Learning reduced dynamics of turbulent flows

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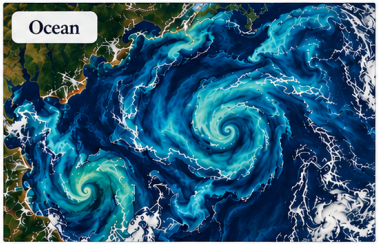
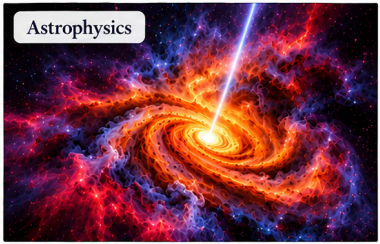
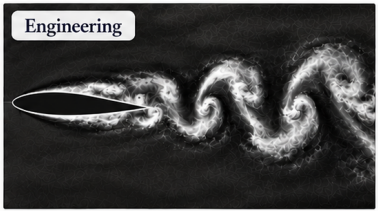
Turbulence: ubiquitous and multiscale







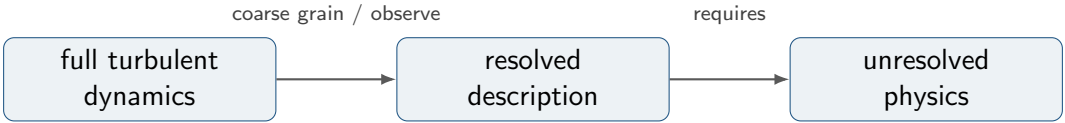






multiscale | nonlinear | chaotic | intermittent | mixing | far from equilibrium

Turbulence beyond resolution



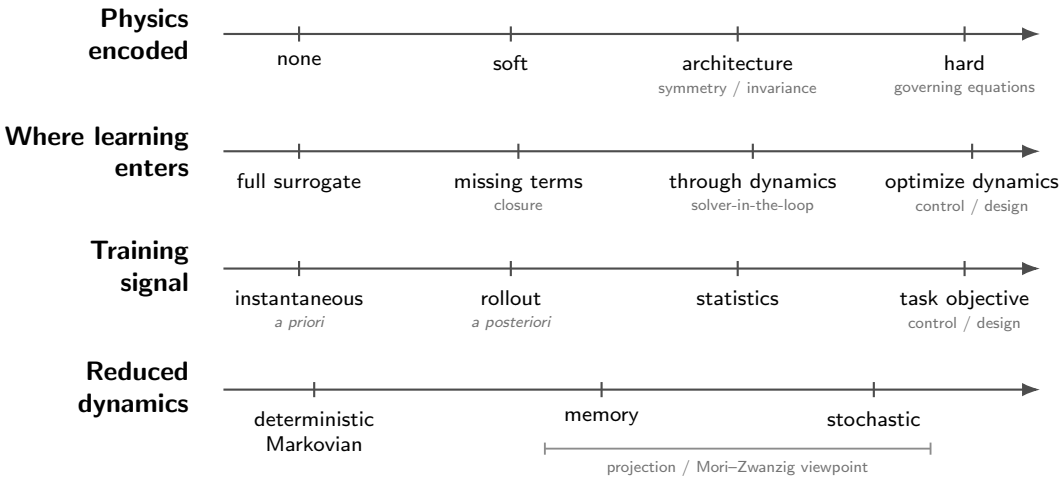
When degrees of freedom are removed, their effect must be modelled.

What is lost when we reduce a turbulent system?

closure	memory	fluctuations	correlations
unresolved cascade and subgrid transfer	multiscale and multitime history dependence	intermittency and departure from self-similarity	non-trivial space–time and cross-scale correlations

resolved variables are usually **not** a closed deterministic Markovian system

A design space for scientific machine learning



Two reductions of the same turbulent system

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{f}, \qquad \nabla\cdot\mathbf{u} = 0, \qquad \mathrm{Re} = \frac{UL}{\nu} \gg 1.$$

Eulerian view

$$\mathbf{u}(\mathbf{x},t) \longrightarrow \bar{\mathbf{u}}(\mathbf{x},t)$$

Question

Can we learn the effect of unresolved scales on resolved fields?

