} \mathscr{U}^\top$$

Positivity-preserving dynamics

- **Assumption**: Let $\hat{S} = \hat{S}_e(\mathrm{Tr}(\mathbf{c}), \mathrm{Tr}(\mathbf{c}^2)) + \frac{1}{2}\sum_{i=1}^{n} \log\det \mathbf{c}_i$ and $\mathscr{E}_i, \mathscr{M}_i, \nabla \hat{S}_e$ bounded

- **Proposition**: Given $\mathbf{c}_i(0) \succ 0$, then $\mathbf{c}_i(t) \succ 0 \quad \forall t > 0$

- **Sketch of Proof**: Consider the dynamics of $\det \mathbf{c}$

$$\frac{\mathrm{d}(\det \mathbf{c}_\mathrm{i})}{\mathrm{dt}} = \mathbf{P}(\mathbf{c}_i) : \left(\nabla \mathbf{u}^\top : \mathscr{E}_i + \mathscr{M}_i : \frac{\partial \hat{S}_e}{\partial \mathbf{c}_i} \right) + \frac{1}{\det \mathbf{c}_i} \left(\mathbf{P}(\mathbf{c}_i) : \mathscr{M}_i : \mathbf{P}(\mathbf{c}_i) \right)$$

$$\mathbf{P}(\mathbf{c}) = \det(\mathbf{c})\mathbf{c}^{-1} = \mathbf{c}^2 - \mathrm{Tr}(\mathbf{c})\mathbf{c} + \frac{1}{2}\left(\mathrm{Tr}(\mathbf{c})^2 - \mathrm{Tr}(\mathbf{c}^2)\right)\mathbf{I}$$

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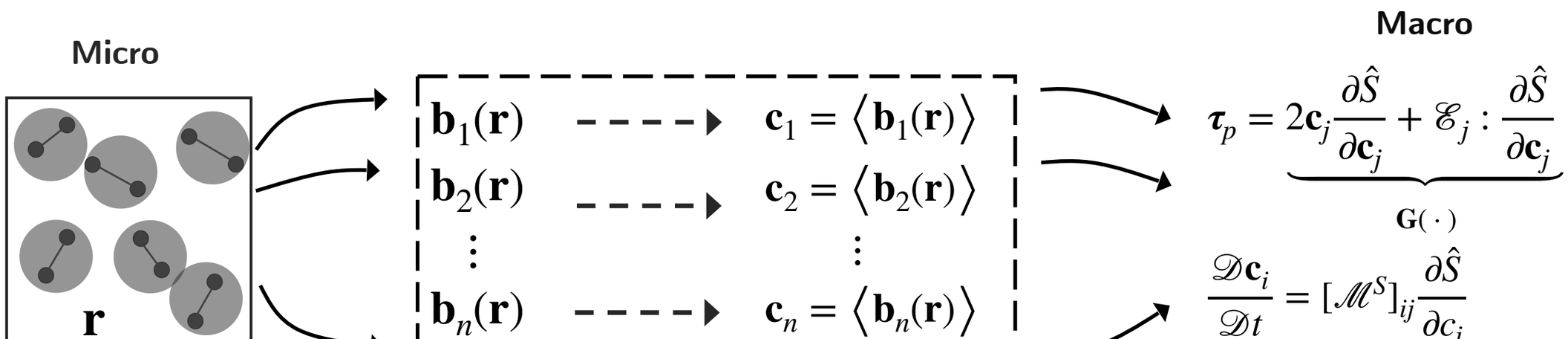
Micro-macro correspondence

Main idea II: seek a set of explicit micro-macro correspondences

$$\langle \mathbf{b}_i(\mathbf{r}) \rangle := \int f(\mathbf{r}) \mathbf{b}_i(\mathbf{r}) \mathrm{d}\mathbf{r} \qquad f(\mathbf{r}) \text{ - PDF of polymer configuration } \mathbf{r}$$



- **Key observation:** polymer configuration PDF $f(\mathbf{r})$ is sufficient but not necessary....
  - $\mathbf{c}_i$ and $\mathbf{b}_i(\mathbf{r})$ are restricted to second-order tensors and are NOT used to approximate $f(\mathbf{r})$
  - $\left\{\mathbf{b}_i(\mathbf{r})\right\}_{i=1}^n$ are jointly learned for the best approximation of $\mathbf{G}(\cdot)$ and $\mathbf{H}(\cdot)$
  - Proper symmetry-preserving form of $\left\{\mathbf{b}_i(\cdot)\right\}_{i=1}^n$ is needed

---

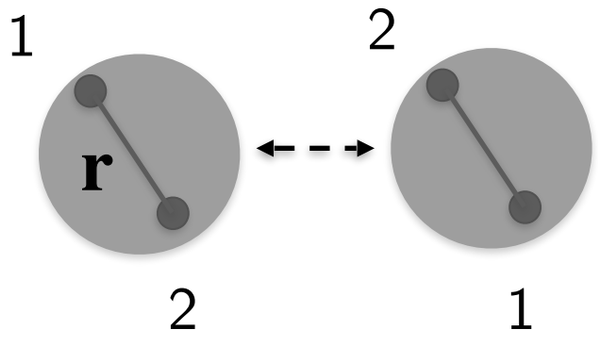
Grad, *Commun. Pure Appl. Math.*, 1949; Yu-Du-Liu, *SIAM MMS,* 2008; Han-Ma-Ma-E, *Proc. Natl. Acad. Sci*, 2019

Symmetry-preserving micro-macro encoder: dumbbell

- Proper choice of $\left\{\mathbf{b}_i(\mathbf{r})\right\}_{i=1}^{n}$ to retain rotational symmetry

  - If $\mathbf{b}_i(\mathbf{r}) \in \mathbb{R}^3$, $\mathbf{b}_i(\mathbf{r})$ needs to satisfy

$$\mathbf{b}_i(\mathcal{U}\mathbf{r}) = \mathcal{U}\mathbf{b}_i(\mathbf{r}), \quad \mathcal{U}\mathcal{U}^{\top} = \mathbf{I}$$



  $\mathbf{b}_i(\mathbf{r})$ must take the form

$$\mathbf{b}_i(\mathbf{r}) = g_i(r)\mathbf{r} \quad g_i : \mathbb{R} \to \mathbb{R} \quad \text{yielding } \left\langle \mathbf{b}_i(\mathbf{r}) \right\rangle \equiv 0$$

  - If $\mathbf{b}_i(\mathbf{r}) \in \mathbb{R}^{3\times3}$, $\mathbf{b}_i(\mathbf{r})$ needs to satisfy

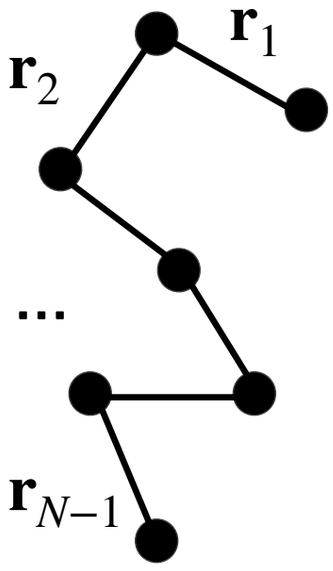
$$\mathbf{b}_i(\mathcal{U}\mathbf{r}) = \mathcal{U}\mathbf{b}_i(\mathbf{r})\mathcal{U}^{\top}$$

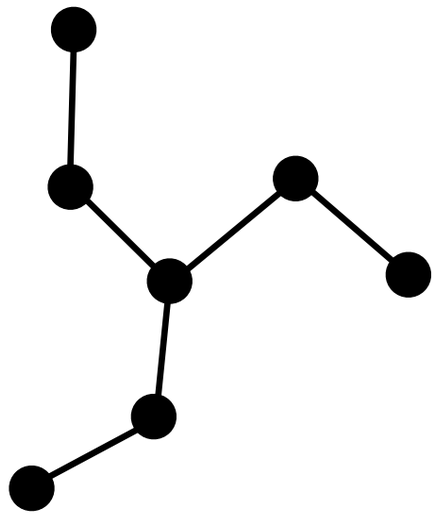
  A simple non-trivial choice is

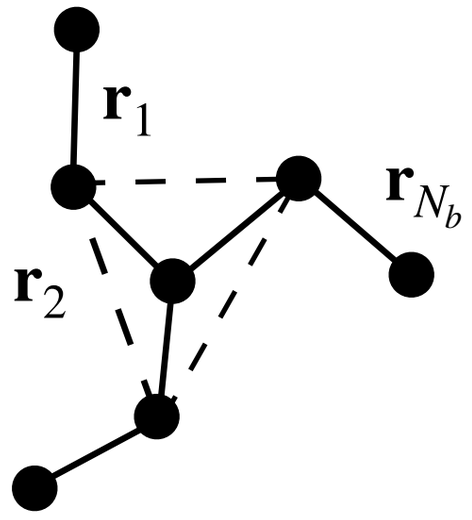
$$\boxed{\mathbf{b}_i = \mathbf{f}_i(\mathbf{r})\mathbf{f}_i(\mathbf{r})^{\top} \quad \mathbf{f}_i(\mathcal{U}\mathbf{r}) = \mathcal{U}\mathbf{f}_i(\mathbf{r}) \quad \text{i.e.,}\ \mathbf{f}_i(\mathbf{r}) = g_i(r)\mathbf{r}}$$

- $g_i(r)$ encodes non-linear features and will be learned jointly from micro-models

Symmetry-preserving micro-macro encoder: arbitrary structure







N - **bead number** N_b - **bond number**

- Rotational-symmetric configuration:

$$\mathbf{r} = \left[\mathbf{r}_1; \mathbf{r}_2; \cdots; \mathbf{r}_{N-1}\right], \quad \widetilde{\mathbf{r}_j} = \mathscr{U}\mathbf{r}_j \qquad 1 \le j \le N-1$$

- Rotational-invariant configuration:

$$\mathbf{r}^* = \left[|\mathbf{r}_1|, |\mathbf{r}_2|, |\mathbf{r}_{12}|, |\mathbf{r}_3|, |\mathbf{r}_{13}|, |\mathbf{r}_{23}|, \cdots, |\mathbf{r}_{N-1}|, |\mathbf{r}_{(N-2)(N-1)}|\right], \quad \widetilde{\mathbf{r}^*} = \mathbf{r}^*$$

