DeePN^2: 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.

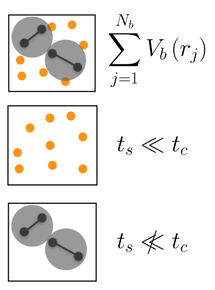
Motivations

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

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

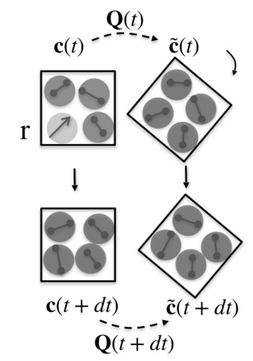
$\mathbf{G}$ stress
$\mathbf{H}_i$ constitutive dynamics
$\frac{\mathcal{D}\mathbf{c}_i}{\mathcal{D}t}$ objective tensor derivative
$\Big\}\rightarrow$ unclosed form $\leftarrow$

Micro-model



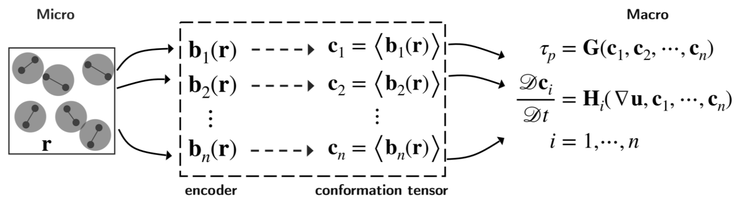
- **Physical constraint:** frame-indifference condition.

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

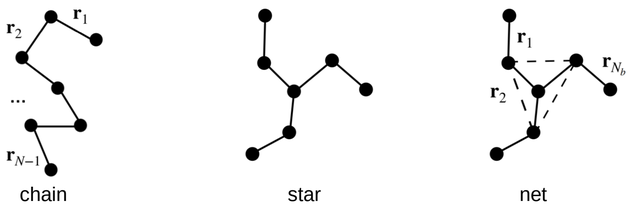


- **Limits of existing empirical models:**
  - Molecular fidelity: heuristic form of **G(c)**
  - Empirical formulation: non-unique choices of $\frac{\mathcal{D}\boldsymbol{c}}{\mathcal{D}t}$
  - Generalization ability: heterogeneous molecule structural micro-mechanics
- **Machine-learning difficulties:**
  - 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

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

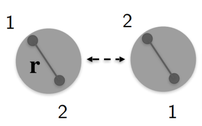
where w_{ij} and g_i will be represented by deep neural networks.

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:

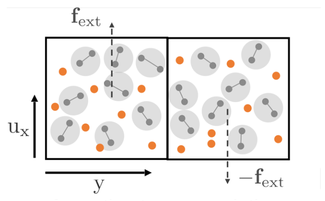
$$\mathbf{H}_{1,i}(\mathbf{c})=\left\langle\sum_{j,k=1}^{N-1}A_{jk}\nabla_{\mathbf{r}_j}\cdot\nabla_{\mathbf{r}_k}\mathbf{b}_i\right\rangle$$
$$\mathbf{H}_{2,i}(\mathbf{c})=\left\langle\sum_{j=1}^{N-1}\sum_{k=1}^{N_b}A_{jk}\nabla_{\mathbf{r}_k}V(\mathbf{r})\cdot\nabla_{\mathbf{r}_j}\mathbf{b}_i\right\rangle$$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

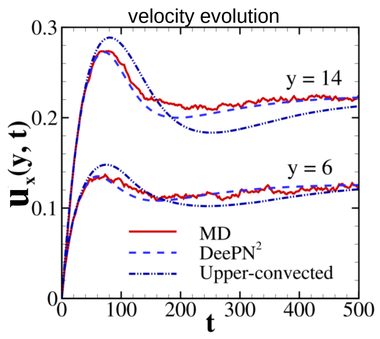
Remark: DeePN^2 achieves the following innovations