Lagrangian view

$$\mathbf{u}(\mathbf{x},t) \longrightarrow \{\mathbf{x}_i(t), \mathbf{v}_i(t)\}_{i=1}^{N_p}$$

Question

Can we learn closed particle dynamics after removing the field?

Talk structure

Eulerian closures

shell models

buoyancy-driven turbulence

Smart Lagrangian agents

active particles

flow control

Lagrangian reduced dynamics

memory
symmetry

multi-particle statistics

Eulerian closure

Motivation

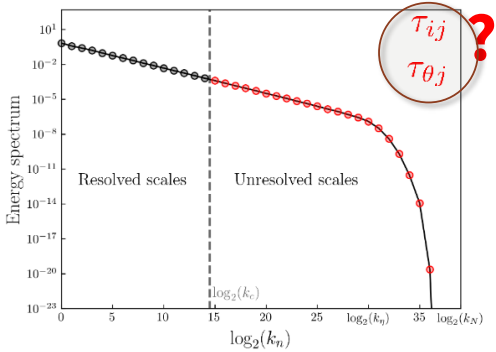
3D turbulence

Modeling

Large Eddy Simulations (LES)

$$\#_{DOF} \sim Re^{9/4}$$

!!



Can we learn a closure model from data?

Closure problem

full field $\mathbf{u}$ $\xrightarrow{\text{filter / truncate}}$ $\bar{\mathbf{u}}$ $+$ missing subgrid physics

$$\partial_t \bar{\mathbf{u}} = \underbrace{\mathcal{N}(\bar{\mathbf{u}})}_{\text{resolved physics}} + \underbrace{\mathcal{C}_\theta(\bar{\mathbf{u}})}_{\text{learned closure}}$$

We keep the equations for the resolved field and learn only the terms created by coarse-graining.

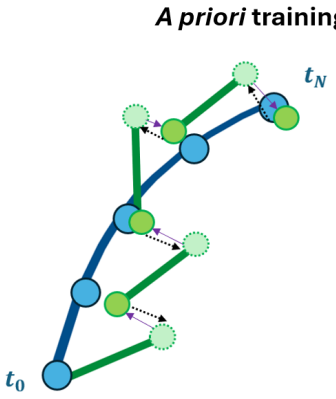
Solver-in-the-loop: pictorial view

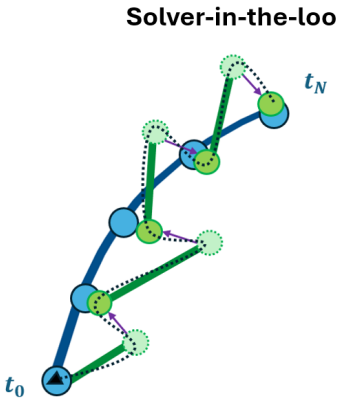
GROUND TRUTH

LES

NN CORRECTION

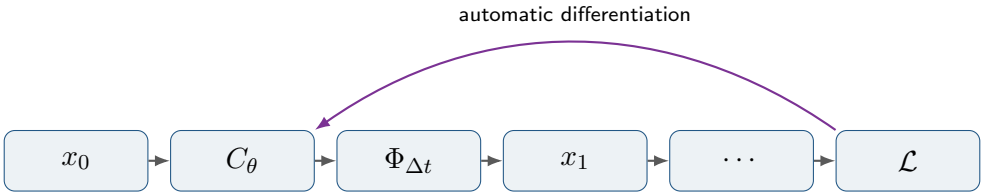
BACKPROP





Learning through the dynamics (solver-in-the-loop)

$$x_{n+1} = \Phi_{\Delta t}\left(x_n, C_\theta(x_n)\right)$$



The neural network is optimized according to its effect on the evolution, not only according to an instantaneous target.