- Symmetry-preserving micro-macro encoder:

$$\mathbf{c}_i = \langle \mathbf{b}_i(\mathbf{r}) \rangle, \ \mathbf{b}_i = \mathbf{f}_i \mathbf{f}_i^{\top}, \ \mathbf{f}_i = g_i(\mathbf{r}^*) \sum_{j=1}^{N-1} w_{ij} \mathbf{r}_k \quad 1 \le i \le n$$

Structure-preserving constitutive dynamics of the encoders

- With the micro-macro encoder $\left\{\mathbf{b}_i\right\}_{i=1}^{n}$, challenges remain on learning physics-interpretable forms of $\left\{\mathbf{H}_i, \dfrac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}\right\}_{i=1}^{n}$ ***without*** using time-series samples

$$\underbrace{\dot{\mathbf{c}}_i - \nabla\mathbf{u}^{\top} : \mathscr{E}_i}_{\dfrac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}} = \underbrace{[\mathscr{M}^S]_{ij}\frac{\partial\hat{S}}{\partial c_j}}_{\mathbf{H}_i(\,\cdot\,)}$$

- Non-uniqueness of $\dfrac{\mathscr{D}\mathbf{c}}{\mathscr{D}t}$

$$\widetilde{\frac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}} = \mathscr{U}\frac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}\mathscr{U}^{\top} \qquad\qquad \mathbf{c}_i = \left\langle \mathbf{b}_i(\mathbf{r}) \right\rangle \quad i = 1,\cdots,n$$

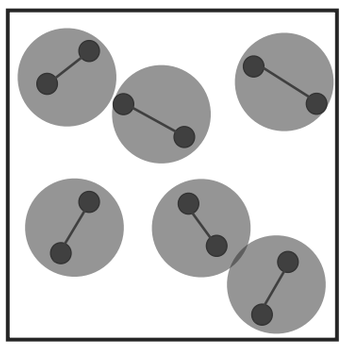
- Frame-indifference constraint

$$\mathbf{H}_i(\widetilde{\mathbf{c}}_1,\cdots,\widetilde{\mathbf{c}}_n) = \mathscr{U}\mathbf{H}_i(\mathbf{c}_1,\cdots,\mathbf{c}_n)\mathscr{U}^{\top} \qquad \widetilde{\mathbf{c}_i} = \mathscr{U}\mathbf{c}_i\mathscr{U}^{\top}$$

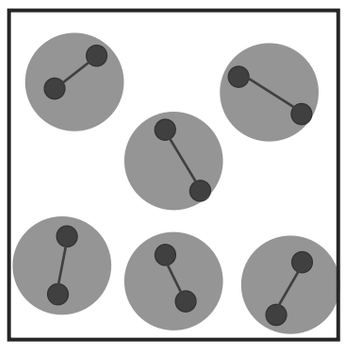
Dynamics of the encoders: formulations from microscale model

Q: Given a snapshot as $\mathbf{r}(t_0) = \mathbf{r}_0$, can we determine $\mathbf{b}(\mathbf{r}_t)$ and $\mathbf{c}_t = \left\langle \mathbf{b}(\mathbf{r}_t) \right\rangle, t \geq t_0$?

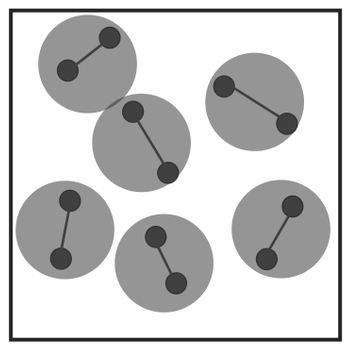
A: **No** if we directly learn the dynamics as a "black-box" on the macro-scale



$\mathbf{r}(t)$



$\mathbf{r}(t + \Delta t)$



$\mathbf{r}(t + 2\Delta t)$ ...

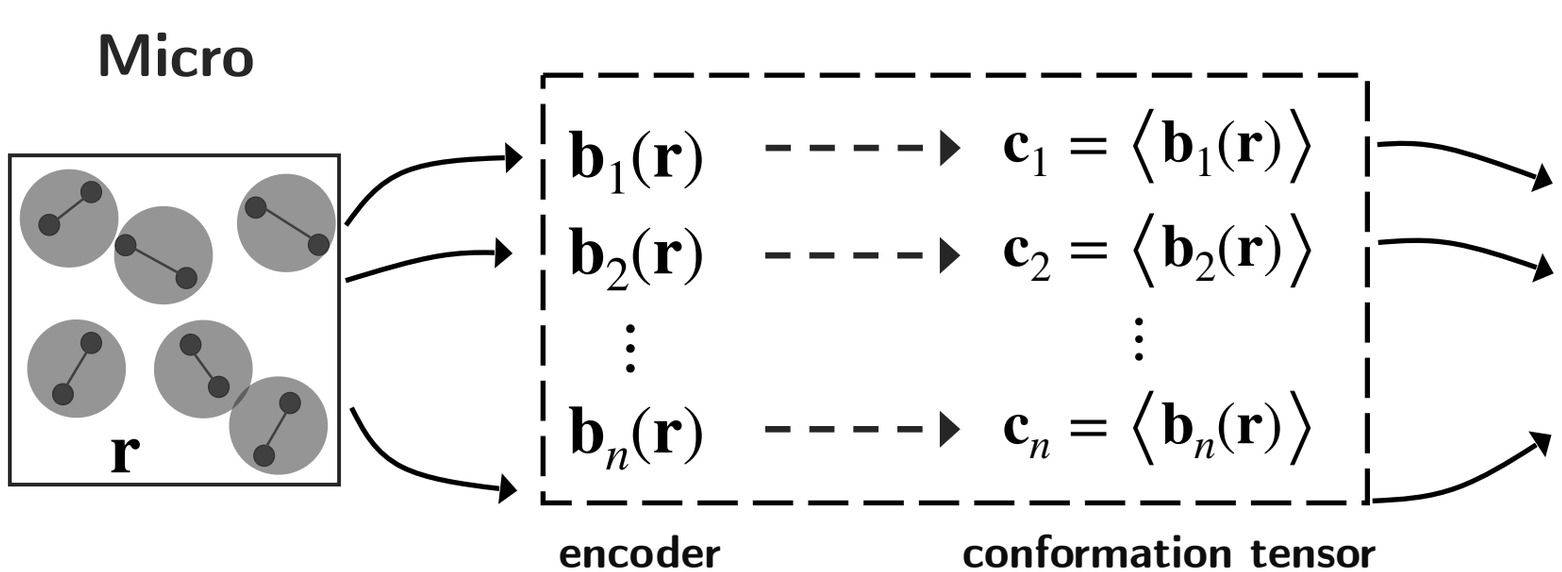
Yes if we use/pass the explicit form of the physical laws on the micro-scale

$$-\nabla V(\mathbf{r}) - \gamma \dot{\mathbf{r}} + \sqrt{2k_B T \gamma}\dot{W}_t = 0 \qquad \text{(over-damping Langevin dynamics)}$$

V - micro-scale intramolecular potential

γ - friction coefficient

Dynamics of the encoders: formulations from microscale model



Key observation: the explicit micro-macro correspondence $\mathbf{c}_i = \int \mathbf{b}_i(\mathbf{r}) f(\mathbf{r}) \mathrm{d}\mathbf{r}$ enables us to derive their evolution from the Fokker-Planck equation (micro-model) of $f(\mathbf{r}, t)$

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathbf{c}_i - \nabla \mathbf{u}^\top : \left\langle \sum_{j=1}^{N-1} \mathbf{r}_j \nabla_{\mathbf{r}_j} \otimes \mathbf{b}_i \right\rangle = \frac{k_B T}{\gamma} \left\langle \sum_{j,k=1}^{N-1} A_{jk} \nabla_{\mathbf{r}_j} \cdot \nabla_{\mathbf{r}_k} \mathbf{b}_i \right\rangle - \frac{1}{\gamma} \left\langle \sum_{j=1}^{N-1} \sum_{k=1}^{N_b} A_{jk} \nabla_{\mathbf{r}_k} V(\mathbf{r}_1, \cdots, \mathbf{r}_{N_b}) \cdot \nabla_{\mathbf{r}_j} \mathbf{b}_i \right\rangle \quad (2)$$

$\mathbf{A}$ - Rouse matrix encodes molecule structures

V - potential function encodes micro-interactions

Proposition: Eq. (2) strictly preserves the rotational frame-indifference constraint

Dynamics of the encoders: formulations from microscale model

Sketch of Proof:

Frame 1 (inertial) $\xrightarrow{\tilde{\boldsymbol{x}} = \mathscr{U}(t)\boldsymbol{x}}$ Frame 2

$\tilde{\boldsymbol{x}}$ $\qquad\qquad$ $\boldsymbol{x}$

$\tilde{\mathbf{u}}(\tilde{\boldsymbol{x}}, t)$ $\qquad\qquad$ $\mathbf{u}(\boldsymbol{x}, t)$

$$\underbrace{\frac{\mathrm{d}}{\mathrm{dt}}\langle \mathbf{b}_i \rangle - \nabla \mathbf{u}^{\top} : \left\langle \sum_{j=1}^{N-1} \mathbf{r}_j \nabla_{\mathbf{r}_j} \otimes \mathbf{b}_i \right\rangle}_{\dfrac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t}} = \frac{k_B T}{\gamma} \left\langle \sum_{j,k=1}^{N-1} A_{jk} \nabla_{\mathbf{r}_j} \cdot \nabla_{\mathbf{r}_k} \mathbf{b}_i \right\rangle - \frac{1}{\gamma} \left\langle \sum_{j=1}^{N-1} \sum_{k=1}^{N_b} A_{jk} \nabla_{\mathbf{r}_k} V(\mathbf{r}_1, \cdots, \mathbf{r}_{N_b}) \cdot \nabla_{\mathbf{r}_j} \mathbf{b}_i \right\rangle$$