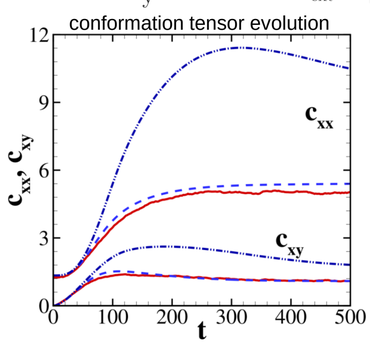
- **Does Not:**
  - Learn constitutive dynamics using timeseries samples.
  - Rely on empirical choices of the constitutive closures.
  - Seek the direct approximation of the high-dimensional PDF.
- **Does:**
  - **Be reliable**: systematically pass the micro-scale heterogenous molecular structures and 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

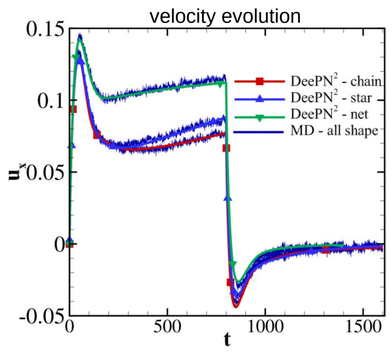
- **Dumbbell:** Empirical form of objective tensor derivative is limited.

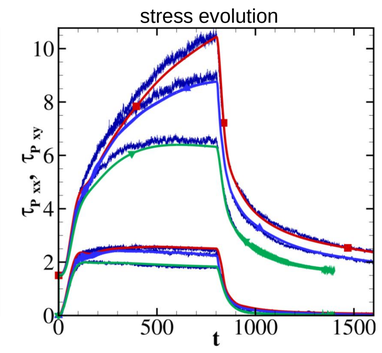




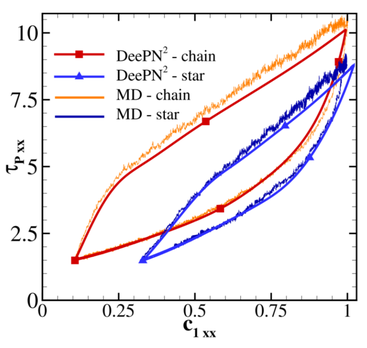


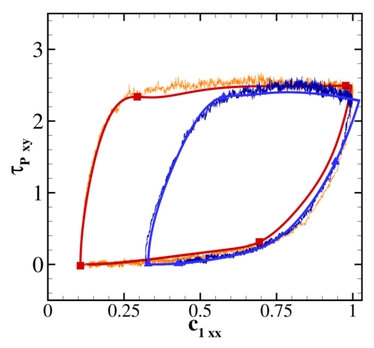
- **Multi-bead molecules (N=7):** our model can capture the different flow responses arising from the different molecule structures **without human intervention**.





