Bridging scales using physically-informed machine learning

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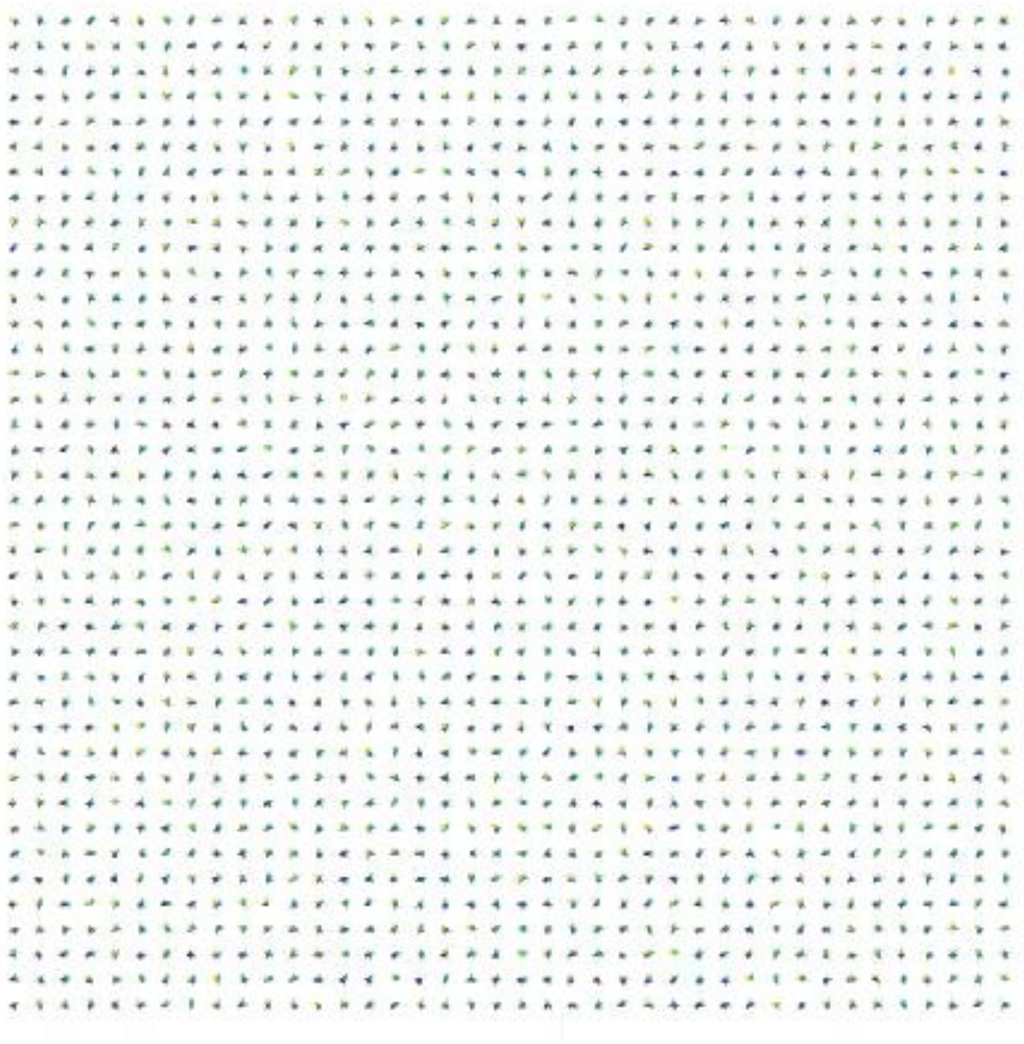
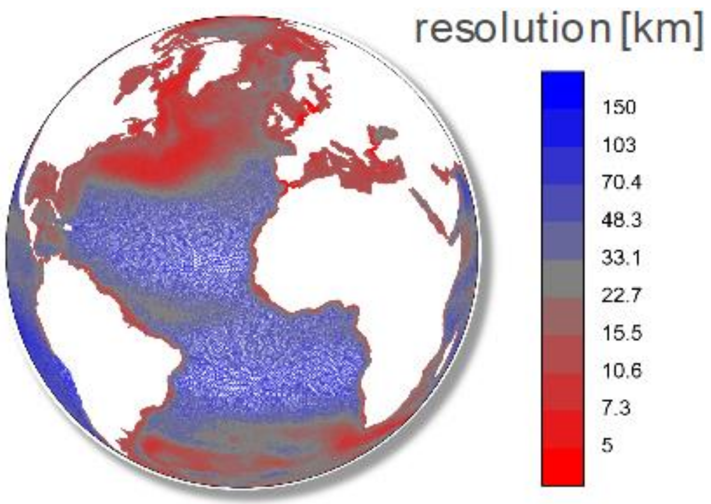
IPAM Workshop: Bridging Scales from Atomistic to Continuum in Electrochemical Systems



Outline

- Motivation (bringing scales in fluid turbulence)
- Physically informed equation inference **framework** (SPIDER)
- Coarse-graining *continuum* microscopic models
- Coarse-graining *discrete* microscopic models

Modeling of multiscale phenomena



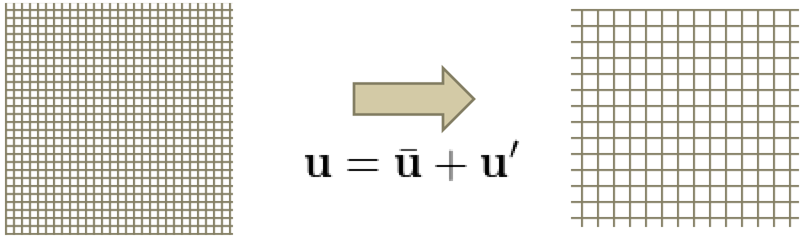
Coupled Model Intercomparison Project 6 using Alfred Wegener Institute Climate Model

Microscopic governing equations

$$\partial_t \rho + \nabla_i(\rho u_i) = 0 \quad \rightarrow \quad \nabla_i u_i = 0$$

$$\partial_t u_i + \nabla_j(u_j u_i) = -\rho^{-1}\nabla_i p + \nu \nabla_j \nabla_j u_i$$

Traditional coarse-graining approach:

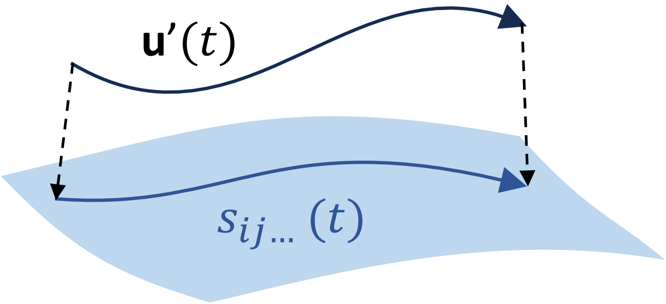


$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$$

$$\dot{u}_i = F_i(\mathbf{u}) \qquad \dot{\bar{u}}_i \approx F_i(\bar{\mathbf{u}}) + W_i(\bar{\mathbf{u}})$$

Closure term

Accounting for information flow from small to large scales:



$$\dot{\bar{u}}_i = F_i(\bar{\mathbf{u}}) + W_i(\bar{\mathbf{u}}, s_{ij\ldots})$$

$$\dot{s}_{ij\ldots} = G(\bar{\mathbf{u}}, s_{ij\ldots})$$

Temporal coarse-graining (RANS)

$$\overline{u}(\mathbf{x},t) \equiv \int G_\Delta(t-t')u(\mathbf{x},t')dt' \quad \Longrightarrow$$

$$\partial_t \bar{u}_i + \bar{u}_j \nabla_j \bar{u}_i = -\rho^{-1}\nabla_i \bar{p} + \nu \nabla_j \nabla_j \bar{u}_i + \nabla_j R_{ij}$$

Reynolds stress tensor: $R_{ij} = \overline{u_i' u_j'}$

Can **derive** an *infinite* system of equations for correlations:

$$\partial_t R_{ij} + \bar{u}_k \nabla_k R_{ij} = -R_{ik}\nabla_k \bar{u}_j - R_{jk}\nabla_k \bar{u}_i + \nu\nabla^2 R_{ij} + \bar{T}_{ij}$$

$$T_{ij} = \frac{2}{\rho} p' S_{ij}' - 2\nu \nabla_k u_i' \nabla_k u_j' - \nabla_k \left(u_i' u_j' u_k' + \frac{1}{\rho}[p' u_i' \delta_{jk} + p' u_j' \delta_{ik}] \right)$$

Eddy viscosity

…or **model** closure in *ad hoc* way: $R_{ij} - \frac{1}{d}\delta_{ij}R_{kk} = 2\nu_e \bar{S}_{ij},\qquad S_{ij} = \frac{1}{2}(\nabla_i u_j + \nabla_j u_i)$

<u>Smagorinsky model:</u>

$$\nu_e = C\Delta^2 \sqrt{\bar{S}_{ij}\bar{S}_{ij}}$$

<u>k-ε model:</u>

$$\nu_e = C_\nu \frac{k^2}{\epsilon}$$

$$\partial_t k + \bar{u}_j \nabla_j k = 2\nu_e I_1 + C_3 \nabla_i(\nu_e \nabla_i k) - \epsilon,$$

$$\partial_t \epsilon + \bar{u}_j \nabla_j \epsilon = C_1 \frac{\epsilon}{k}\nu_e I_1 + C_4 \nabla_i(\nu_e \nabla_i \epsilon) - C_2 \frac{\epsilon^2}{k}$$