- LHS terms follows

$$\frac{\mathrm{d}}{\mathrm{dt}} \left\langle \widetilde{\mathbf{b}} \right\rangle \Big|_{\text{frame 1}} = \dot{\mathscr{U}} \langle \mathbf{b} \rangle \mathscr{U}^{\top} + \mathscr{U} \langle \mathbf{b} \rangle \dot{\mathscr{U}}^{\top} + \mathscr{U} \frac{\mathrm{d}}{\mathrm{dt}} \langle \mathbf{b} \rangle \Big|_{\text{frame 2}} \dot{\mathscr{U}}^{\top}$$

$$\begin{aligned} \widetilde{\nabla \mathbf{u}^{\top}} : \left\langle \widetilde{\mathbf{r}} \nabla_{\tilde{\mathbf{r}}} \otimes \widetilde{\mathbf{b}} \right\rangle \Big|_{\text{frame1}} &= \left[\left(\mathscr{U} \nabla \mathbf{u}^{\top} \mathscr{U}^{\top} + \dot{\mathscr{U}} \mathscr{U}^{\top} \right) \cdot \mathscr{U} \mathbf{r} \right] \cdot \mathscr{U} \nabla_{\mathbf{r}} \left(\mathscr{U} \mathbf{b} \mathscr{U}^{\top} \right) \\ &= \mathscr{U} (\nabla \mathbf{u}^{\top} \cdot \mathbf{r}) \cdot \nabla_{\mathbf{r}} \mathbf{b} \mathscr{U}^{\top} \Big|_{\text{frame2}} + \left(\dot{\mathscr{U}} \mathbf{b} + \mathbf{b} \dot{\mathscr{U}}^{\top} \right) \Big|_{\text{frame2}} \end{aligned}$$

$$\frac{\mathrm{d}}{\mathrm{dt}} \left\langle \widetilde{\mathbf{b}} \right\rangle \Big|_{\text{frame 1}} - \widetilde{\nabla \mathbf{u}^{\top}} : \left\langle \widetilde{\mathbf{r}} \nabla_{\tilde{\mathbf{r}}} \otimes \widetilde{\mathbf{b}} \right\rangle \Big|_{\text{frame 1}} \equiv \mathscr{U} \left[\frac{\mathrm{d}}{\mathrm{dt}} \langle \mathbf{b} \rangle \Big|_{\text{frame 2}} - \nabla \mathbf{u}^{\top} : \left\langle \mathbf{r} \nabla_{\mathbf{r}} \otimes \mathbf{b} \right\rangle \Big|_{\text{frame 2}} \right] \mathscr{U}^{\top} \quad \square$$

DeePN²

- **DeePN²**: A variational-informed machine-learning model of non-Newtonian fluids

$$\chi = (\mathbf{u}, \mathbf{c}_1, \cdots, \mathbf{c}_n)$$

$$\dot{\chi} = \mathscr{L}\frac{\delta E}{\delta \chi} + \mathscr{M}\frac{\delta S}{\delta \chi}$$

$$\mathscr{L}\frac{\delta S}{\delta \chi} = \mathscr{M}\frac{\delta E}{\delta \chi} \equiv 0$$

$$\mathbf{H}_i = [\mathscr{M}^S]_{ij}\frac{\partial \hat{S}}{\partial \mathbf{c}_j}$$

$$\boldsymbol{\tau}_p = \mathscr{E}_j : \frac{\partial \hat{S}}{\partial \mathbf{c}_j}$$

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

$$\rho\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} = -\nabla p + \nabla \cdot (\tau_s + \tau_\mathrm{p})$$

$$\frac{\mathscr{D}\mathbf{c}_i}{\mathscr{D}t} := \frac{\mathrm{d}\mathbf{c}_\mathrm{i}}{\mathrm{dt}} - \nabla \mathbf{u}^\top : \mathscr{E}_i = \mathbf{H}_i(\mathbf{c}_1, \cdots, \mathbf{c}_n)$$

- $\left\{\mathscr{M}_i^S, \mathscr{E}_i\right\}_{i=1}^n$ and $\hat{S}$ represented by neural networks preserving the rotational symmetries

$$\mathbf{H}_i \text{ - } [\mathscr{M}^S]_{ij}\frac{\partial \hat{S}}{\partial c_j} = \frac{k_B T}{\gamma}\left\langle \sum_{j,k=1}^{N-1} A_{jk}\nabla_{\mathbf{r}_j} \cdot \nabla_{\mathbf{r}_k}\mathbf{b}_i \right\rangle - \frac{1}{\gamma}\left\langle \sum_{j=1}^{N-1}\sum_{k=1}^{N_b} A_{jk}\nabla_{\mathbf{r}_k} V_b \cdot \nabla_{\mathbf{r}_j}\mathbf{b}_i \right\rangle$$

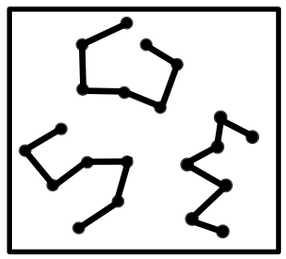
$$\boldsymbol{\tau}_p \text{ - } \mathscr{E}_j : \frac{\partial \hat{S}}{\partial \mathbf{c}_j} = \left\langle \sum_{k=1}^{N_b} \mathbf{r}_k \otimes \nabla_{\mathbf{r}_k} V(r) \right\rangle \qquad \frac{\mathscr{D}\mathbf{c}}{\mathscr{D}t} \text{ - } \mathscr{E}_i(\mathbf{c}_1, \cdots, \mathbf{c}_n) = \left\langle \sum_{j=1}^{N-1} \mathbf{r}_j \otimes \nabla_{\mathbf{r}_j} \otimes \mathbf{b}_i \right\rangle$$

$\langle \cdot \rangle$ - discrete samples collected from micro-scale molecular dynamics simulations

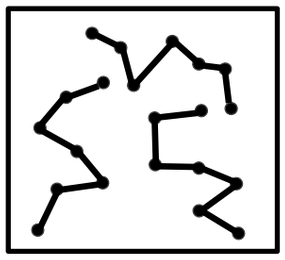
- **No time-series sample is needed**

DeePN^2: training sample collection

- Discrete samples (snapshots) collected from shear flow of different shear rates

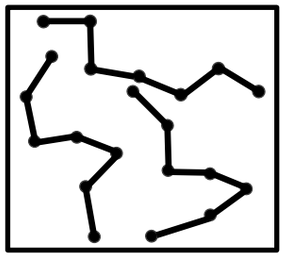


$\mathbf{r}^{(1)}$



$\mathbf{r}^{(2)}$

...



$\mathbf{r}^{(m)}$

- The phase space sampling is independent of the initial conditions, enabling efficient parallel sampling, enhanced sampling, etc.

- DeePN^2 model is validated with ***different*** flow types using the ***same*** training set

DeePN^2: Energy variational structure informed learning

- Joint learning of both micro-macro encoders $\left\{\mathbf{b}_i(\cdot)\right\}_{i=1}^n$ and structures $\mathscr{V} = \left\{E, S, \mathscr{L}, \mathscr{M}\right\}$

$$L = \sum_{j=1}^{N_s} \left(\left\| \tau_p(\cdot)^{(j)} - \widetilde{\tau_p}^{(j)} \right\|^2 + \left\| \mathscr{E}(\cdot)^{(j)} - \widetilde{\mathscr{E}}^{(j)} \right\|^2 + \sum_{i=1}^{n} \left\| \mathbf{H}_i(\cdot)^{(j)} - \widetilde{\mathbf{H}}_i^{(j)} \right\|^2 \right)$$

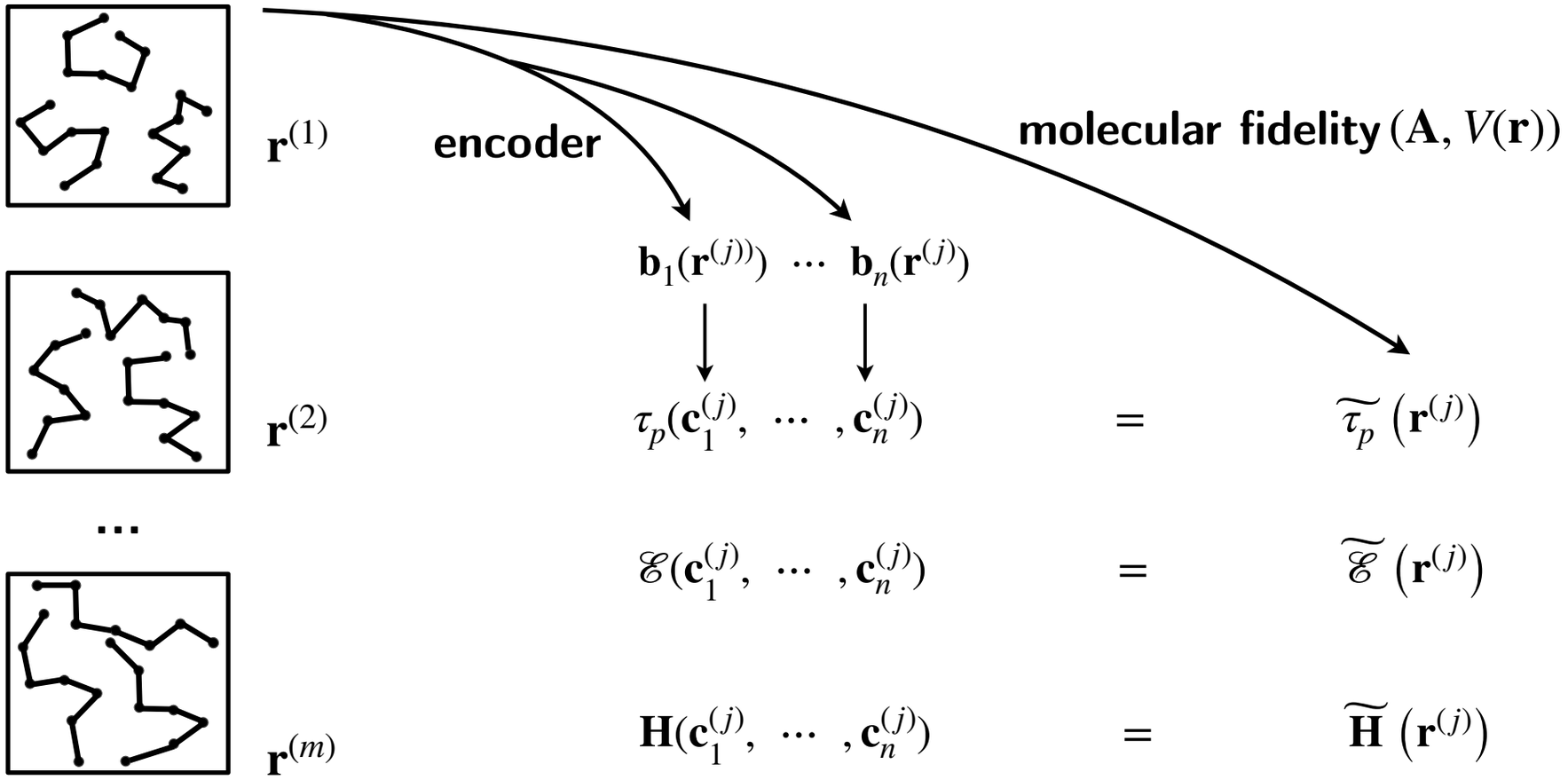
$\square(\cdot)$ - macro-model terms constructed by the variational form $\mathscr{V}$

