DeePN2: A deep learning-based non-Newtonian hydrodynamic model

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Introduction

A deep learning-based non-Newtonian hydrodynamic model, which retains a multi-scaled nature by mapping the polymer configurations into a set of symmetry-preserving macro-scale features.

Our goals are:

- Faithfully inherit the micro-scale interactions beyond empirical models.
- Automatically capture specific molecular structural mechanics without human intervention.
- Strictly preserve the frame indifference constraints.
- Only utilize discrete samples for model training.

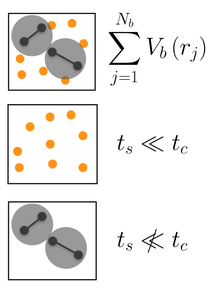
Motivations

- **Macro-model:** hydrodynamic equations for non-Newtonian fluid

$$\nabla\cdot\mathbf{u}=0,\quad \rho\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}=-\nabla p+\nabla\cdot(\boldsymbol{\tau}_{\mathrm{s}}+\boldsymbol{\tau}_{\mathrm{p}}),$$
$$\boldsymbol{\tau}_{\mathrm{p}}=\mathbf{G}(\mathbf{c}),\quad \frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}=\mathbf{H}_i(\mathbf{c}).$$

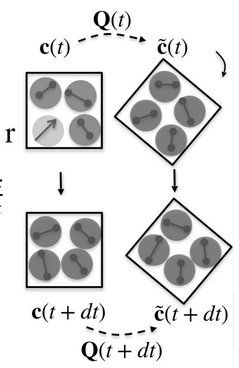
$\mathbf{G}$ stress
$\mathbf{H}_i$ constitutive dynamics
$\frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}$ objective tensor derivative
$\}\rightarrow$ unclosed form $\leftarrow$

Micro-model



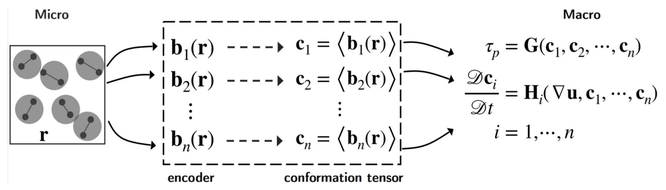
- **Physical constraint:** frame-indifference condition.

$$\mathbf{G}(\widetilde{\mathbf{c}})=\mathbf{Q}\mathbf{G}(\mathbf{c})\mathbf{Q}^T,\quad \widetilde{\frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}}=\mathbf{Q}\frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}\mathbf{Q}^T.$$

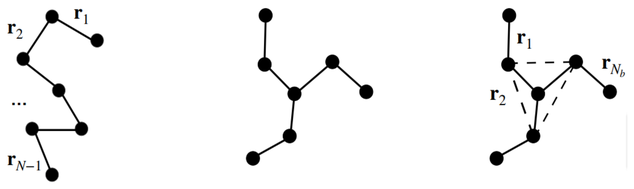


- **Limits of existing empirical models:**
  - ☐ Molecular fidelity: heuristic form of **G(c)**
  - ☐ Empirical formulation: non-unique choices of $\frac{\mathcal{D}\boldsymbol{c}}{\mathcal{D}t}$
  - ☐ Generalization ability: heterogeneous molecule structural micro-mechanics
- **Machine-learning difficulties:**
  - ☐ Retain physical interpretation
  - ☐ Require error-prone time-series samples
  - ☐ Preserve symmetry constraints

Model Construction from Micro Description



- **Main idea 1:** seek explicit micro-macro encoders to best approximate the macro-scale features.



$\boldsymbol{r}$ is the bond which is rotational-symmetric, $\boldsymbol{r}^*$ is the length and the distance of bonds which is rotational-invariant. Then we can construct the symmetry-preserving micro-macro encoder by

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

where w_{ij} and g_i will be represented by deep neural networks.