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



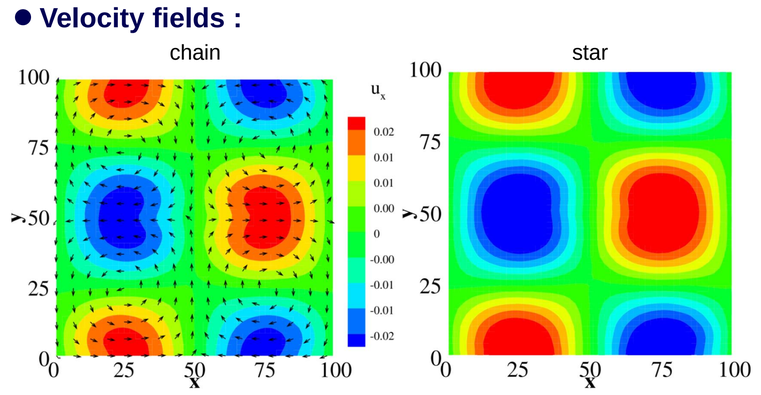


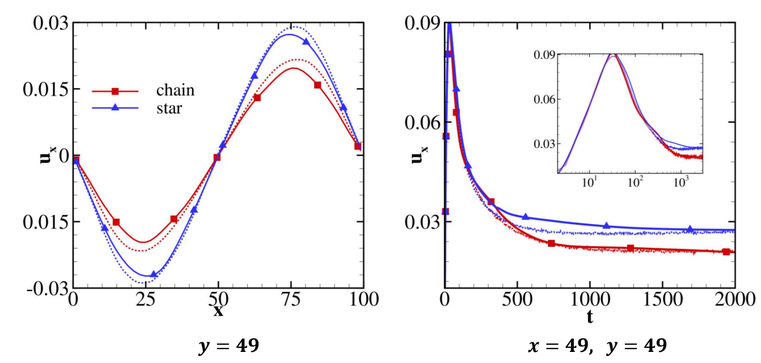
Numerical Example: 2D Green-Taylor flow

Vortex generated by:

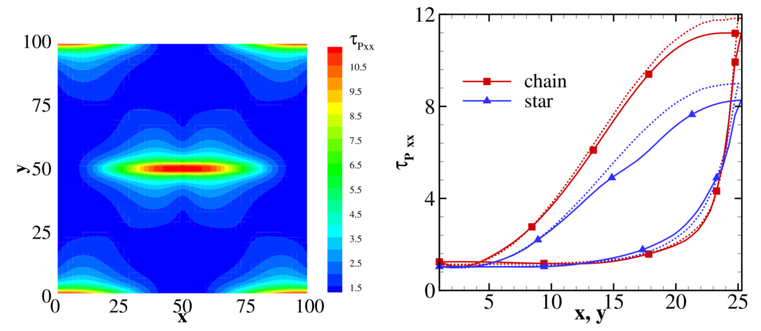
$$f_x(x,y)=-2f_0\sin(\frac{2\pi x}{L})\cos(\frac{2\pi y}{L}),\quad f_y(x,y)=2f_0\cos(\frac{2\pi x}{L})\sin(\frac{2\pi y}{L})$$

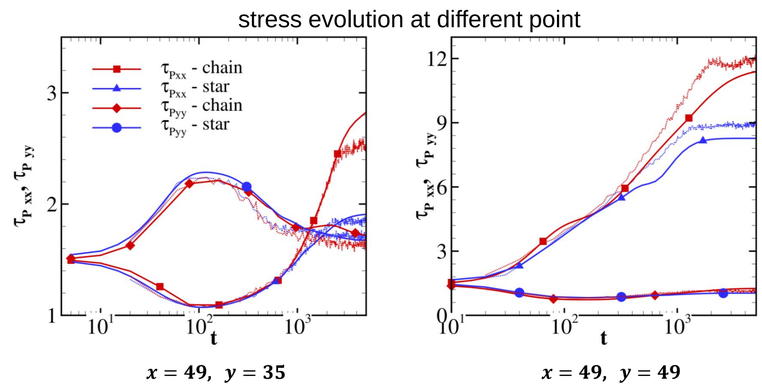
- **Velocity fields :**





- **Stress field:**





- **Effects of heterogenous molecular structure:** the chain-shaped molecule suspension exhibits larger polymer stress variation, also reflected in the larger hysteresis loop area. Such difference is also consistent with the more pronounced asymmetric velocity field.

Future Work

Use the generalized Langevin equation with state-dependent memory formulation[2] into the friction term and derive a better continuous dynamics in DeePN^2 model.

References

[1] Lidong Fang, Pei Ge, Lei Zhang, Weinan E, and Huan Lei. DeePN^2: A deep learning-based non-newtonian hydrodynamic model. Journal of Machine Learning, 1(1):114–140, 2022.

[2] Pei Ge, Zhongqiang Zhang and Huan Lei. Data-driven learning of the generalized Langevin equation with state-dependent memory. arXiv:2310.18582

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

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

Acknowledgment

The work is supported by the National Science Foundation under Grant DMS-2110981, CAREER DMS-2143739, and the ACCESS program through allocation MTH210005.