$\widetilde{\square}$ - micro-scale correspondences determined by the first-principle descriptions

- Adaptive choice of the number of encoder $\left\{\mathbf{b}_i(\mathbf{r})\right\}_{i=1}^n$

- Macro-terms $\tau_p(\mathbf{c}_1, \cdots, \mathbf{c}_n)$, $\left\{\mathscr{E}_i(\mathbf{c}_1, \cdots, \mathbf{c}_n), \mathbf{H}_i(\mathbf{c}_1, \cdots, \mathbf{c}_n)\right\}_{i=1}^n$ represented by the variational form $\mathscr{V}$

DeePN²: End-to-end training



Micro-scale full model $(\mathbf{A}, V(\mathbf{r}))$

macro-scale DeePN² $(\mathbf{b}, E, S, \mathscr{L}, \mathscr{M})$

Main features

- Training only requires time-discrete samples (challenge 1)
- Analytical forms of the micro-scale physical laws can be passed across scales (challenge 2)
- Variational structure enables the energy stable numerical scheme (challenge 3)

DeePN^2: energy-stable numerical scheme

- ***Scalar auxiliary variable*** approach: introduce an auxiliary variable $r = \sqrt{S + C}$ and re-write the extended dynamics of (χ, z) with modified **quadratic** free energy $F = E - z^2$

$$\begin{pmatrix} \dot{\chi} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & 0 \\ \phi_z^* & 1 \end{pmatrix} \begin{pmatrix} \mathscr{L} + \mathscr{M} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{I} & \phi_z \\ 0 & 1 \end{pmatrix} \nabla F \qquad \phi_z = \frac{1}{2\sqrt{S + C}} \frac{\delta S}{\delta \chi}$$

$$\Longleftrightarrow$$

$$\dot{\chi} = \mathscr{L} \frac{\delta E}{\delta \chi} + \mathscr{M} \left(\frac{-r}{\sqrt{S + C}} \frac{\delta S}{\delta \chi} \right) \qquad \dot{z} = \frac{1}{2\sqrt{S + C}} \left\langle \frac{\delta S}{\delta \chi}, \dot{\chi} \right\rangle \tag{3}$$

- It is possible to design linearly-implicit schemes for Eq. (3) such that $F^{(n+1)} < F^{(n)}$

- ***Remark***: Other energy stable schemes (e.g., invariant energy quadratization, discrete variational derivative method) can be naturally inherited.

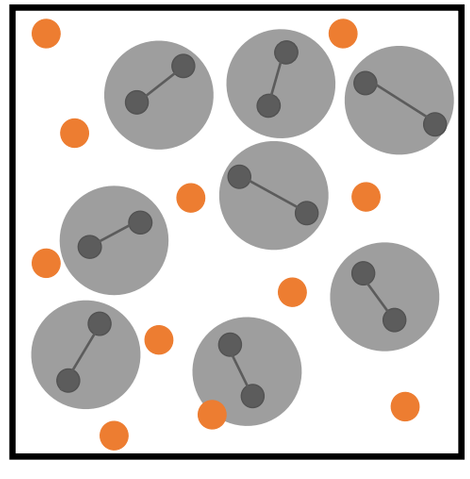
Furihata, *Numerische Mathematik*, 2001; Yang, *J. Compt. Phys*, 2016; Shen-Xu-Yang, *J. Compt. Phys*, 2018

Numerical examples: dumbbell solution

- Micro-scale polymer solution model
  - Elastic bond (FENE) bond potential

$$V(r) = -\frac{k_s}{2} r_0^2 \log\left[1 - \frac{r}{r_0^2}\right]$$

k_s - spring constant r_0 - maximum bond extension

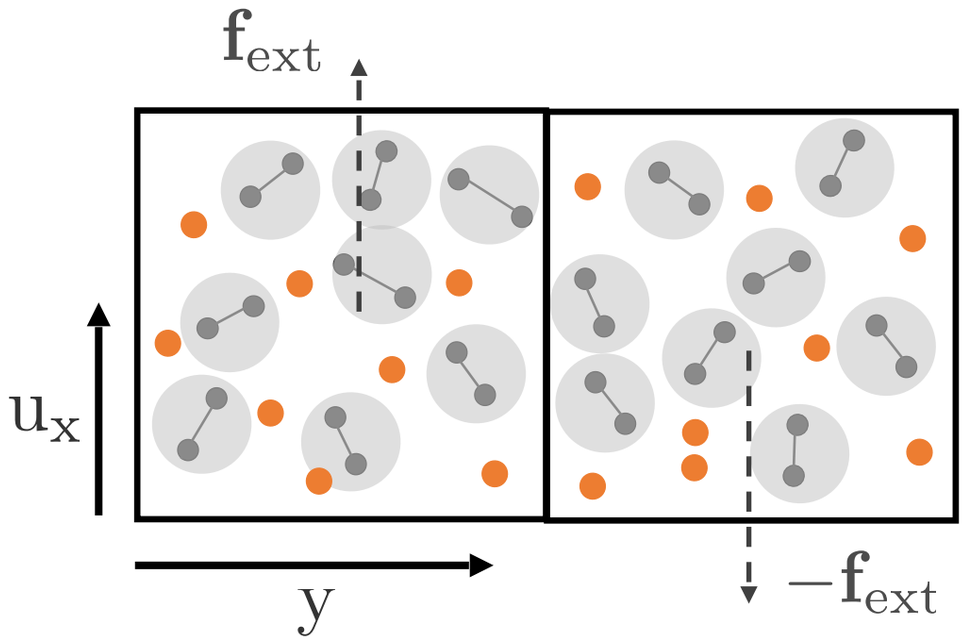


  - Pairwise interactions imposed between solvent-solvent, solvent-polymer

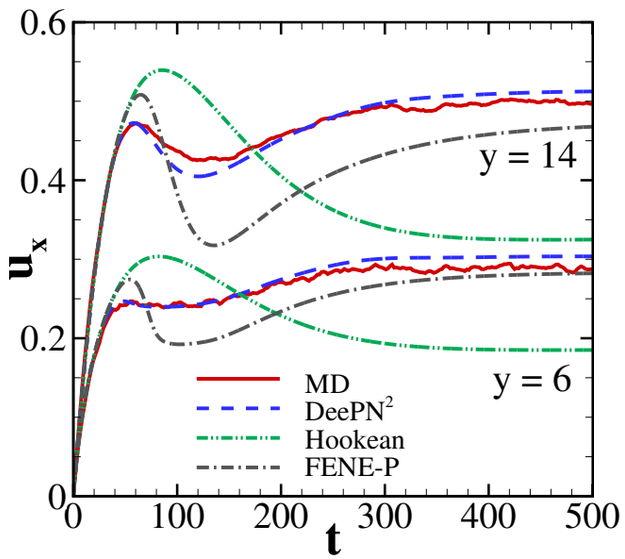
- Two popular empirical continuum non-Newtonian fluid models
  - Hookean model: $\tau_p \propto \mathbf{c}$, $\overset{\triangledown}{\mathbf{c}} \propto \mathbf{I} - \lambda\mathbf{c}$ (linear)
  - FENE-P model: $\tau_p \propto \frac{\mathbf{c}}{1 - \mathrm{Tr}(\mathbf{c})/r_0^2}$, $\overset{\triangledown}{\mathbf{c}} \propto \mathbf{I} - \lambda\frac{\mathbf{c}}{1 - \mathrm{Tr}(\mathbf{c})/r_0^2}$ (mean-field)

Dumbbell solution: reverse-Poiseuille flow

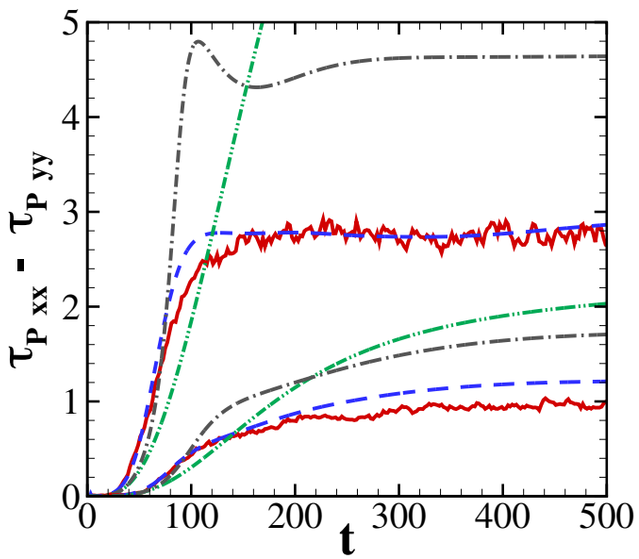
- Development of the reverse Poiseuille flow