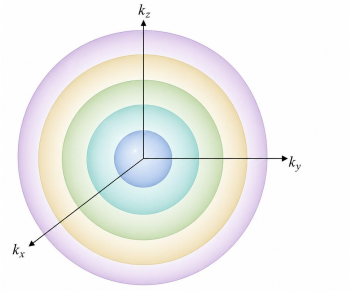
Research Questions

Can we improve subgrid scale closure in LES by using ML-based solver-in-the-loop / differentiable unrolled training ?

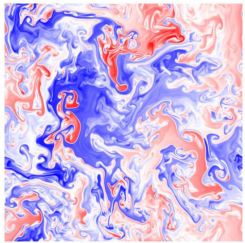
- Does it improve upon phenomological closures ? And data-driven ones ?
- Can we have an unconditionally stable model ?
- Can we reproduce statistical quantities of interest within error bars? (e.g. flatness, Eulerian and Lagrangian structure functions, energy flux)
- What is the ideal time *in the loop* before backpropagation ? How much do we gain from unrolling in time ?

Systems considered

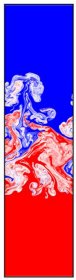
Shell models



Rayleigh-Bénard



Rayleigh-Taylor

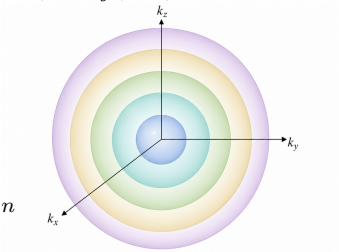


Shell Models

Navier–Stokes equation in Fourier Space:

$$\left(\frac{d}{dt} + \nu|\mathbf{k}|^2\right) u_j(\mathbf{k},t) = -ik_l P_{j\alpha}(\mathbf{k}) \sum_{\mathbf{k}'} u_\alpha(\mathbf{k}',t)\, u_l(\mathbf{k}-\mathbf{k}',t) + f_j(\mathbf{k},t)$$

- Sum over all wave vector triads: $\mathbf{k} + \mathbf{k}' = \mathbf{k}''$
- To solve numerically the dissipative scale: $\#\mathrm{DOF} \sim Re^{9/4}$



Dynamical system mimics the energy cascade:

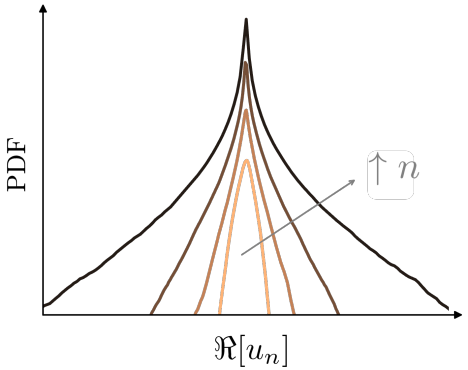
$$\{u_n \in \mathbb{C},\ n = 0, 1, \ldots, N\} \qquad k_n = k_0 2^n$$

$$\frac{du_n}{dt} = i\left(ak_n u^*_{n+1}u_{n+2} + bk_n u^*_{n-1}u_{n+1} - ck_{n-1}u_n u_{n-2}\right) - \nu k_n^2 u_n + f_n$$

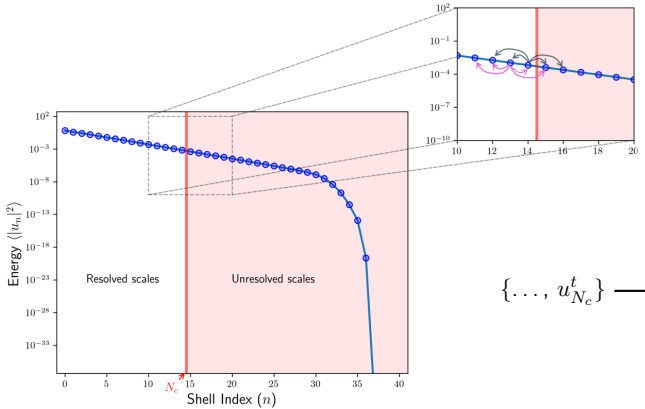
- Sum over the first and second neighbours
- To solve numerically the dissipative scale: $\#\mathrm{DOF} \sim \ln Re$