Remark:

- ☐ $\{\boldsymbol{c}_i\}$ are not standard moments to approximate the polymer configuration density.
- ☐ $\{\mathbf{b}_i\}$ are jointly learned for the best approximation of **G**(·) and **H**(·).
- ☐ $\{\boldsymbol{c}_i\}$ strictly preserve symmetry constraints

Dumbbell Example:

$$\mathbf{b}_i(\mathbf{r})=\mathbf{f}_i(\mathbf{r})\mathbf{f}_i^T(\mathbf{r}),\quad \mathbf{f}_i(\mathbf{r})=g_i(|\mathbf{r}|)\mathbf{r},$$
$$\text{s.t. } \mathbf{b}_i(\mathbf{Q}\mathbf{r})=\mathbf{Q}\mathbf{b}_i(\mathbf{r})\mathbf{Q}^T,\quad \mathbf{f}_i(\mathbf{Q}\mathbf{r})=\mathbf{Q}\mathbf{f}_i(\mathbf{r})$$

- **Main idea 2:** discrete-sample-based learning with molecular fidelity.

The explicit form of micro-macro correspondence enables us to derive their evolution from the Fokker-Planck equation

$$\frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}=\frac{\mathrm{d}\mathbf{c}_i}{\mathrm{d}t}-\boldsymbol{\kappa}:\left\langle\sum_{j=1}^{N-1}\mathbf{r}_j\otimes\nabla_{\mathbf{r}_j}\otimes\mathbf{b}_i\right\rangle$$
$$=\frac{k_BT}{\gamma}\left\langle\sum_{j,k=1}^{N-1}A_{jk}\nabla_{\mathbf{r}_j}\cdot\nabla_{\mathbf{r}_k}\mathbf{b}_i\right\rangle-\frac{1}{\gamma}\left\langle\sum_{j=1}^{N-1}\sum_{k=1}^{N_b}A_{jk}\nabla_{\mathbf{r}_k}V(\mathbf{r})\cdot\nabla_{\mathbf{r}_j}\mathbf{b}_i\right\rangle$$

Remark:

- ☐ A - generalized Rouse matrix encodes various molecule structures
- ☐ V - potential function encodes micro-scale intramolecular interactions
- ☐ The LHS provides a generalized objective tensor derivative with clear micro-scale physical interpretation.

DeePN^2 Model

- **DeePN^2:** A machine-learning-based model of non-Newtonian fluids.

$$\rho\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}=-\nabla p+\nabla\cdot(\boldsymbol{\tau}_{\mathrm{s}}+\boldsymbol{\tau}_{\mathrm{p}}),\quad \nabla\cdot\mathbf{u}=0,$$
$$\boldsymbol{\tau}_{\mathrm{p}}=\mathbf{G}(\mathbf{c}),\quad \frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}=\mathbf{H}_i(\mathbf{c}),$$
$$\frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}=\frac{\mathrm{d}\mathbf{c}_i}{\mathrm{d}t}-\boldsymbol{\kappa}:\mathcal{E}_i,\quad \mathbf{H}_i(\mathbf{c})=\frac{k_BT}{\gamma}\mathbf{H}_{1,i}(\mathbf{c})-\frac{1}{\gamma}\mathbf{H}_{2,i}(\mathbf{c})$$

$\mathbf{G},\mathbf{H}_{1,i},\mathbf{H}_{2,i},\mathbf{b}_i,\boldsymbol{\mathcal{E}}_i$ are represented by DNNs that rigorously **preserve rotational symmetry** and are jointly learned by:

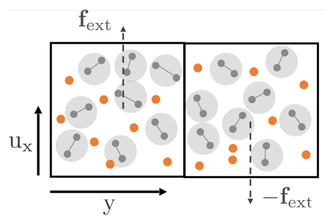
$$\mathbf{H}_{1,i}(\mathbf{c})=\left\langle\sum_{j,k=1}^{N-1}A_{jk}\nabla_{\mathbf{r}_j}\cdot\nabla_{\mathbf{r}_k}\mathbf{b}_i\right\rangle$$
$$\mathbf{H}_{2,i}(\mathbf{c})=\left\langle\sum_{j=1}^{N-1}\sum_{k=1}^{N_b}A_{jk}\nabla_{\mathbf{r}_k}V(\mathbf{r})\cdot\nabla_{\mathbf{r}_j}\mathbf{b}_i\right\rangle$$
$$\mathcal{E}_i(\mathbf{c})=\left\langle\sum_{j=1}^{N-1}\mathbf{r}_j\otimes\nabla_{\mathbf{r}_j}\otimes\mathbf{b}_i\right\rangle$$
$$\mathbf{G}(\mathbf{c})=\left\langle\sum_{k=1}^{N_b}\mathbf{r}_k\otimes\nabla_{\mathbf{r}_k}\otimes V_b(r)\right\rangle$$