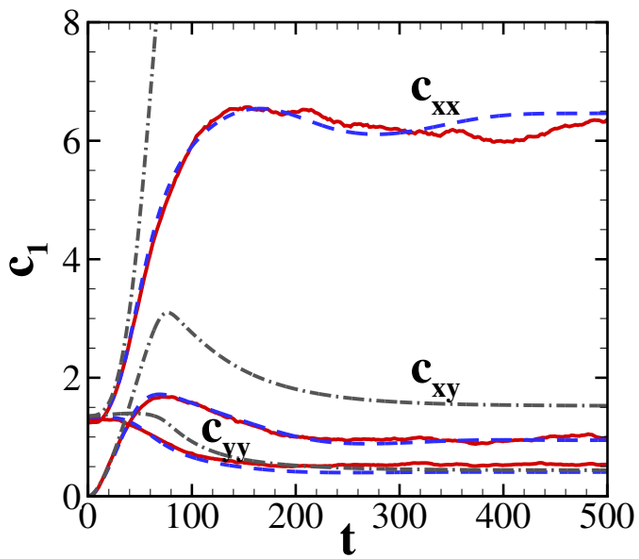
- Micro-macro correspondence



velocity evolution



stress evolution



conformation tensor evolution

Dumbbell solution: generalized objective tensor derivative

- ***Generalized*** objective tensor derivative with micro-scale interpretations

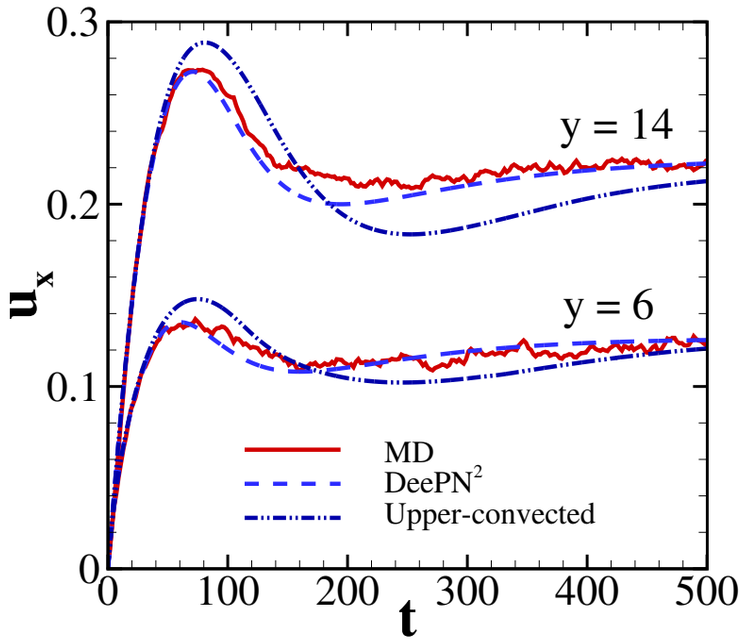
$$\frac{\mathscr{D}\mathbf{c}}{\mathscr{D}t} = \frac{\mathrm{d}\mathbf{c}}{\mathrm{dt}} - \nabla\mathbf{u}^{\top} : \mathscr{E}$$

$$= \frac{\mathrm{d}\mathbf{c}}{\mathrm{dt}} - \nabla\mathbf{u}^{\top}\mathbf{c} - \mathbf{c}\nabla\mathbf{u} - \nabla\mathbf{u}^{\top} : \sum_{k=1}^{9} \mathbf{E}_1^{(k)} \otimes \mathbf{E}_2^{(k)}$$

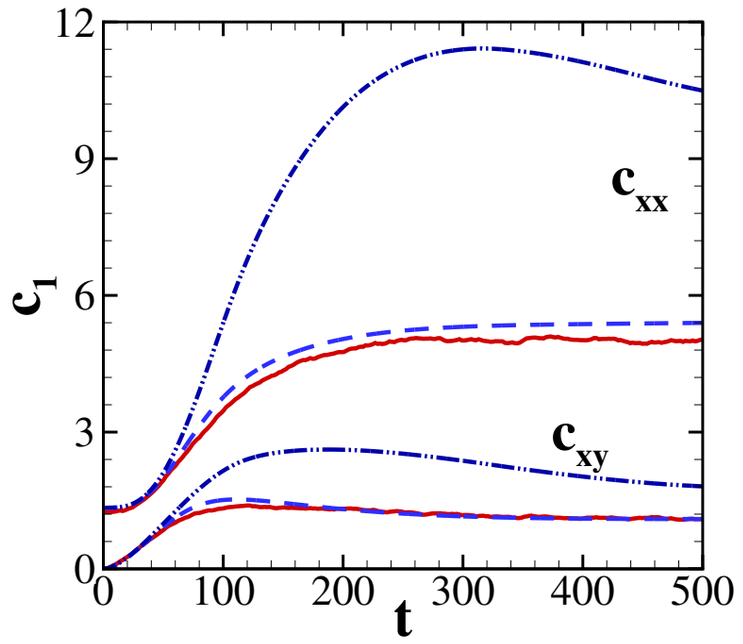
$$= \overset{\nabla}{\mathbf{c}} - \underbrace{\nabla\mathbf{u}^{\top} : \sum_{k=1}^{9} \mathbf{E}_1^{(k)} \otimes \mathbf{E}_2^{(k)}}$$

additional source term

- Limitations of the empirical form



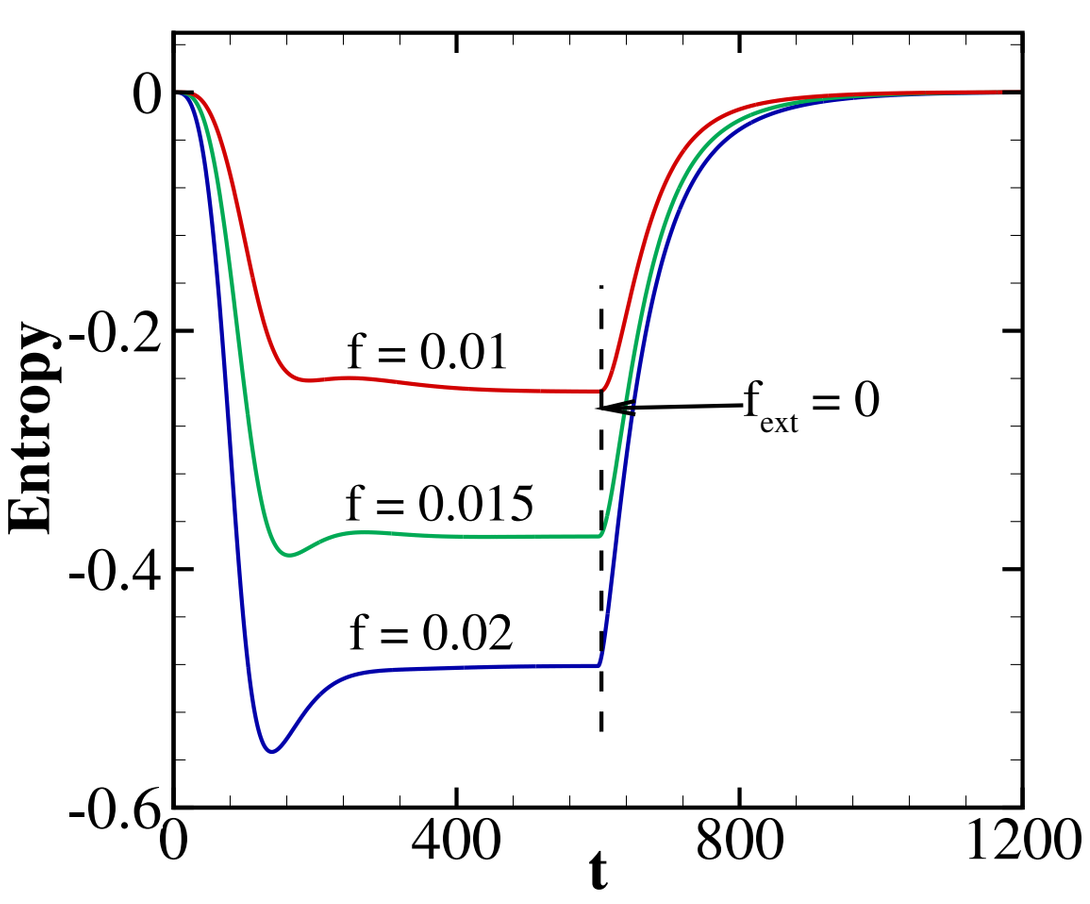
velocity evolution



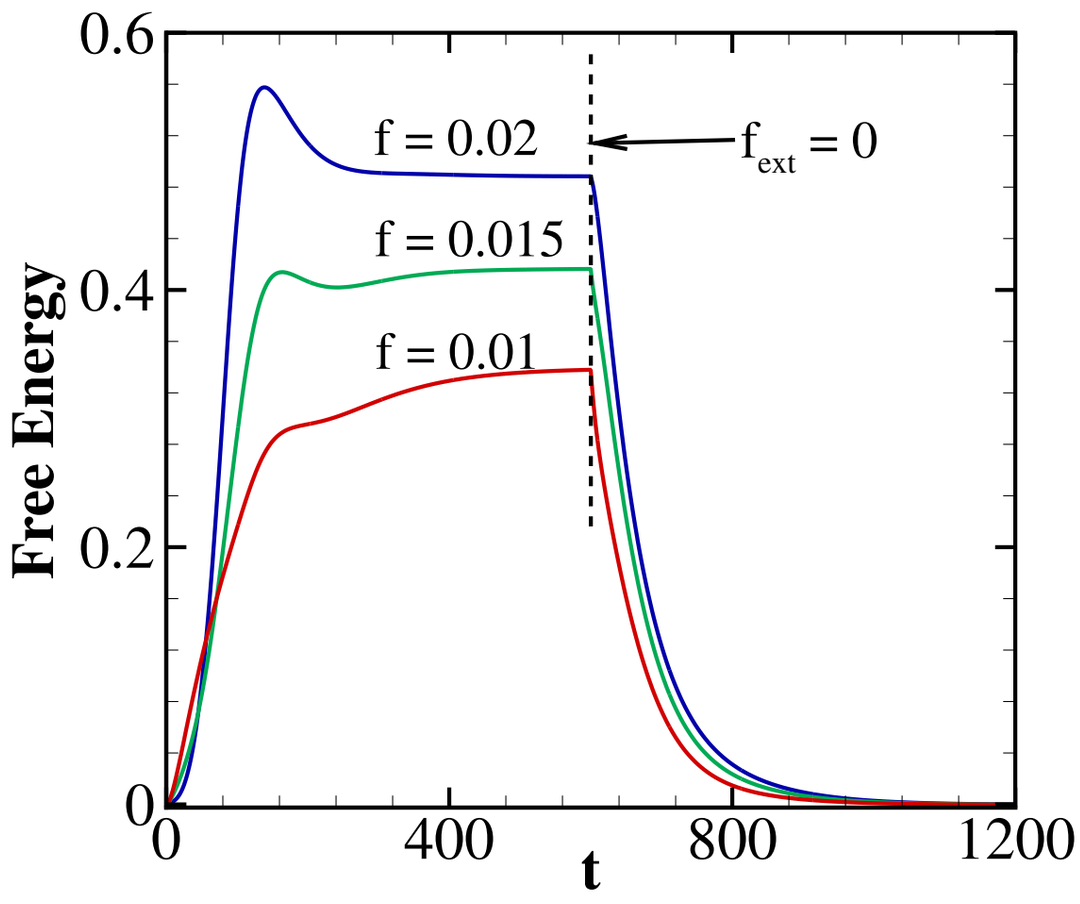
conformation tensor evolution

Dumbbell solution: energy-stable numerical discretization

- The explicit energy variational structure enables the inheritance of the pre-existing energy-stable numerical discretization schemes.