Spatial coarse-graining (LES)

$$\bar{u}(\mathbf{x},t) \equiv \int G_\Delta(\mathbf{x}-\mathbf{y})u(\mathbf{y},t)d\mathbf{y} \quad \Longrightarrow \quad \partial_t\bar{u}_i + \bar{u}_j\nabla_j\bar{u}_i = -\rho^{-1}\nabla_i\bar{p} + \nu\nabla_j\nabla_j\bar{u}_i + \nabla_j\tau_{ij}$$

SGS stress tensor:

$$\tau_{ij} \equiv \bar{u}_i\bar{u}_j - \overline{u_i u_j} = f(\bar{\mathbf{u}})$$

Model $f(\mathbf{u})$ using:

- Empirical considerations
- Scaling & symmetry
- Formal expansions

…the correct way to do this

$$\bar{u}(\mathbf{x},t) \equiv \int G_\Delta(\mathbf{x}-\boldsymbol{y})u(\mathbf{y},t)d\mathbf{y} \quad \Longrightarrow \quad \partial_t\bar{u}_i + \bar{u}_j\nabla_j\bar{u}_i = -\rho^{-1}\nabla_i\bar{p} + \nu\nabla_j\nabla_j\bar{u}_i + \nabla_j\tau_{ij}$$

SGS stress tensor:

$$\tau_{ij} \equiv \bar{u}_i\bar{u}_j - \overline{u_i u_j}$$
$$= L_{ij} + C_{ij} + R_{ij}$$

Leonard (1975)

Large scales:

$$L_{ij} \equiv \overline{\bar{u}_i\bar{u}_j} - \bar{\bar{u}}_i\bar{\bar{u}}_j = f_L(\bar{u}_i)$$

Scale interaction:

$$C_{ij} \equiv \overline{\bar{u}_i u_j' + \bar{u}_j u_i'} - \bar{\bar{u}}_i\bar{u}_j' - \bar{\bar{u}}_j\bar{u}_i' = f_C(\bar{u}_i, R_{ij})$$

Small scales:

$$R_{ij} \equiv \overline{u_i' u_j'} - \bar{u}_i'\bar{u}_j' = ?$$

Closing the system…

Dynamical subgrid-scale (SGS) model:

$$\partial_t R_{ij} = f_R(\bar{u}_i, R_{ij})$$

Data-driven inference of equivariant models

What do we do when **formal** homogenization approaches fail?

<ins>The idea:</ins> infer the **governing equations** of an *effective* physical theory in *explicit*, *interpretable form* from data using primarily the most fundamental physical constraint: *symmetry*

Use *specific domain knowledge* and *formal analytical methods* mostly to identify the relevant **variables** (effective degrees of freedom)

Equivariant structure of physical models

Governing equations for fluids

$$\nabla_i u_i = 0, \qquad \nabla_i \nabla_i p = \rho \nabla_i (u_j \nabla_j u_i)$$

$$\partial_t \bar{u}_i + \bar{u}_j \nabla_j \bar{u}_i = -\rho^{-1} \nabla_i \bar{p} + \nu \nabla_j \nabla_j \bar{u}_i + \nabla_j R_{ij}$$

$$\partial_t R_{ij} + \bar{u}_k \nabla_k R_{ij} + R_{ik} \nabla_k \bar{u}_j + R_{jk} \nabla_k \bar{u}_i = \nu \nabla_k \nabla_k R_{ij} + \overline{T}_{ij}$$

O(3) group representation

rank-0 tensor (scalar)

rank-1 tensor (vector)

rank-2 tensor

Symmetry equivariant search space

Most "physical laws" can be written in the form:

$$\sum_n c_n F^n = 0$$

Translation symmetry: all coefficients c_n are constant (with respect to group transformations)

Rotation + reflection symmetry: every term F^n transforms according to the same *irreducible* representation $k = 0,1,2,\ldots$ of $O(d)$

Libraries of potential terms: $\mathcal{L}_k = \{F^1, F^2, \cdots, F^{N_k}\}$ $\rightarrow$ Search space

Term libraries

Symmetries: E(3) = T(3) × O(3) (translations, rotations, reflections)

Original variables: p, $\mathbf{u}$

Differential operators: ∂_t, ∇

Derivative variables: $\mathbf{u}, p, \partial_t \mathbf{u}, \partial_t p, \nabla \mathbf{u}, \nabla p, \partial_t^2 p, \nabla\nabla \mathbf{u}, \cdots$

Truncation: complexity, order of derivatives, scaling, …

Rank-0: $\mathcal{L}_0 = \{1, p, \nabla \cdot \mathbf{u}, \partial_t p, p^2, u^2, p^3, \mathbf{u} \cdot \nabla p, \nabla^2 p, p\partial_t p, \partial_t^2 p, p\nabla \cdot \mathbf{u}, u^2 p, \mathbf{u} \cdot \partial_t \mathbf{u}\}$

Rank-1:

$$\mathcal{L}_1 = \{\mathbf{u}, \partial_t \mathbf{u}, \nabla p, p\mathbf{u}, (\mathbf{u} \cdot \nabla)\mathbf{u}, \nabla^2 \mathbf{u}, \partial_t^2 \mathbf{u}, u^2 \mathbf{u}, p^2 \mathbf{u}, \partial_t \nabla p, p\nabla p, \mathbf{u}(\nabla \cdot \mathbf{u}), (\nabla \mathbf{u}) \cdot \mathbf{u}, \nabla(\nabla \cdot \mathbf{u}), p\partial_t \mathbf{u}, \mathbf{u}\partial_t p\}$$

Term libraries

Symmetries: E(3) × G(3) (translations, rotations, reflections, Galilean)

Original variables: p, $\mathbf{u}$

Differential operators: $\partial_t + \mathbf{u} \cdot \nabla, \nabla$

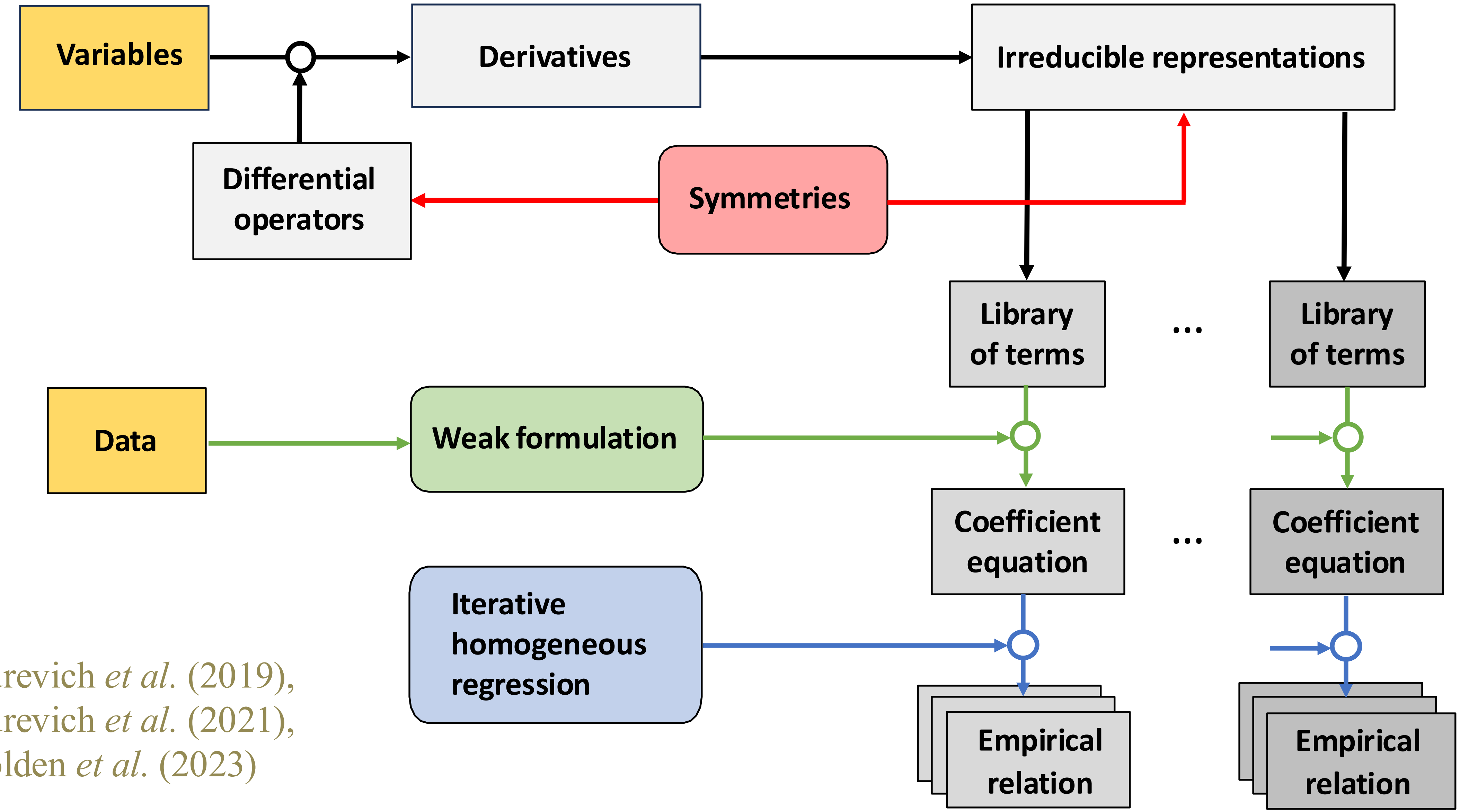
Derivative variables: $\cancel{\mathbf{u}}, p, \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}, \partial_t p + (\mathbf{u} \cdot \nabla)p, \nabla \mathbf{u}, \nabla p, \cdots$