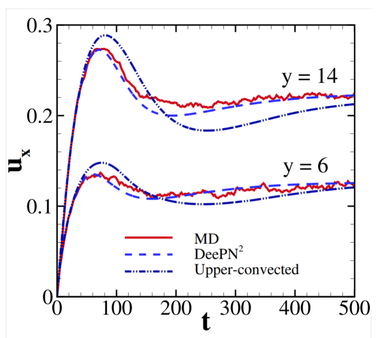
Remark: DeePN^2 achieves the following innovations

- **Does Not:**
  - ☐ Learn constitutive dynamics using timeseries samples.
  - ☐ Rely on empirical choices of the constitutive closures.
  - ☐ Seek the direct approximation of the high-dimensional PDF.
- **Does:**
  - ☐ **Be reliable**: systematically pass the micro-scale heterogenous molecular structures and interactions.
  - ☐ **Retain physical interpretation**: provide a generalized form of the objective tensor derivative.
  - ☐ **Respect constraints**: strictly preserve the rotational frame-indifference symmetries.

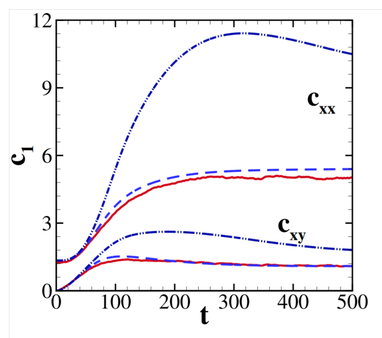
Numerical Example: Reverse Poiseuille Flow

- **Dumbbell:** Empirical form of objective tensor derivative is limited.



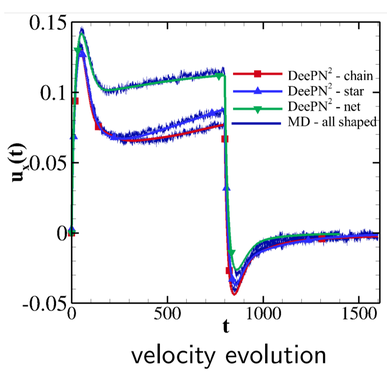


velocity evolution

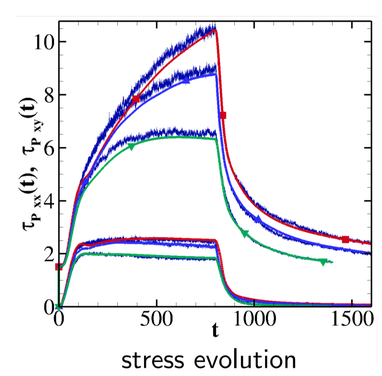


conformation tensor evolution

- **Multi-bead molecules:** the polymer suspensions exhibit different flow responses due to the different molecule structures.

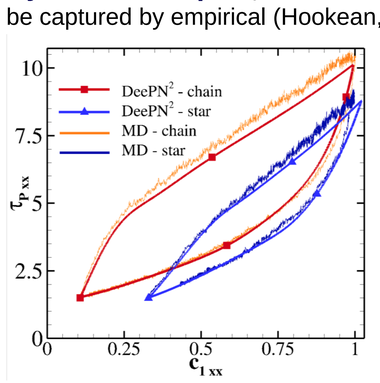


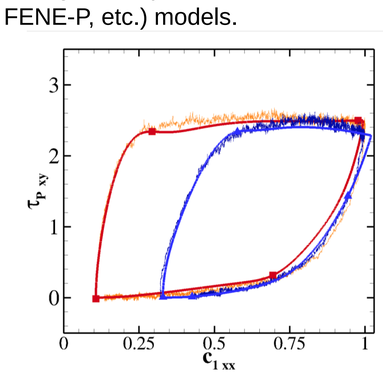
velocity evolution



stress evolution

Hysteresis loop: represents the strong memory effect that can not be captured by empirical (Hookean, FENE-P, etc.) models.