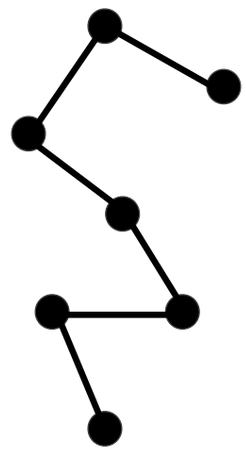
Development of entropy $S = r^2$



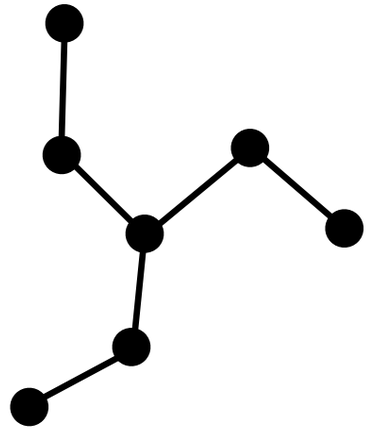
Development of free energy $F = E - r^2$

Suspensions of multi-bead molecules

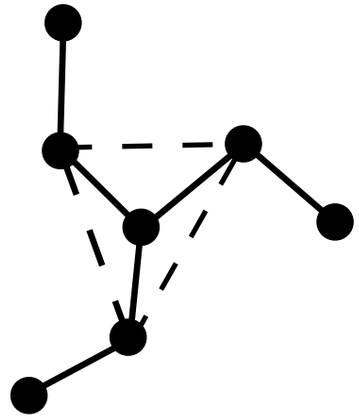
- ***Heterogeneous*** molecular structural mechanics can be naturally encoded into DeePN^2



chain

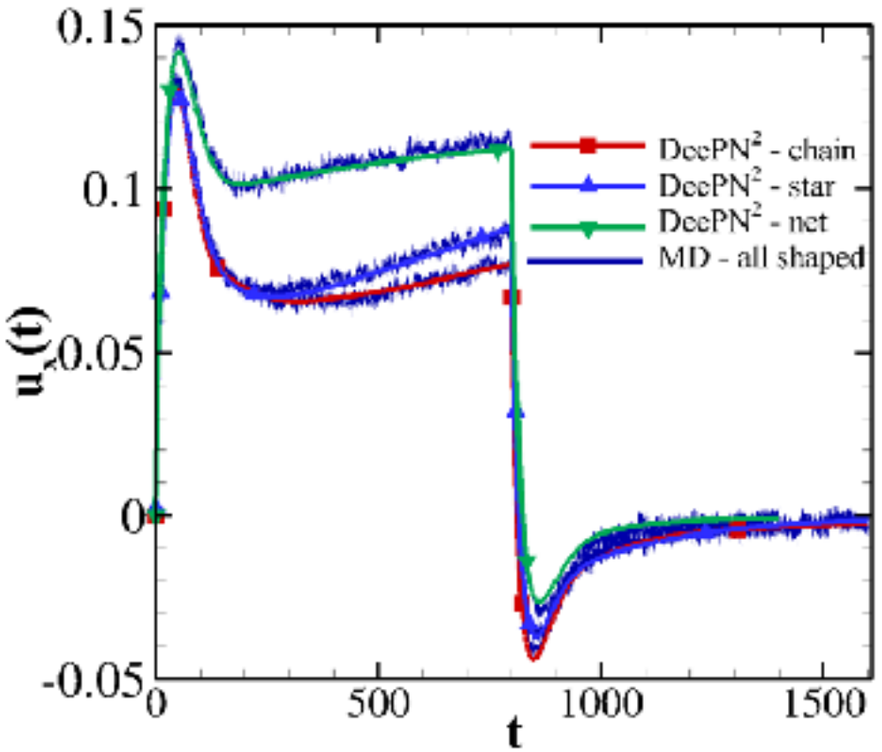


star

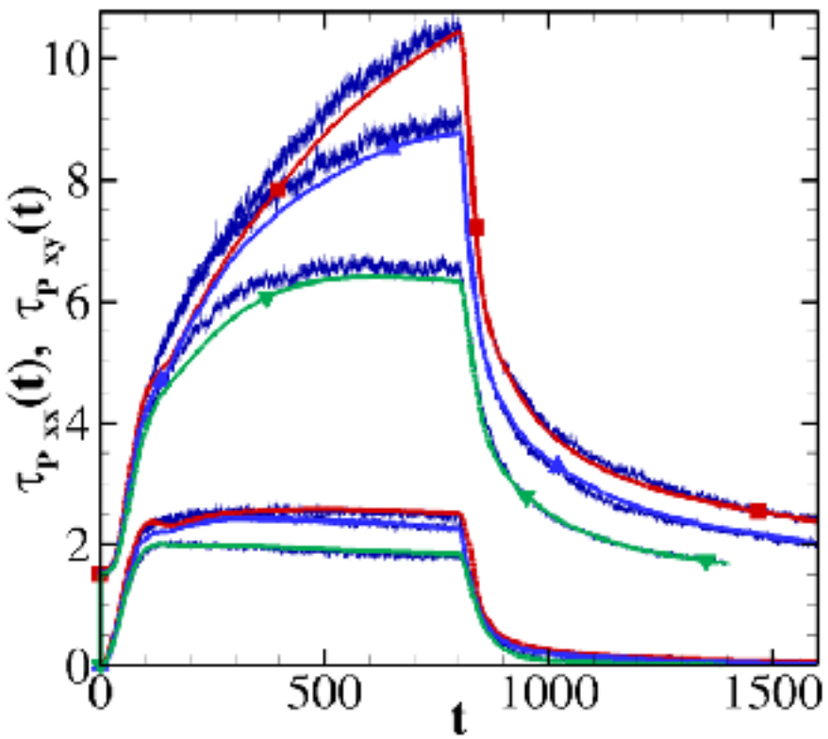


net

- Molecules with the same bead number and bond interaction exhibits different viscoelastic response