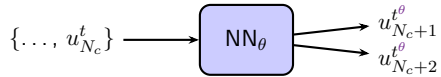
Shell Models

- Extreme events, strongly non-Gaussian statistics, anomalous scaling and multifractality



Methodology





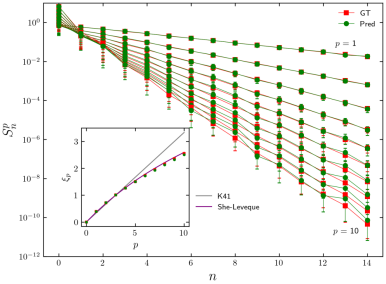
$$\frac{du_{N_c-1}}{dt} = i\left(ak_{N_c}u^{\theta}_{N_c+1}u^{*}_{N_c} + bk_{N_c-1}u_{N_c}u^{*}_{N_c-2} - ck_{N_c-2}u_{N_c-2}u_{N_c-3}\right) + D_{N_c-1} \tag{1}$$

$$\frac{du_{N_c}}{dt} = i\left(ak_{N_c+1}u^{\theta}_{N_c+2}u^{*^\theta}_{N_c+1} + bk_{N_c}u^{\theta}_{N_c+1}u^{*}_{N_c-1} - ck_{N_c-1}u_{N_c-1}u_{N_c-2}\right) + D_{N_c} \tag{2}$$

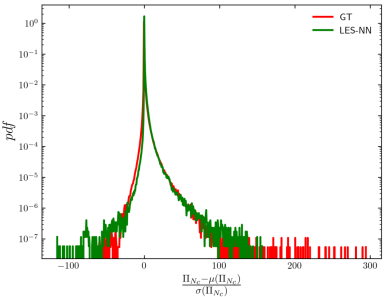
Results

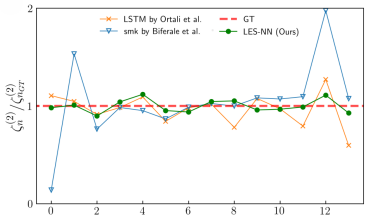
$S_n^p = \langle |u_n|^p \rangle$

$S_n^p \propto k_n^{-\xi_p}$



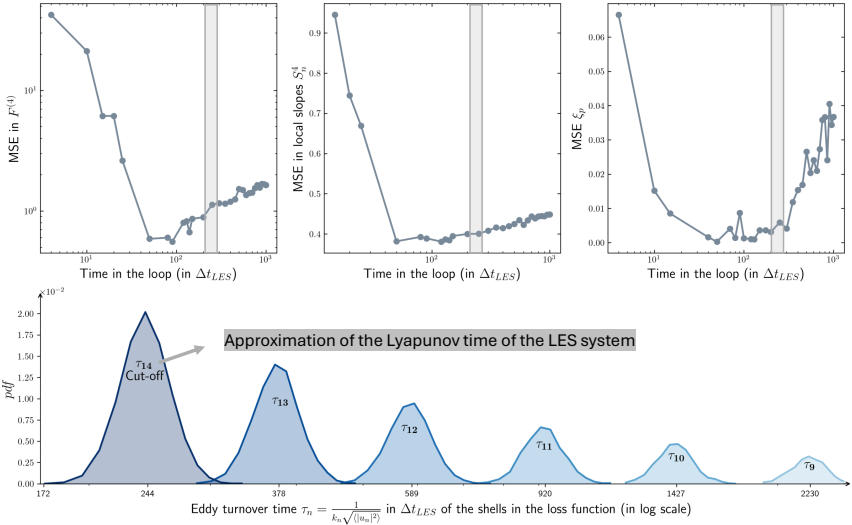
$\Pi_{N_c} = k_0 \lambda^{N_c} \left(\lambda a u_{N_c+2} u^*_{N_c+1} u^*_{N_c} + b u_{N_c+1} u^*_{N_c} u^*_{N_c-1} \right)$