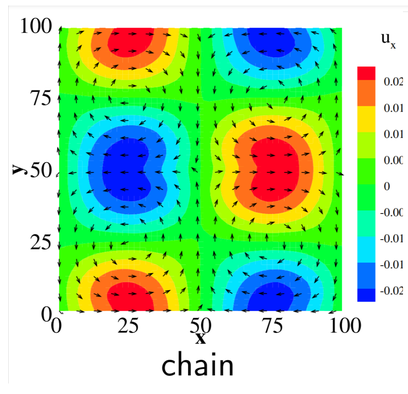




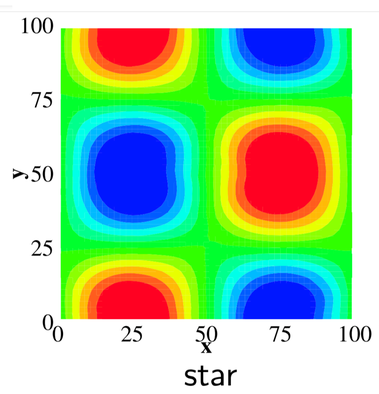
Numerical Example: 2D Green-Taylor flow

Vortex generated by:

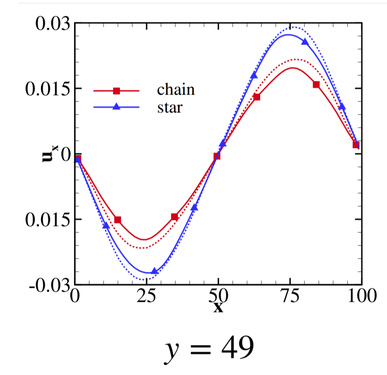
$$f_x(x,y)=-2f_0\sin(\frac{2\pi x}{L})\cos(\frac{2\pi y}{L}),\quad f_y(x,y)=2f_0\cos(\frac{2\pi x}{L})\sin(\frac{2\pi y}{L})$$



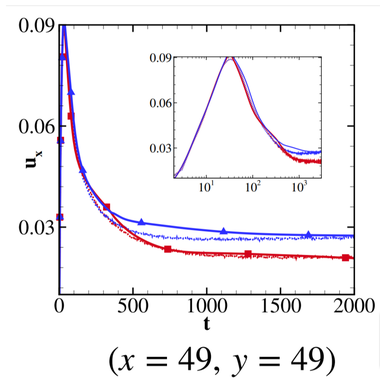
chain



star



$y=49$



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

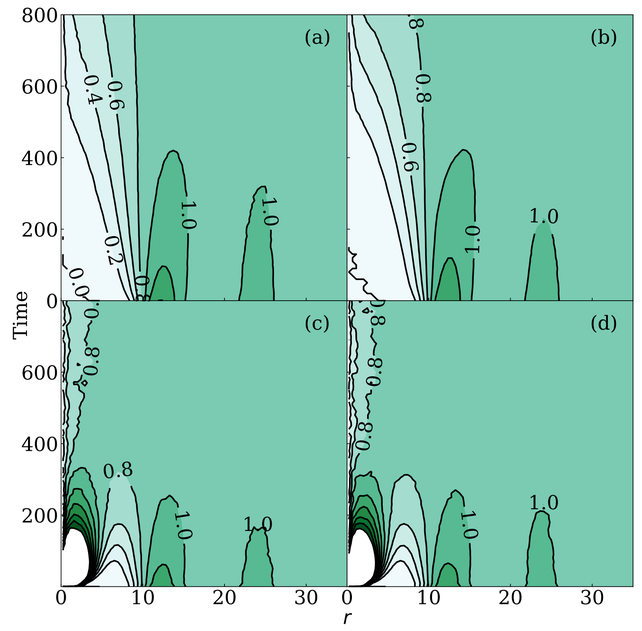
Future Work

Integrate the inter-molecule interactions into the DeePN^2 model

$$V_i(\mathbf{r}^i,\mathbf{Q})=V_{\text{intra}}(\mathbf{r}^i)+V_{\text{inter}}(\mathbf{Q})$$
$$V_{\text{intra}}(\mathbf{r}^i)=\sum_{j=1}^{N_b}V_b(r_j^i)$$
$$V_{\text{inter}}(\mathbf{Q})=V_{\text{CG}}(\mathbf{Q}_1,\cdots,\mathbf{Q}_N)$$

r - intramolecular coordinate
Q - center of mass of polymer molecules

The intermolecular interaction is many-body and further effect the hydro dynamics (van-Hove function) on the collective scale.



(a) Full micro-model (b) ML-model
(c) GLE (Empirical) (d) DPD (Empirical)

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