velocity evolution

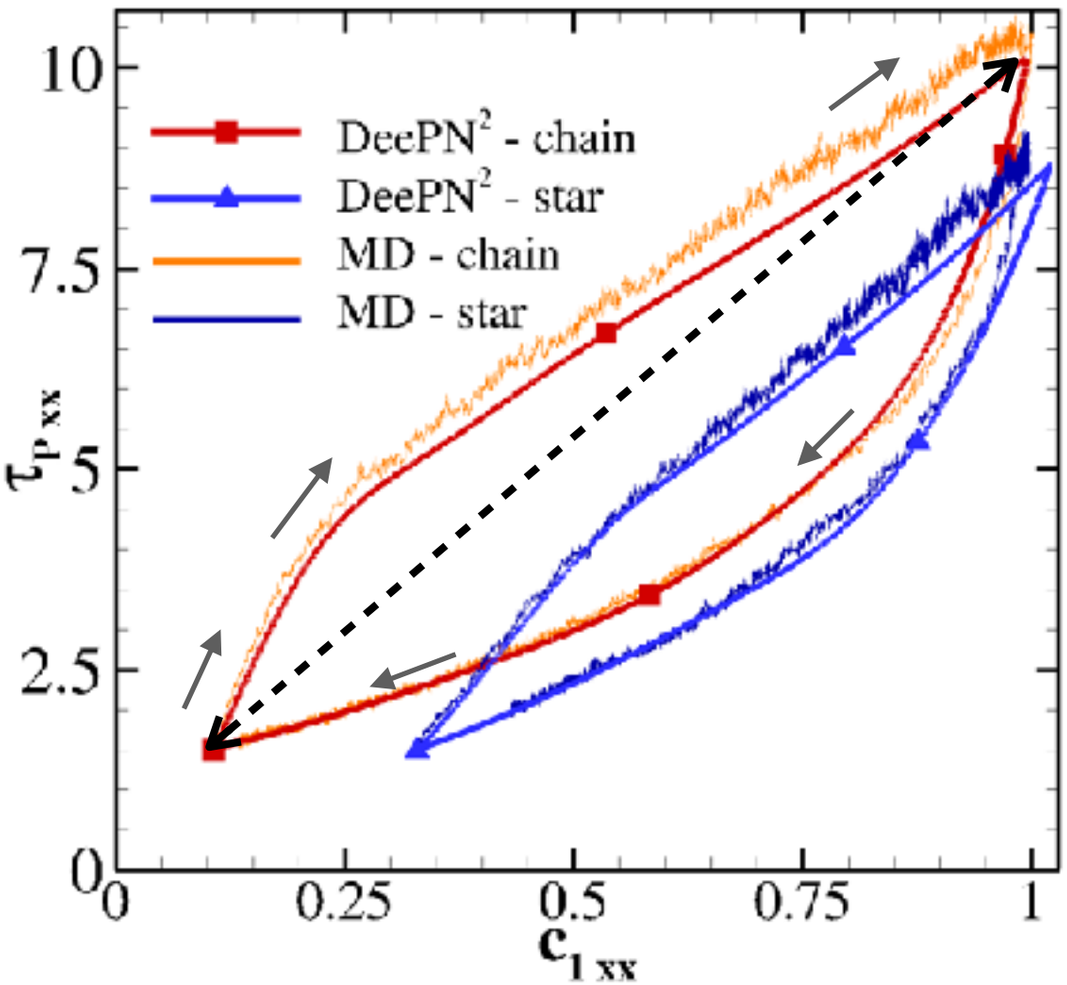


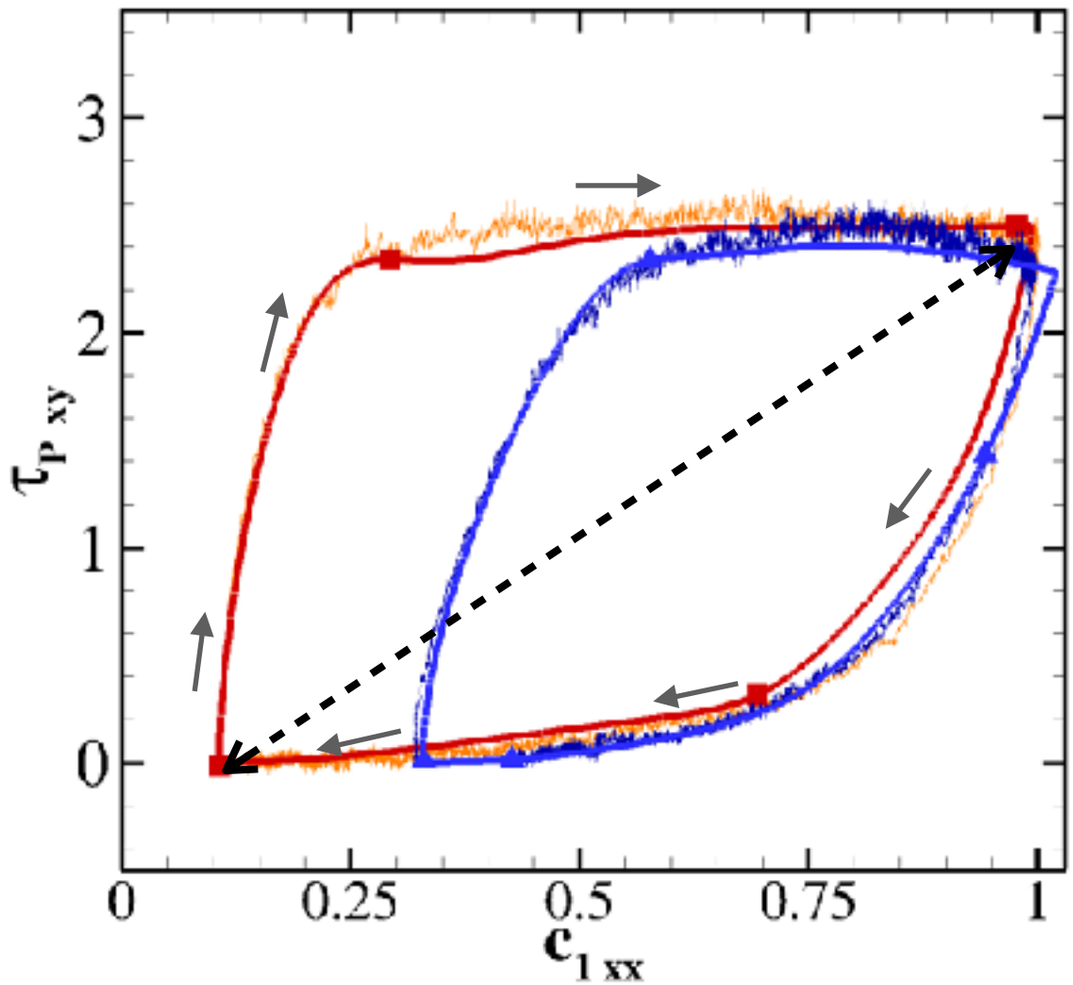
stress evolution

Development of the reverse Poiseuille flow (force removed at t = 800)

Heterogeneous structural induced viscoelastic responses

- ***Hysteresis loop***



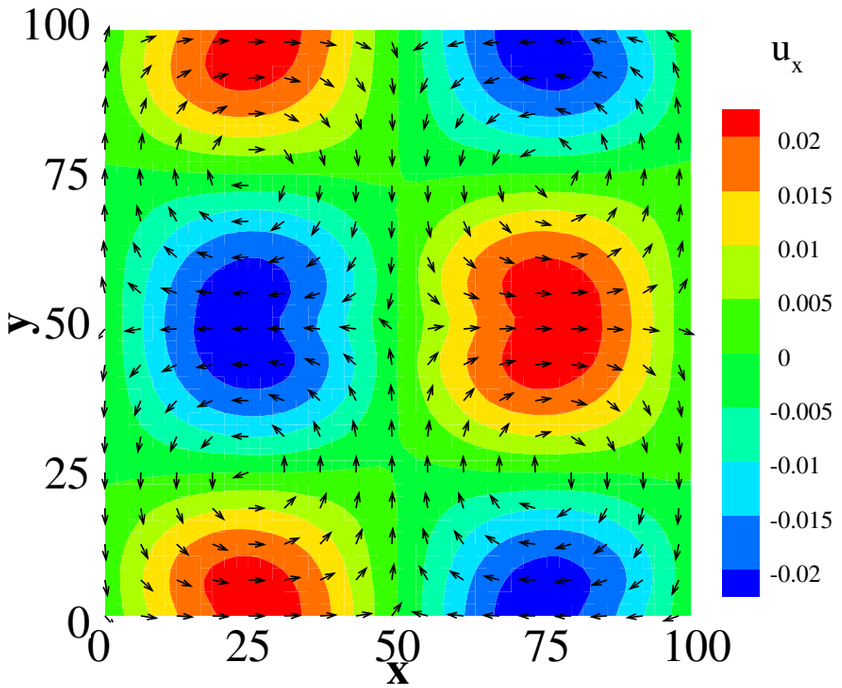


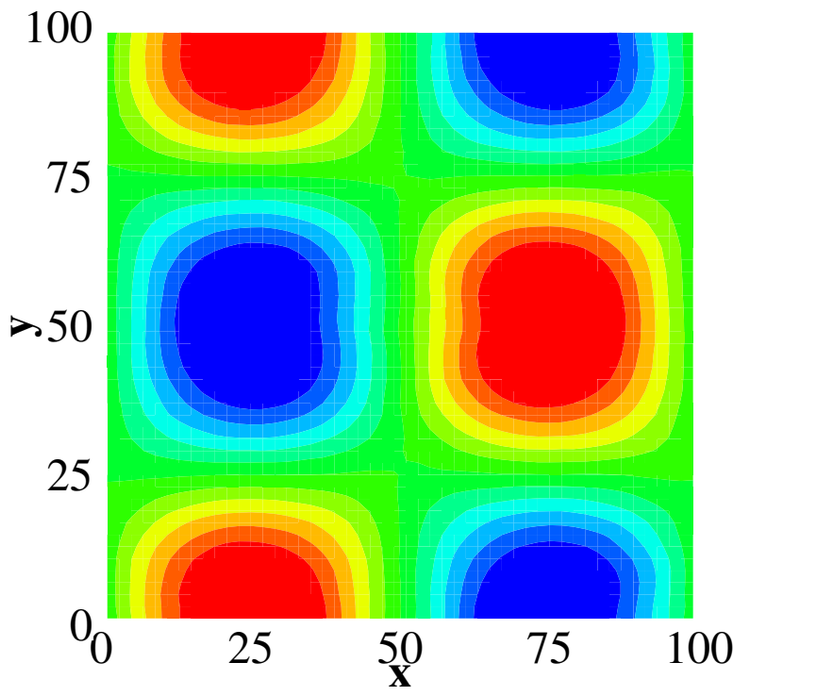
- ***Micro-model interpretation:***
  - The chain-shaped molecule is less symmetric than the star-shaped molecule and therefore exhibits larger dispersion in the phase space
  - DeePN² automatically encodes the heterogeneous structural mechanics
  - Hookean (←- - - - →) and FENE-P based on linear and mean-field approximation are not able to predict the hysteresis loop

2D Green-Taylor flow

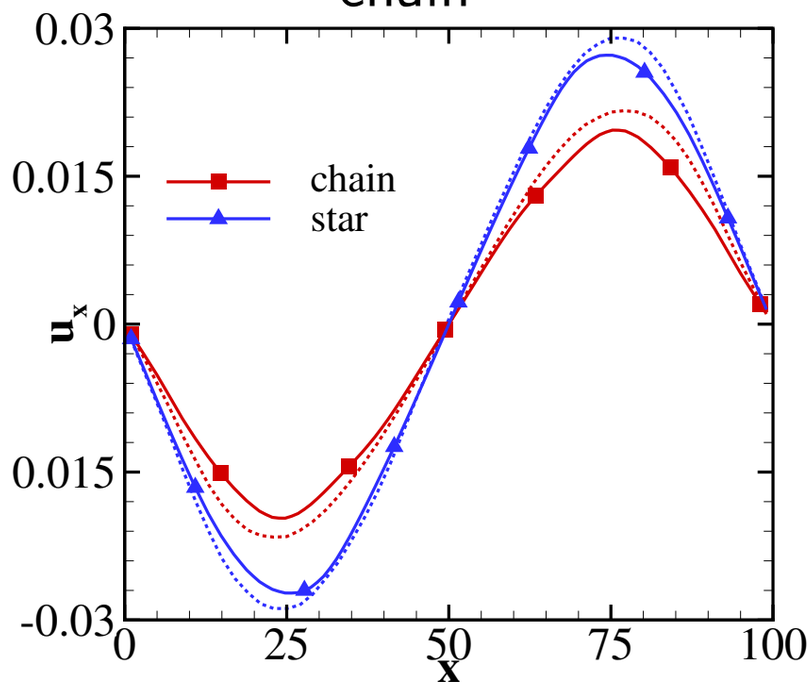
- ***Vortex generated by***

$$f_x(x,y) = -2f_0 \sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{2\pi y}{L}\right), \quad f_y(x,y) = 2f_0 \cos\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)$$