$\zeta_n^{(p)} = \frac{\log[S_{n+1}^p - S_n^p]}{\log[\lambda]}$

Results - Optimal Time in the Loop



Conclusions

- Unrolled training with a differentiable solver provides improvements compared to an *a priori* static training paradigm.
- The optimal number of time steps in the loop before backprop is related to the time scale of the shells in the loss function.
- Using the solver-in-the-loop approach we are able to build a closure model for the shell models that is unconditionally stable and that reproduces with accuracy high order statistical moments.
- Ongoing work: extending to 2D/3D buoyancy driven turbulent flows (RB, RT).

Rayleigh–Bénard convection

$$\mathbf{x} \in \mathbb{T}^2, \qquad \omega, \theta, \psi \text{ periodic.}$$

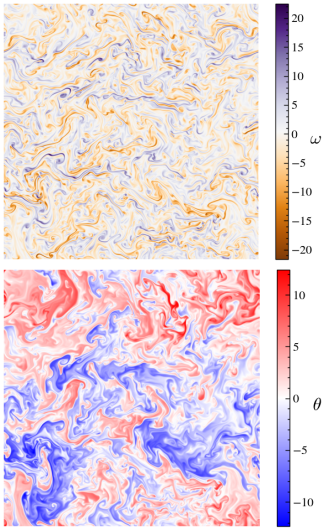
$$\frac{\partial \omega}{\partial t} + \mathbf{u}\cdot\nabla\omega = \mathrm{Pr}\ \nabla^2\omega + \mathrm{Pr}\ \mathrm{Ra}\ \frac{\partial \theta}{\partial x} - \mathrm{Rh}\,(\mathrm{Pr}\ \mathrm{Ra})^{1/2}\,\omega,$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u}\cdot\nabla\theta = \nabla^2\theta + \Gamma u_y,$$

$$\nabla^2\psi = -\,\omega,$$

$$\mathbf{u} = \big(\partial_y\psi,\ -\partial_x\psi\big).$$

$$\mathrm{Pr} = \frac{\nu}{\kappa}, \qquad \mathrm{Ra} = \frac{g\alpha\Gamma L^4}{\nu\kappa}, \qquad \mathrm{Rh} = \frac{\mu L^2}{\kappa(\mathrm{Pr}\,\mathrm{Ra})^{1/2}}.$$



Rayleigh–Bénard convection – LES

$$\mathbf{x} \in \mathbb{T}^2, \qquad \tilde{\omega}, \tilde{\theta}, \tilde{\psi} \text{ periodic.}$$

$$\frac{\partial \tilde{\omega}}{\partial t} + \tilde{\mathbf{u}}\cdot\nabla\tilde{\omega} = \mathrm{Pr}\ \nabla^2\tilde{\omega} + \mathrm{Pr}\ \mathrm{Ra}\frac{\partial \tilde{\theta}}{\partial x} - \mathrm{Rh}\,(\mathrm{Pr}\ \mathrm{Ra})^{1/2}\tilde{\omega} - \left[\nabla \times (\nabla\cdot\boldsymbol{\tau})\right]_z,$$

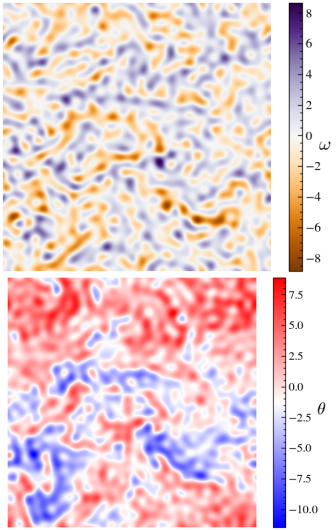
$$\frac{\partial \tilde{\theta}}{\partial t} + \tilde{\mathbf{u}}\cdot\nabla\tilde{\theta} = \nabla^2\tilde{\theta} + \Gamma\tilde{u}_y - \nabla\cdot\boldsymbol{\tau}^{\theta},$$