Truncation: complexity, order of derivatives, scaling, …

Rank-0: $\mathcal{L}_0 = \{1, p, \nabla \cdot \mathbf{u}, p^2, p^3, \partial_t p + \mathbf{u} \cdot \nabla p, \nabla^2 p, p \nabla \cdot \mathbf{u}\}$

Rank-1: $\mathcal{L}_1 = \{\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}, \nabla p, \nabla^2 \mathbf{u}, p \nabla p, \nabla(\nabla \cdot \mathbf{u})\}$

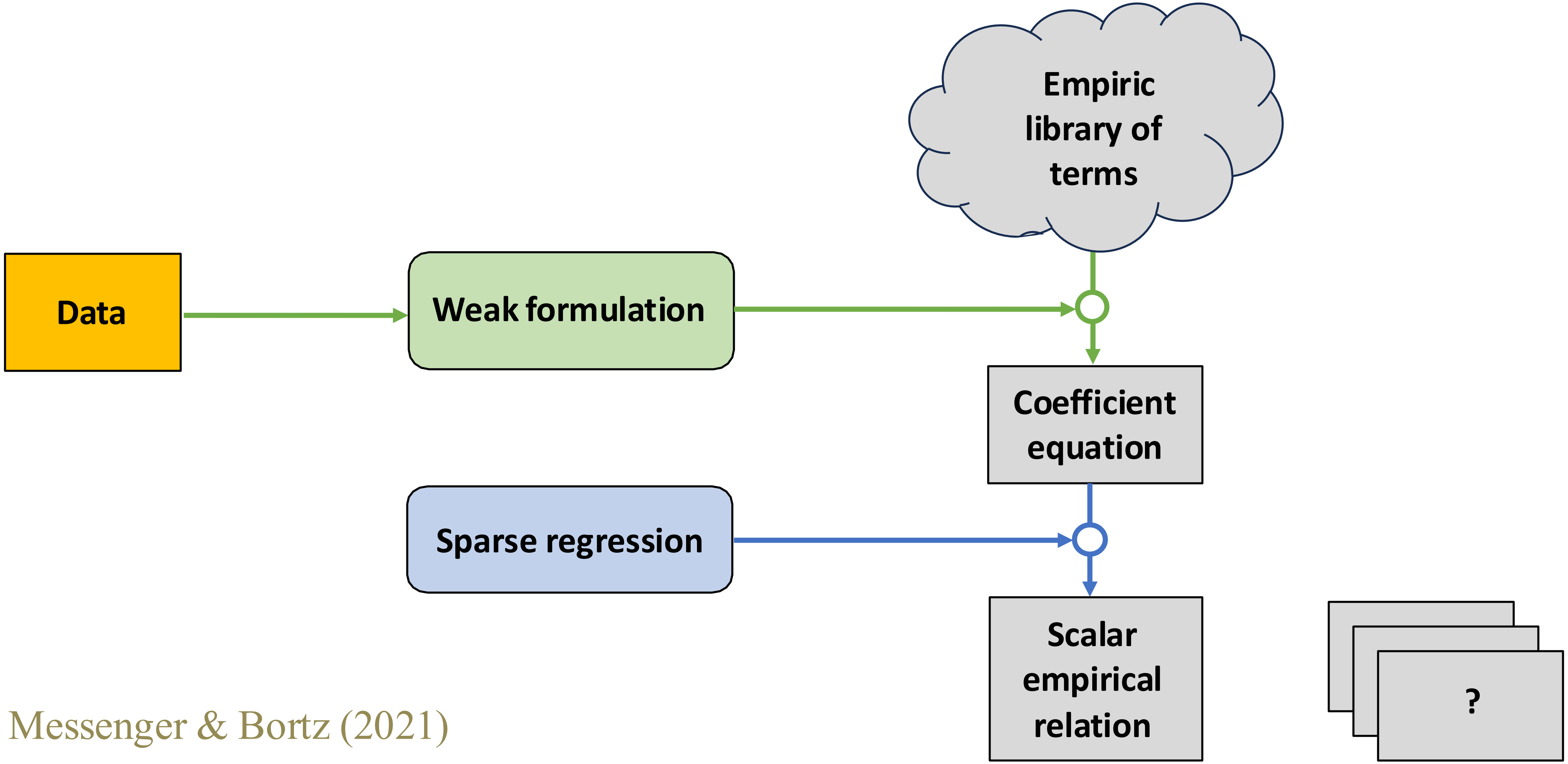
Sparse physically-informed discovery of empirical relations (SPIDER)



Gurevich *et al.* (2019),
Gurevich *et al.* (2021),
Golden *et al.* (2023)

WSINDy

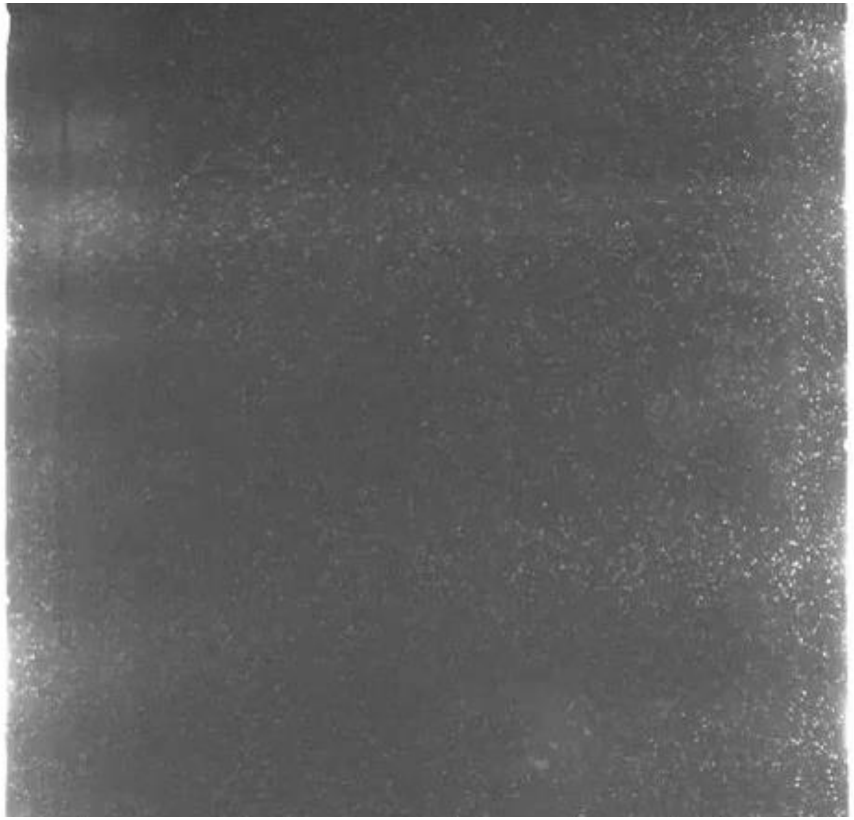
To put things in proper perspective…



Messenger & Bortz (2021)

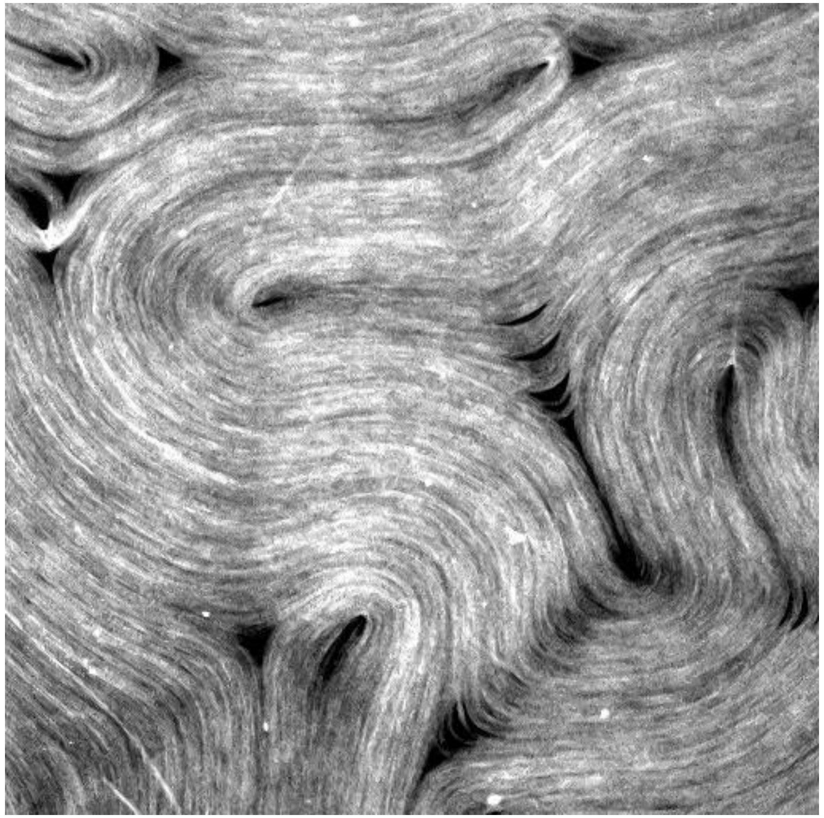
Governing equations from experiment

Lorenz-force-driven electrolyte



Kageorge *et al.* (2021)