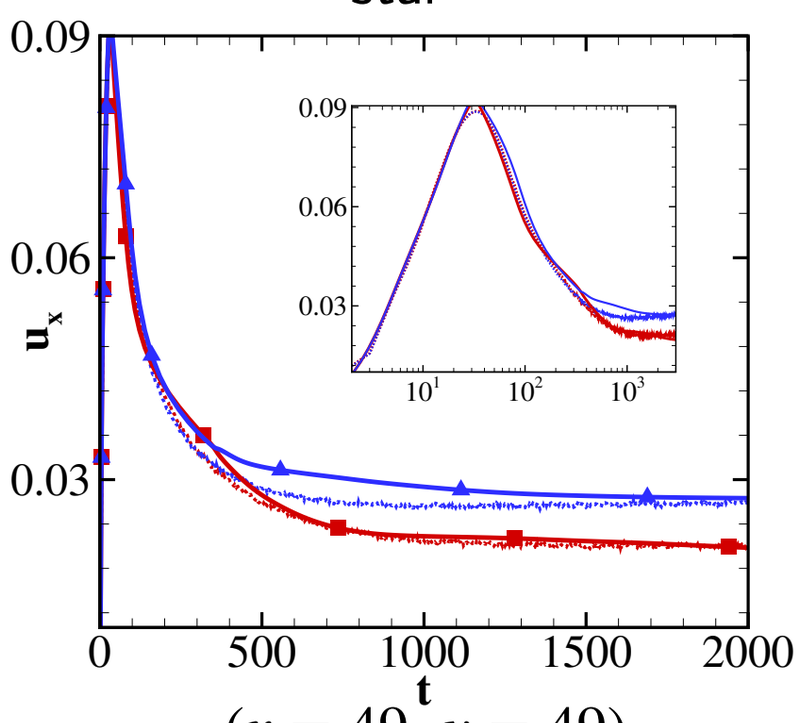


chain



$y = 49$

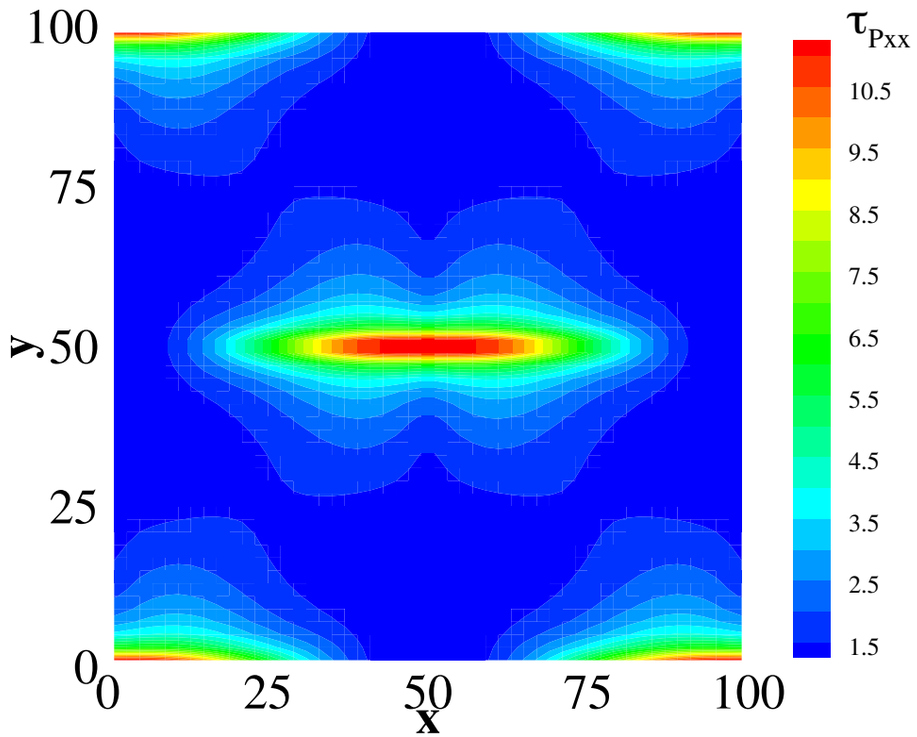
star

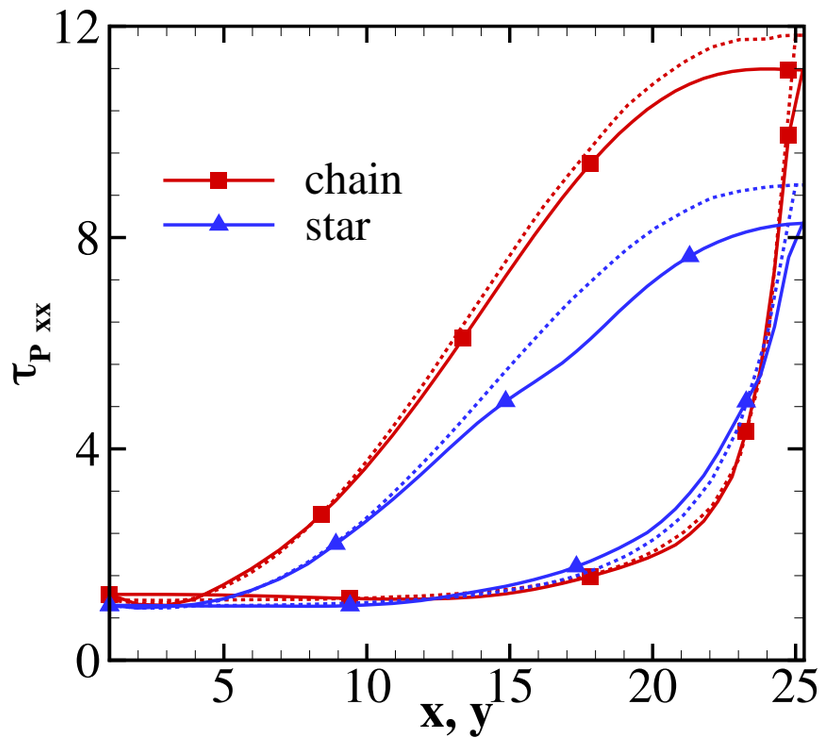


$(x = 49, y = 49)$

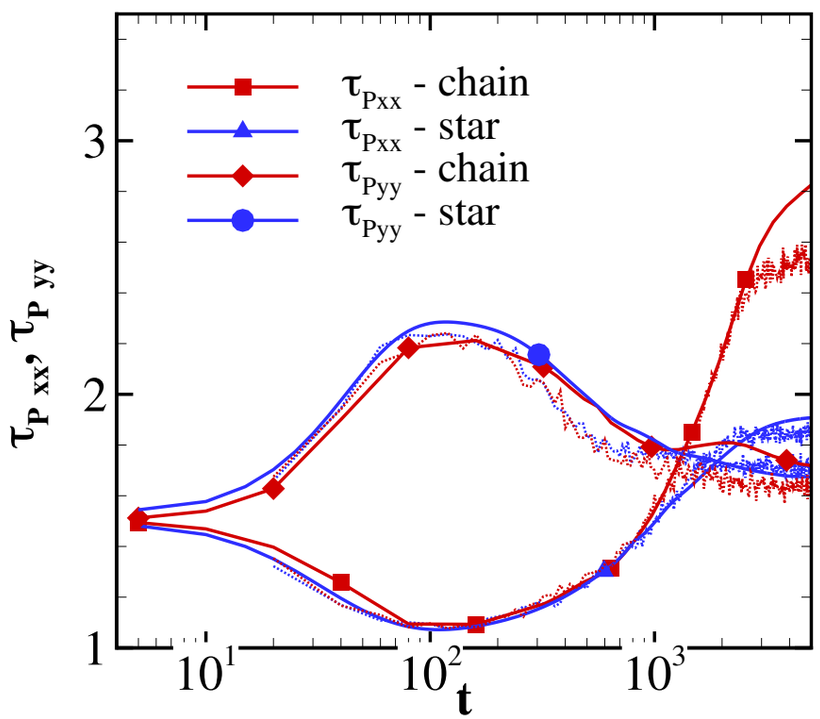
2D Green-Taylor flow

- ***Micro-macro correspondence***

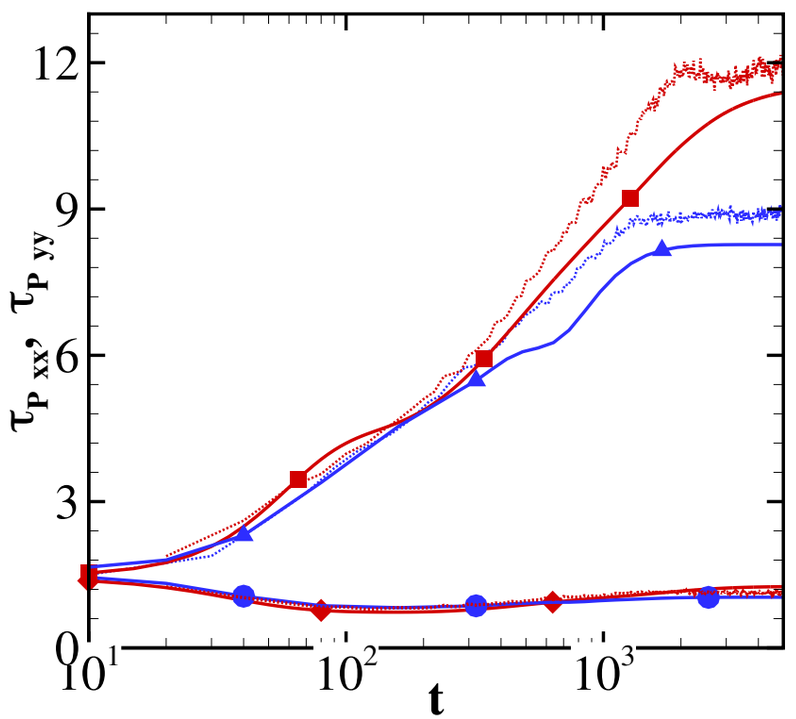




$(x = 49,\ y)$ and $(x,\ y = 49)$



$(x = 49,\ y = 35)$



$(x = 49,\ y = 49)$

Summary

does not	**does**
Learn reduced dynamics using time-series samples	***Retain micro-model fidelity*:** systematically pass the analytical form micro-models across scales
Rely on empirical choices of the constitutive closures	***Respect symmetry and physical constraints*:** provide a generalized form of the objective tensor derivative
Seek the direct approximation of the high-dimensional PDF	***Be reliable*:** strictly preserve the energy structure and ensure numerical stability

Open problems

- Generalized PB and PNP models for charge fluids with molecular-level fidelity?

- Interface and boundary conditions?

- Can we improve the semi-supervised micro-macro training process?

References

[1] Huan Lei, Lei Wu, and Weinan E. Machine-learning-based non-newtonian fluid model with molecular fidelity. *Phys. Rev. E*, 102:043309, 2020.

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[3] Weinan E, Huan Lei, Pinchen Xie, and Linfeng Zhang. Machine learning-assisted multi-scale modeling. *Journal of Mathematical Physics*, 64(7):071101, 2023.

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Thank you

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