$$\nabla^2\tilde{\psi} = -\tilde{\omega},$$

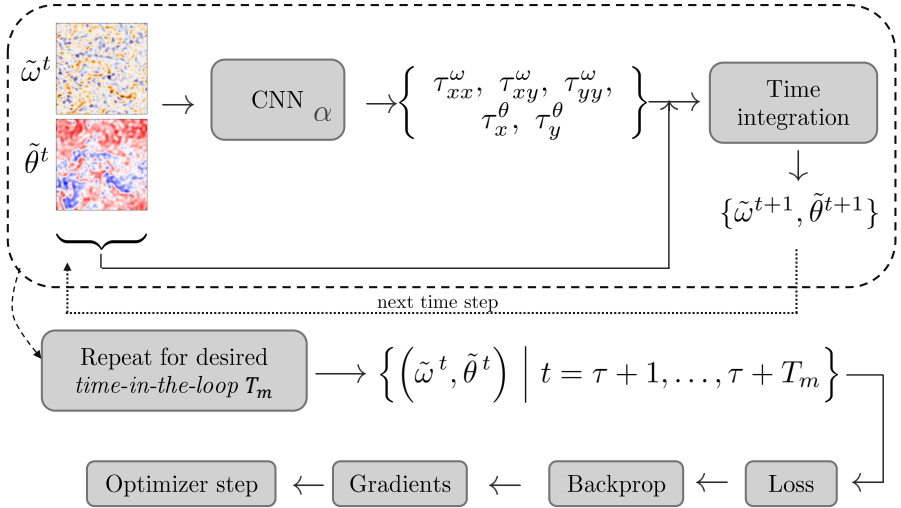
$$\tilde{\mathbf{u}} = \left(\partial_y\tilde{\psi},\ -\partial_x\tilde{\psi}\right).$$

Unclosed SGS terms:

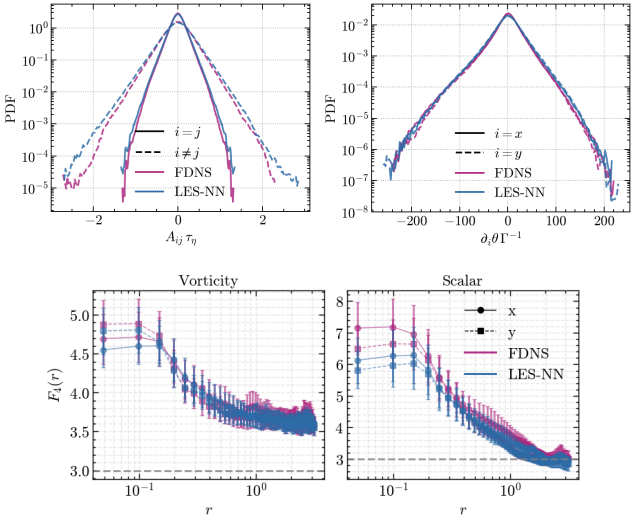
$$\tau_{ij} = \widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j, \qquad \tau_j^{\theta} = \widetilde{u_j\theta} - \tilde{u}_j\tilde{\theta}.$$