Active nematic (microtubules)



Golden *et al.* (2023)

(Invalidated a universally accepted model)

Inference of boundary conditions

Symmetries: E(2) = T(2) × O(2) (translations, rotations, reflections)

Original variables: **u**, **n**

Differential operators: $\nabla, \cancel{\partial_t}$

Derivative variables: $n_i, u, \nabla_i u_j, \nabla_i \nabla_j u_k, \ldots$

Truncation: complexity, order of derivatives, scaling, …

Rank-0: $\mathcal{L}_{0,n} = \{1, n_i u_i, u_i u_i, \nabla_i u_i, \ldots\}$

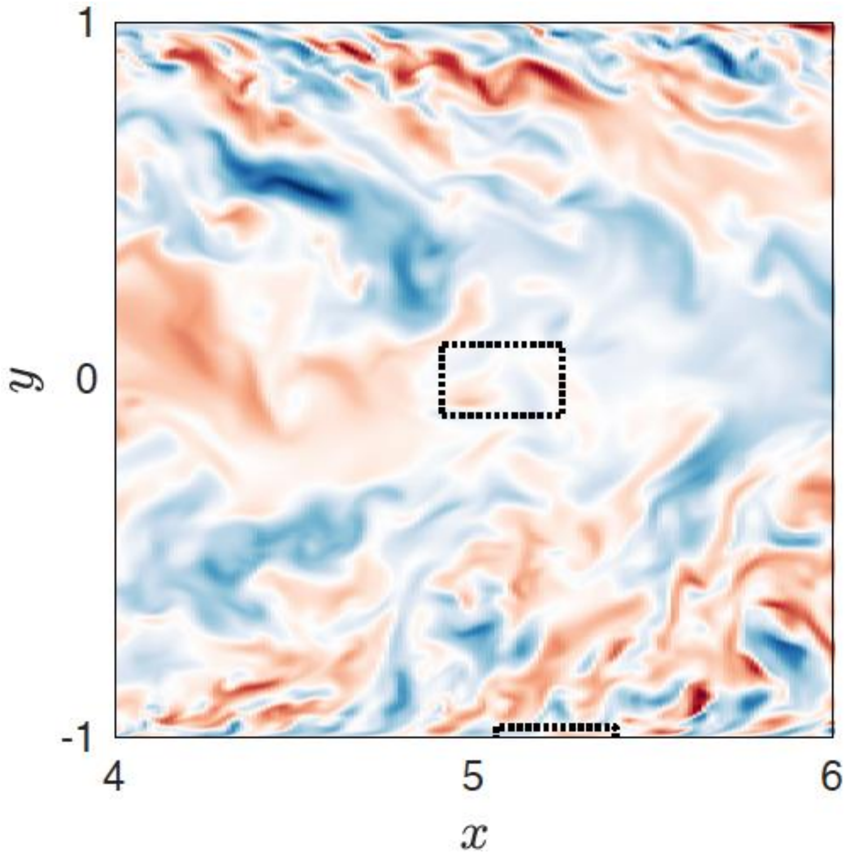
Rank-1: $\mathcal{L}_{1,n} = \{n_i, u_i, n_j \nabla_j u_i, \nabla_j \nabla_j u_i, \ldots\}$

$\mathcal{L}_{\perp} = \{n_k, n_k n_i u_i, n_k n_i n_j \nabla_j u_i, \ldots\}$

$\mathcal{L}_{\parallel} = \{P_{\parallel} n_i, P_{\parallel} u_i, P_{\parallel} n_j \nabla_j u_i, P_{\parallel} \nabla_j \nabla_j u_i, \ldots\}$

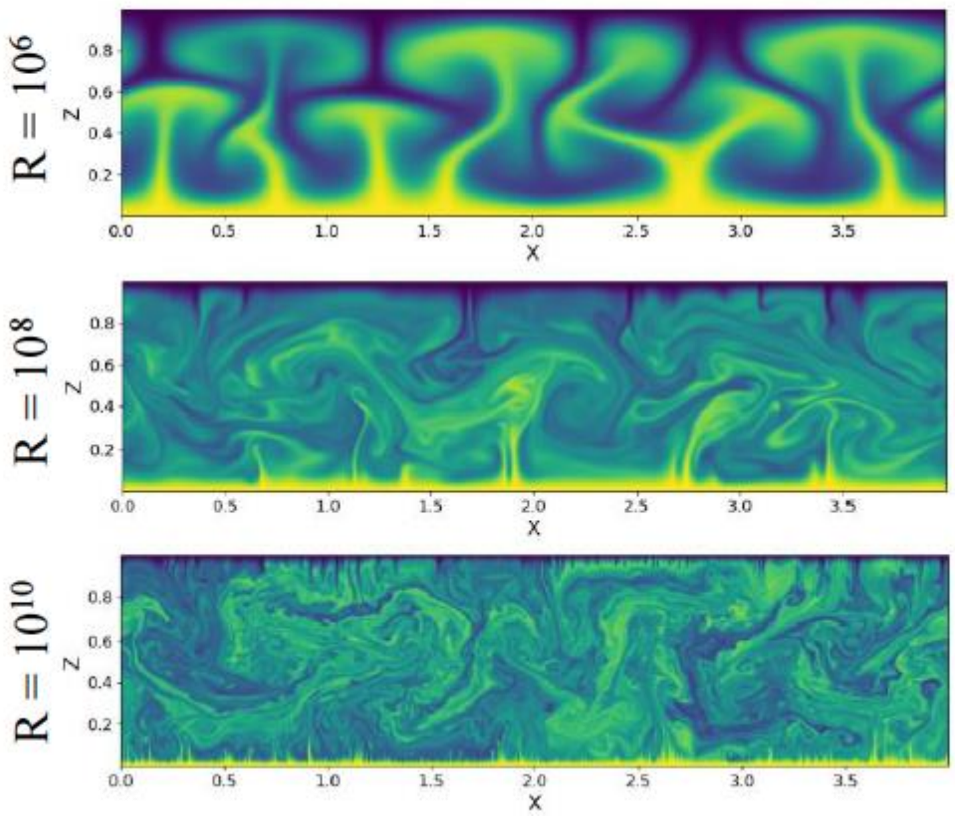
Governing equations *and* boundary conditions from DNS

Pressure-driven turbulence @ $Re \sim 10^5$



Gurevich *et al.* (2024)

Buoyancy-driven turbulence

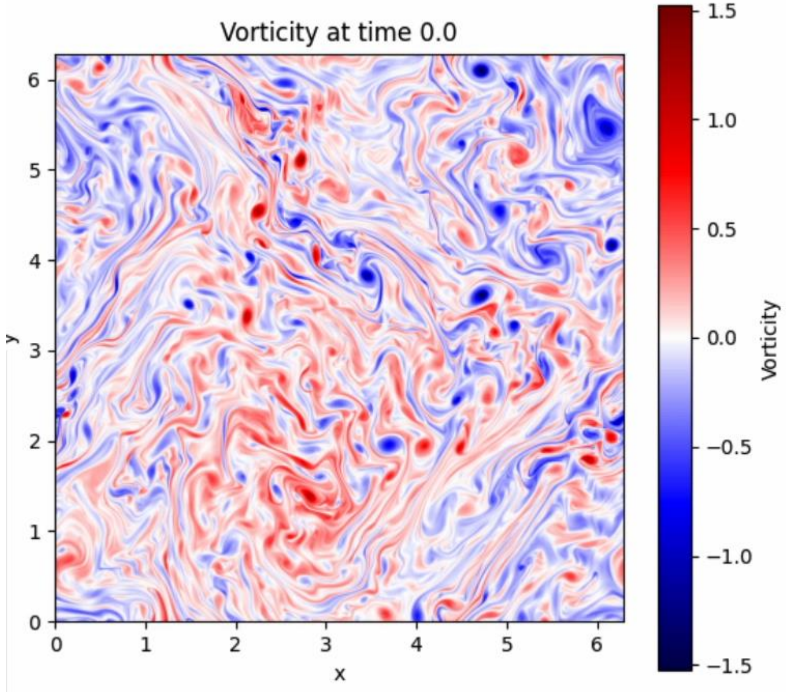


Wareing *et al.* (2025)

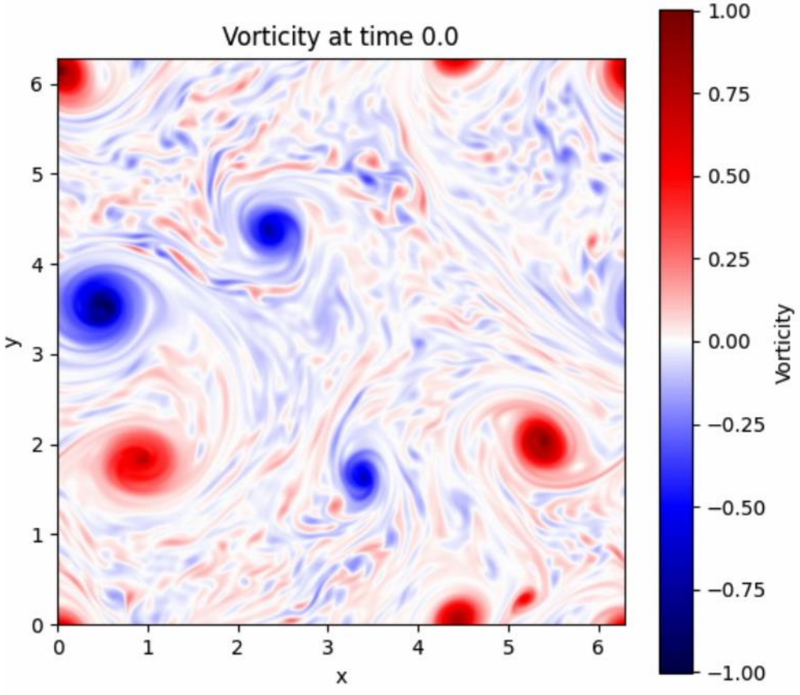
(WSINDy mostly fails)

Coarse-graining *continuum* microscopic models

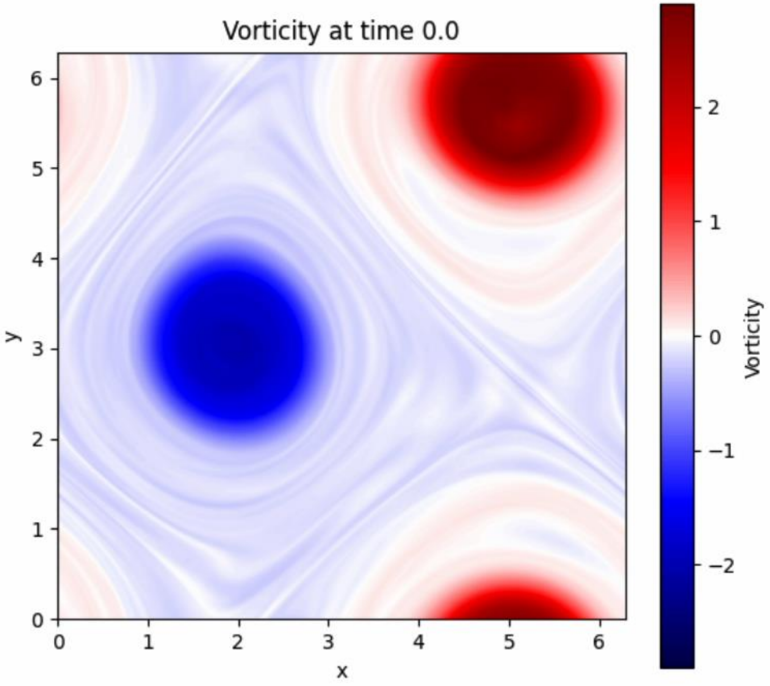
Data generated by fully resolved DNS



Inverse cascade

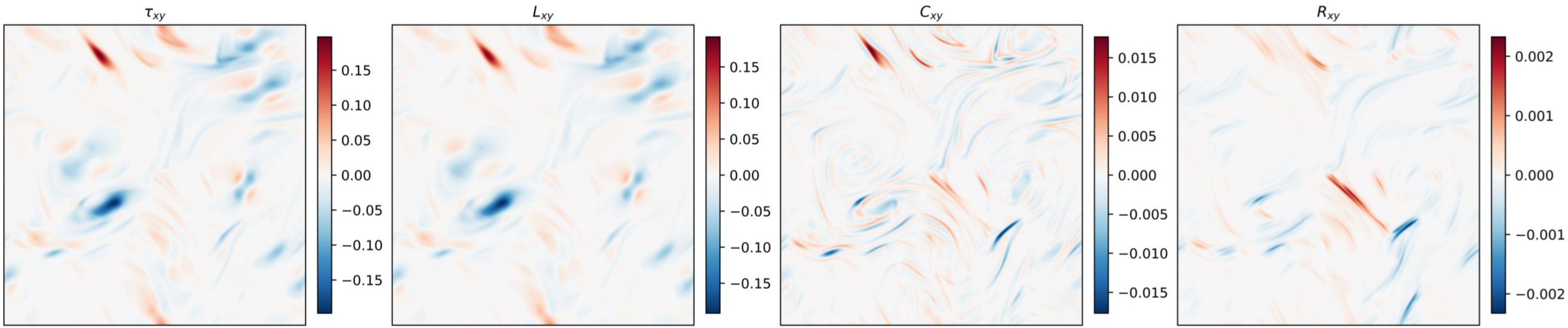


Freely decaying



Direct cascade

Learning the closure term



Constitutive relation for SGS stress tensor inferred from data:

$$\tau_{ij}(\bar{u}_i, R_{ij}) = c_1(\nabla_k \bar{u}_i)\left(\nabla_k \bar{u}_j\right) + c_2(\nabla_k \nabla_l \bar{u}_i)\left(\nabla_k \nabla_l \bar{u}_j\right) + R_{ij}$$

What is the relation between *microscopic* and *macroscopic* parameters $c_n(\nu, \Delta, \ldots)$?

- Scaling
- Dimensional analysis
- Formal expansions

Moment Expansion

For a filter $G_\Delta(\boldsymbol{r})$ with finite moments:

$$\bar{\phi}(\boldsymbol{x}) = \int G_\Delta(\boldsymbol{r})\, \phi(\boldsymbol{x}-\boldsymbol{r}) d^{\mathrm{d}}r = \phi(\boldsymbol{x}) M_0 + \frac{1}{2} M_{ij} \partial_i \partial_j \phi(\boldsymbol{x}) + \frac{1}{24} M_{ijkl} \partial_i \partial_i \partial_i \partial_j \phi(\boldsymbol{x}) \ + \ \ldots$$

$$M_{i_1 i_2 \ldots i_n} = \int r_{i_1} r_{i_2} \cdots r_{i_n} G_\Delta(\boldsymbol{r}) d^d r$$

For a Gaussian filter

$$G_\Delta(\boldsymbol{r}) = \exp\left(-\frac{\boldsymbol{r}^2}{\sigma^2}\right), \qquad \sigma^2 = \frac{\Delta^2}{12}$$

…the SGS stress tensor can be derived *in continuum space*:

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j = \underbrace{\underbrace{\underbrace{\sigma^2 (\nabla_k \bar{u}_i)(\nabla_k \bar{u}_j)}_{L_{ij}} + \frac{\sigma^4}{2} (\nabla_m \nabla_k \bar{u}_i)(\nabla_m \nabla_k \bar{u}_j)}_{L_{ij} + C_{ij}} + \frac{\sigma^6}{3!} (\nabla_m \nabla_k \nabla_l \bar{u}_i)(\nabla_m \nabla_k \nabla_l \bar{u}_j)}_{L_{ij} + C_{ij} + R_{ij}} + \cdots$$

Moment Expansion

For a filter $G_\Delta(\boldsymbol{r})$ with finite moments:

$$\bar{\phi}(\boldsymbol{x}) = \int G_\Delta(\boldsymbol{r})\,\phi(\boldsymbol{x}-\boldsymbol{r})d^{\mathrm{d}}r = \phi(\boldsymbol{x})M_0 + \frac{1}{2}M_{ij}\partial_i\partial_j\phi(\boldsymbol{x}) + \frac{1}{24}M_{ijkl}\partial_i\partial_i\partial_i\partial_j\phi(\boldsymbol{x}) + \ldots$$

$$M_{i_1 i_2 \ldots i_n} = \int r_{i_1} r_{i_2} \cdots r_{i_n} G_\Delta(\boldsymbol{r})d^d r$$

For a Gaussian filter

$$G_\Delta(\boldsymbol{r}) = \exp\left(-\frac{\boldsymbol{r}^2}{\sigma^2}\right), \qquad \sigma^2 = \frac{\Delta^2}{12}$$

…have to *model* high orders *on a discrete computational grid*:

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i\bar{u}_j \approx \underbrace{\underbrace{\sigma^2(\nabla_k\bar{u}_i)(\nabla_k\,\bar{u}_j)}_{L_{ij}} + \frac{\sigma^4}{2}(\nabla_m\nabla_k\bar{u}_i)(\nabla_m\nabla_k\bar{u}_j)}_{L_{ij}+C_{ij}} + R_{ij}$$

Closing the system

Evolution equation for the closure variable (Reynolds stress) inferred from data:

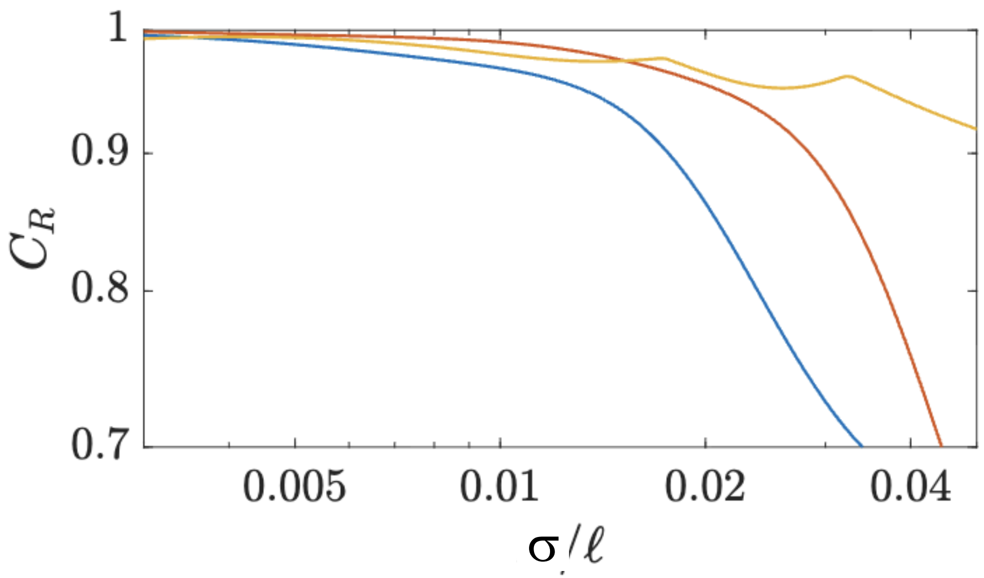
$$\partial_t R_{ij} + c_1 \bar{u}_k \nabla_k R_{ij} = c_2 (R_{ik} \nabla_k \bar{u}_j + R_{jk} \nabla_k \bar{u}_i) + c_3 \nabla^2 R_{ij} + c_4 R_{ij}$$

Dimensional analysis + scaling:

$$c_1 \approx 1, \qquad c_2 \approx +1,$$
$$c_3 \approx \nu, \qquad [c_4] = T^{-1}$$

Buckingham Pi theorem:

$$c_4 = \frac{\nu}{\sigma^2} f\left(\frac{\sigma\sqrt{E}}{\nu}, \frac{\sigma^2 I_1}{\nu}, \frac{\sigma^2 I_2}{\nu}, \ldots\right)$$



Tensor invariants:

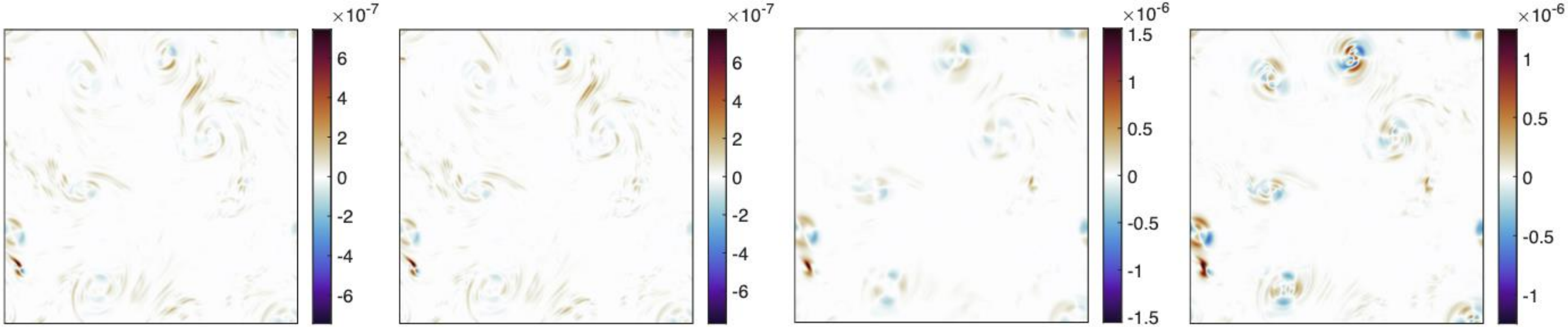
$$E = \tfrac{1}{2} \bar{u}_k \bar{u}_k, \qquad I_1 = \sqrt{\bar{S}_{ij} \bar{S}_{ij}}, \qquad I_2 = \sqrt{\bar{\Omega}_{ij} \bar{\Omega}_{ij}}$$
$$\bar{S}_{ij} = \tfrac{1}{2}(\nabla_i \bar{u}_j + \nabla_j \bar{u}_i), \qquad \bar{\Omega}_{ij} = \tfrac{1}{2}(\nabla_i \bar{u}_j - \nabla_j \bar{u}_i)$$

Regression output: $c_4 \approx -0.5 I_1$

Energy flux between scales

Energy flux:

$$\Pi = -\tau_{ij}\bar{S}_{ij}$$



DNS

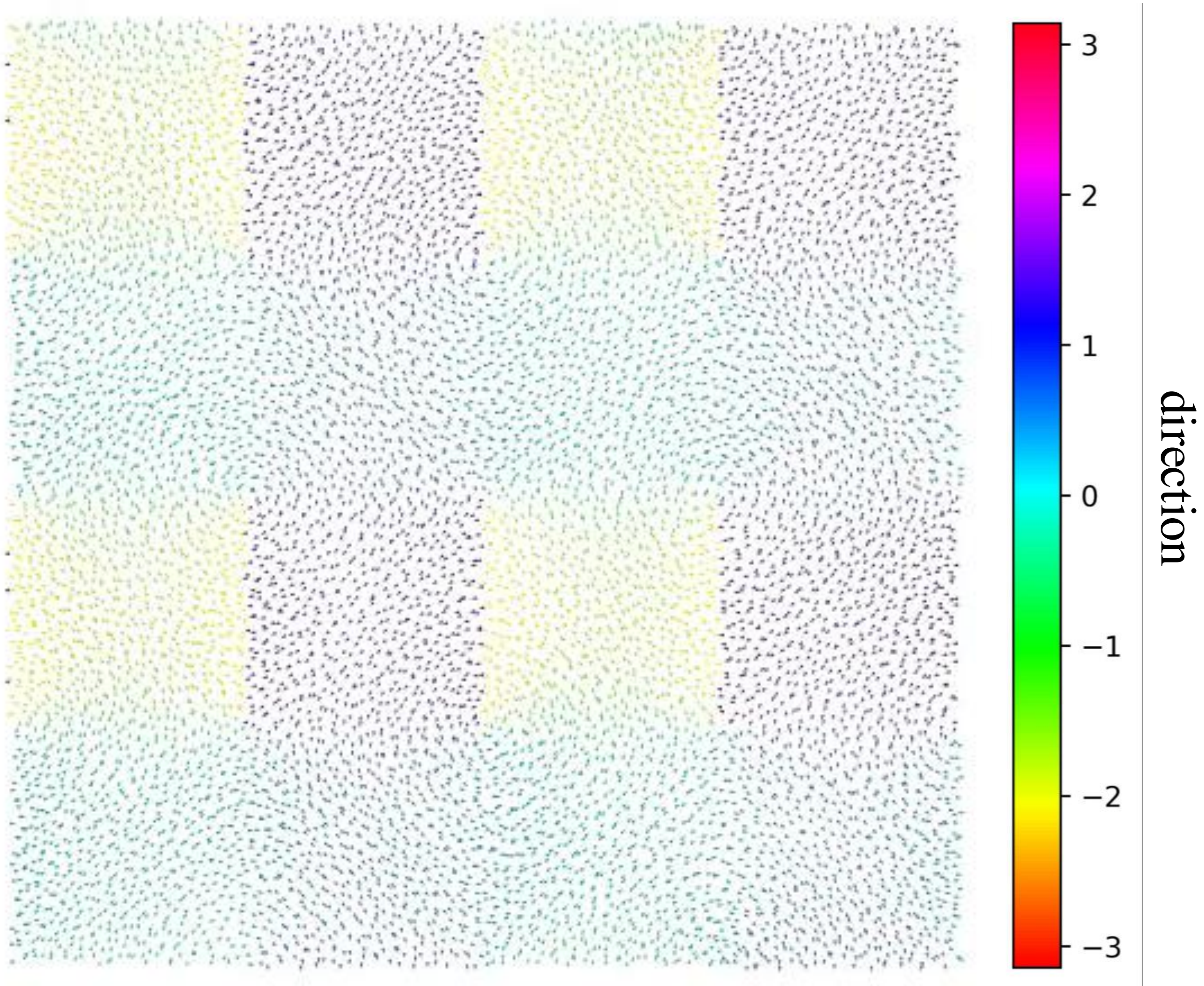
Model inferred from data

LES model (dynamic Smagorinsky)

LES model (dynamic mixed)

Coarse-graining *discrete* microscopic models

MD simulation of a compressible liquid



Spatial coarse-graining

Discrete data:

$$\mathbf{x}^{(n)}(t) \;\rightarrow\; \dot{\mathbf{x}}^{(n)}(t), \ddot{\mathbf{x}}^{(n)}(t), \ldots.$$

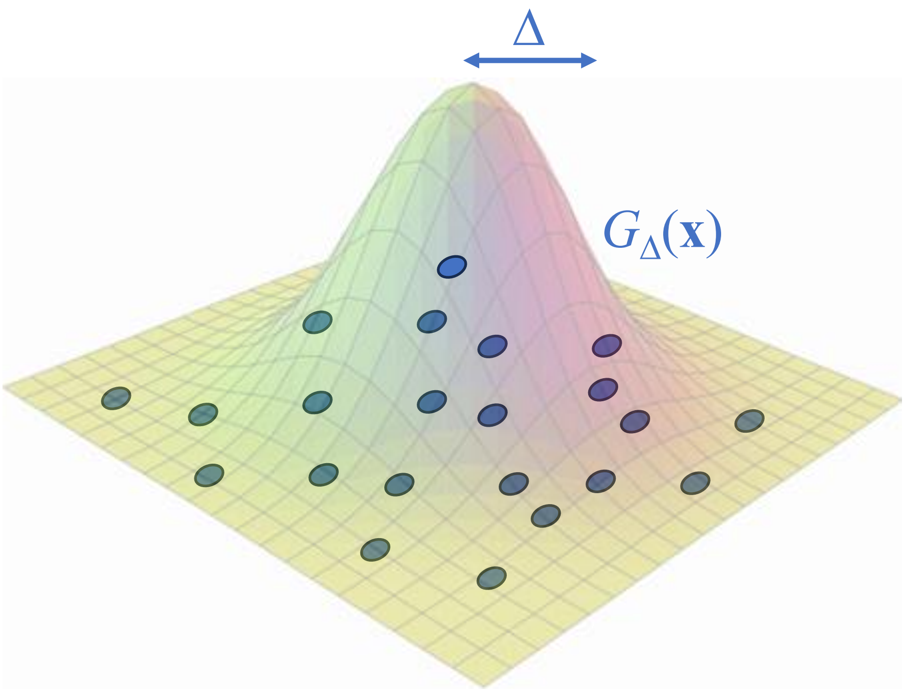
Kernel coarse-graining:

$$\rho[u](\mathbf{x},t) = \sum_n G_\Delta\left(\mathbf{x} - \mathbf{x}^{(n)}(t)\right) u^{(n)}(t)$$

Continuous fields:

$$\rho(\mathbf{x},t) = \sum_n G_\Delta(\mathbf{x} - \mathbf{x}^{(n)}(t))$$

$$\rho[v_i](\mathbf{x},t) = \sum_n G_\Delta\left(\mathbf{x} - \mathbf{x}^{(n)}(t)\right) v_i^{(n)}(t)$$



Spatial coarse-graining

Discrete data:

$$\mathbf{x}^{(n)}(t) \;\rightarrow\; \dot{\mathbf{x}}^{(n)}(t), \ddot{\mathbf{x}}^{(n)}(t), \ldots.$$

⇩

Kernel coarse-graining:

$$\rho[u](\mathbf{x}, t) = \sum_n G_\Delta\left(\mathbf{x} - \mathbf{x}^{(n)}(t)\right) u^{(n)}(t)$$

⇩

Continuous fields:

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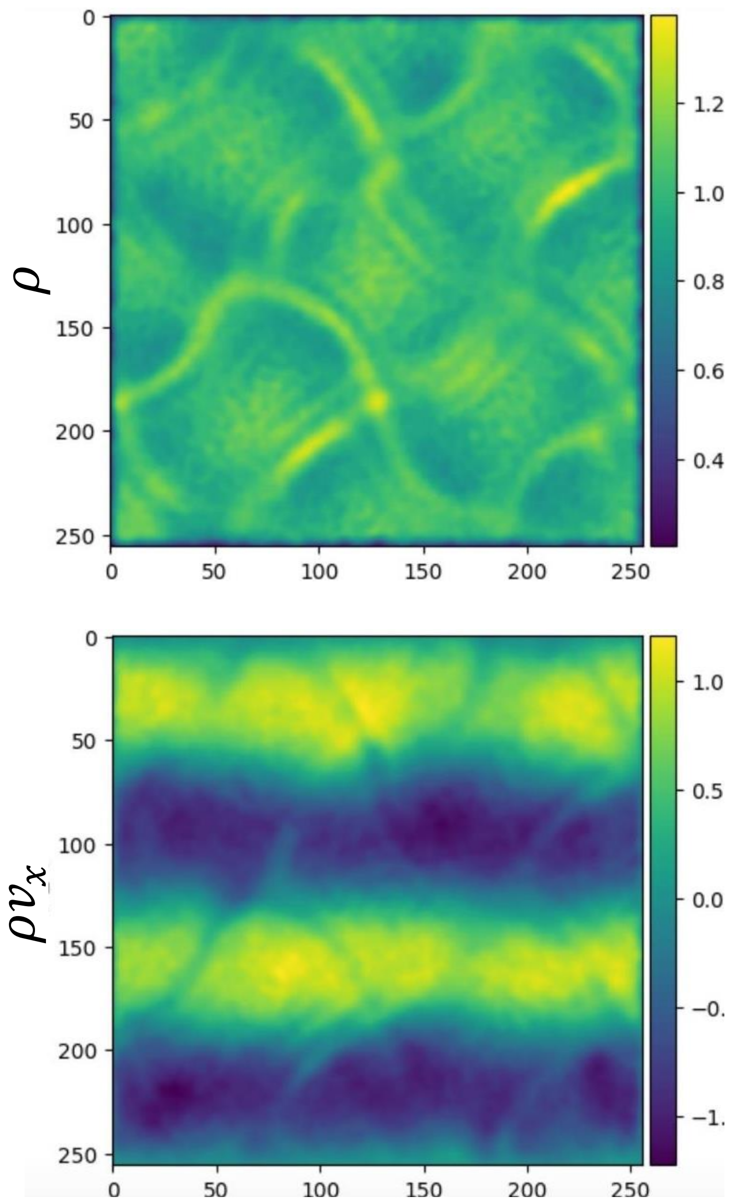


Inferred equations for an athermal liquid

eqn. ID	sublibrary	equation
(a)	rank 0, $\mathcal{C} = 3$	$\partial_t \rho + \partial_\alpha \rho[v_\alpha] = 0$
(b)	rank 0, $\mathcal{C} = 4$	$-0.996 \cdot \rho \cdot \partial_\alpha^2 \rho + 0.268 \cdot \rho \cdot \partial_t^2 \rho + \partial_\alpha^2 \rho - 0.27 \cdot \partial_t^2 \rho = 0$
(c)	rank 1, $\mathcal{C} = 4$	$-0.997 \cdot \rho \cdot \partial_\alpha \rho - 0.191 \cdot \rho \cdot \partial_t \rho[v_\alpha] + \partial_\alpha \rho + 0.192 \cdot \partial_t \rho[v_\alpha] = 0$
(d)	rank 0, $\mathcal{C} = 5$	$0.714 \cdot \rho - 0.709 \cdot \rho \cdot \rho + \rho \cdot \rho[v_\alpha \cdot v_\alpha] - 0.992 \cdot \rho[v_\alpha \cdot v_\alpha] = 0$
(e)	rank 0, $\mathcal{C} = 5$	$\partial_\alpha^2 \rho + 3.46 \times 10^{-5} \cdot \partial_\alpha^2 \partial_\beta^2 \rho - 0.167 \cdot \partial_t^2 \rho + 0.162 \cdot \partial_\alpha \partial_\beta \rho[v_\alpha \cdot v_\beta] = 0$
(f)	rank 1, $\mathcal{C} = 5$	$-\rho \cdot \partial_\alpha \rho + \partial_\alpha \rho = 0$
(g)	rank 1, $\mathcal{C} = 5$	$\rho \cdot \rho[v_\alpha] - 0.727 \cdot \rho \cdot \rho[v_\alpha \cdot v_\beta \cdot v_\beta] - 0.997 \cdot \rho[v_\alpha] + 0.718 \cdot \rho[v_\alpha \cdot v_\beta \cdot v_\beta] = 0$
(h)	rank 1, $\mathcal{C} = 5$	$\partial_\alpha \rho + 4.33 \times 10^{-5} \cdot \partial_\alpha \partial_\beta^2 \rho + 0.158 \cdot \partial_t \rho[v_\alpha] + 0.16 \cdot \partial_\beta \rho[v_\alpha \cdot v_\beta] = 0$
(i)	rank 2 STF, $\mathcal{C} = 5$	$\mathrm{STF}\big[-0.5 \cdot \partial_\gamma^2 \rho[v_\alpha \cdot v_\beta] + \partial_\alpha \partial_\gamma \rho[v_\beta \cdot v_\gamma] - 0.5 \cdot \partial_\alpha \partial_\beta \rho[v_\gamma \cdot v_\gamma]\big] = 0$

Continuity (mass conservation)

Lighthill's equation or aeroacoustics

Momentum balance

Gurevich (2025)

Inferred equations for an athermal liquid

eqn. ID	sublibrary	equation
(a)	rank 0, $\mathcal{C}=3$	$\partial_t \rho + \partial_\alpha \rho[v_\alpha] = 0$
(b)	rank 0, $\mathcal{C}=4$	$-0.996 \cdot \rho \cdot \partial_\alpha^2 \rho + 0.268 \cdot \rho \cdot \partial_t^2 \rho + \partial_\alpha^2 \rho - 0.27 \cdot \partial_t^2 \rho = 0$
(c)	rank 1, $\mathcal{C}=4$	$-0.997 \cdot \rho \cdot \partial_\alpha \rho - 0.191 \cdot \rho \cdot \partial_t \rho[v_\alpha] + \partial_\alpha \rho + 0.192 \cdot \partial_t \rho[v_\alpha] = 0$
(d)	rank 0, $\mathcal{C}=5$	$0.714 \cdot \rho - 0.709 \cdot \rho \cdot \rho + \rho \cdot \rho[v_\alpha \cdot v_\alpha] - 0.992 \cdot \rho[v_\alpha \cdot v_\alpha] = 0$
(e)	rank 0, $\mathcal{C}=5$	$\partial_\alpha^2 \rho + 3.46 \times 10^{-5} \cdot \partial_\alpha^2 \partial_\beta^2 \rho - 0.167 \cdot \partial_t^2 \rho + 0.162 \cdot \partial_\alpha \partial_\beta \rho[v_\alpha \cdot v_\beta] = 0$
(f)	rank 1, $\mathcal{C}=5$	$-\rho \cdot \partial_\alpha \rho + \partial_\alpha \rho = 0$
(g)	rank 1, $\mathcal{C}=5$	$\rho \cdot \rho[v_\alpha] - 0.727 \cdot \rho \cdot \rho[v_\alpha \cdot v_\beta \cdot v_\beta] - 0.997 \cdot \rho[v_\alpha] + 0.718 \cdot \rho[v_\alpha \cdot v_\beta \cdot v_\beta] = 0$
(h)	rank 1, $\mathcal{C}=5$	$\partial_\alpha \rho + 4.33 \times 10^{-5} \cdot \partial_\alpha \partial_\beta^2 \rho + 0.158 \cdot \partial_t \rho[v_\alpha] + 0.16 \cdot \partial_\beta \rho[v_\alpha \cdot v_\beta] = 0$
(i)	rank 2 STF, $\mathcal{C}=5$	$\mathrm{STF}\big[-0.5 \cdot \partial_\gamma^2 \rho[v_\alpha \cdot v_\beta] + \partial_\alpha \partial_\gamma \rho[v_\beta \cdot v_\gamma] - 0.5 \cdot \partial_\alpha \partial_\beta \rho[v_\gamma \cdot v_\gamma]\big] = 0$

Spurious relations:

$$(1-\rho) f\big(\rho, \rho[v_\alpha], \rho[v_\alpha v_\beta]\big) = 0$$

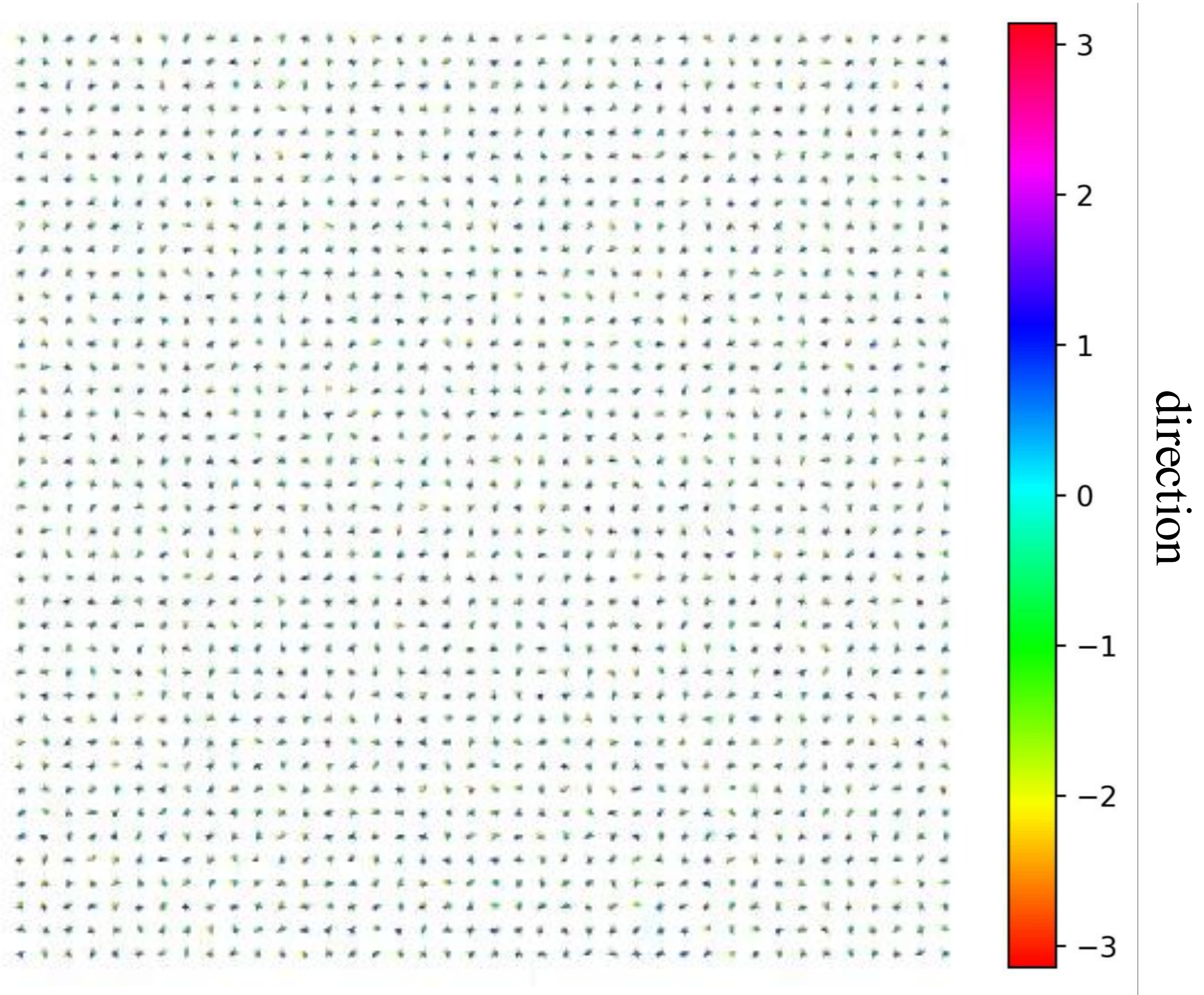
$$\Downarrow$$

Incorrect choice of variables:

$$\rho \to \bar{\rho}, \rho'$$

2D indentity

MD simulation of low-T argon (Lennard-Jones potential)



Spatio-*temporal* coarse-graining for "thermal" data

Temporal filtering:

$$\mathbf{x}^{(n)}(t) \;\rightarrow\; \bar{\mathbf{x}}^{(n)}(t), \mathbf{x}'^{(n)}(t), \ldots.$$

⇩

Spatial coarse-graining:

$$\rho[u](\mathbf{x},t) = \sum_n G_\Delta\left(\mathbf{x} - \bar{\mathbf{x}}^{(n)}(t)\right) u^{(n)}(t)$$

⇩

Continuous fields:

$$\rho(\mathbf{x},t) = \sum_n G_\Delta(\mathbf{x} - \bar{\mathbf{x}}^{(n)}(t))$$

Mass density

$$\rho[\bar{v}_i](\mathbf{x},t) = \sum_n G_\Delta\left(\mathbf{x} - \bar{\mathbf{x}}^{(n)}(t)\right) \bar{v}_i^{(n)}(t)$$

Momentum density

$$\rho[\overline{v_i' v_j'}](\mathbf{x},t) = \sum_n G_\Delta\left(\mathbf{x} - \bar{\mathbf{x}}^{(n)}(t)\right) \overline{v_i'^{(n)}(t) v_j'^{(n)}(t)}$$

Stresses & internal energy density

Chapman-Enskog theory:

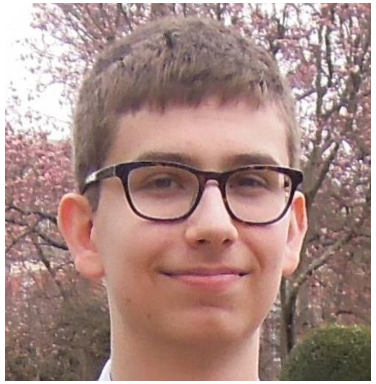
$$n = \int f(\mathbf{x},\mathbf{v})d\mathbf{v}$$

$$nv = \int \mathbf{v}f(\mathbf{x},\mathbf{v})d\mathbf{v}$$

$$3k_B nT = \int mv^2 f(\mathbf{x},\mathbf{v})d\mathbf{v}$$

(requires small Knudsen number and thermodynamic equilibrium)

Thank you!



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pySPIDER: https://github.com/sibirica/PySPIDER