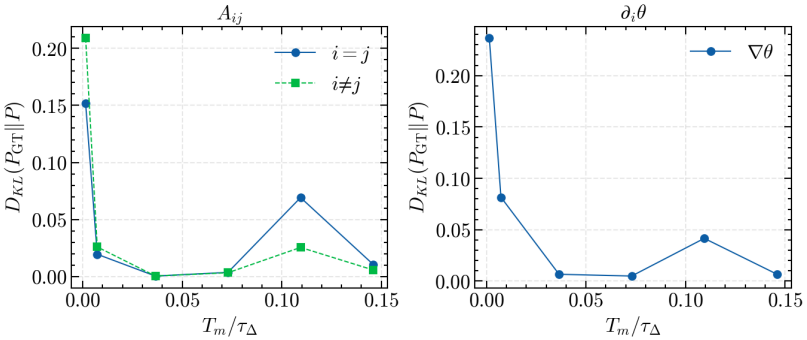
Methodology



Results


PDF
$A_{ij}\,\tau_\eta$
$i=j$
$i\neq j$
FDNS
LES-NN
PDF
$\partial_i\theta\,\Gamma^{-1}$
$i=x$
$i=y$
FDNS
LES-NN
Vorticity
Scalar
$F_4(r)$
r
x
y
FDNS
LES-NN

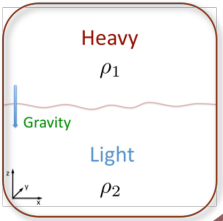
Results – optimal time-in-the-loop



Ongoing and future work

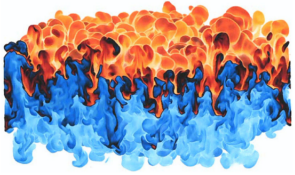
- Extend time in the loop study
- Extend to 3d
- Generalisation to higher Rayleigh numbers

Rayleigh–Taylor turbulence

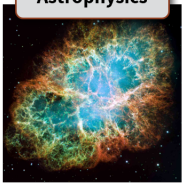


Rayleigh Taylor instability

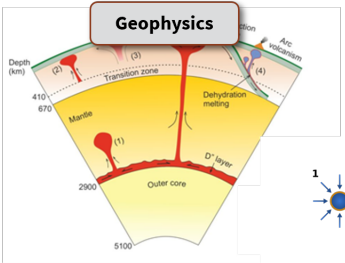
Livescu et al., Physica D (2021)



Astrophysics

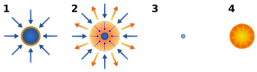


Geophysics



Tech devices





Relevant at different spatial and temporal scales

RT modeling problem

$$\boxed{N_{\mathrm{DOF}} \sim Re^{9/4}}$$

$$L(t) \sim t^2, \qquad U(t) \sim t$$

$$\boxed{Re(t) \sim \frac{U(t)L(t)}{\nu} \sim t^3}$$

RT: research directions and state of the art

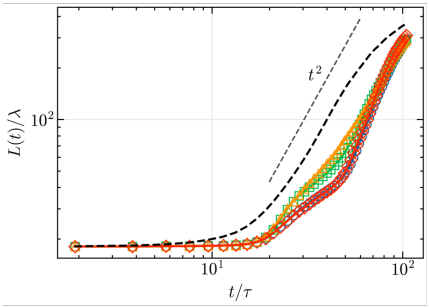
Research directions

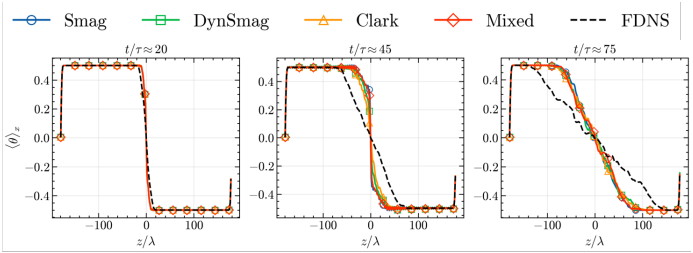
1. Large-scale dynamics
2. Generalization across regimes and retraining
3. Optimizing initial conditions for control of instability growth

State of the art

- **Eddy-viscosity models** $\rightarrow$ typically overdiffusive
- **Gradient-based models** $\rightarrow$ potentially unstable due to backscatter
- Need for **ad hoc tuning** of model parameters
- **No consensus** on a robust model for both **velocity and scalar SGS stresses**
- **Deep learning** provides a new route for learning closures, but *a priori* training has limitations in **stability, accuracy, and generalization**

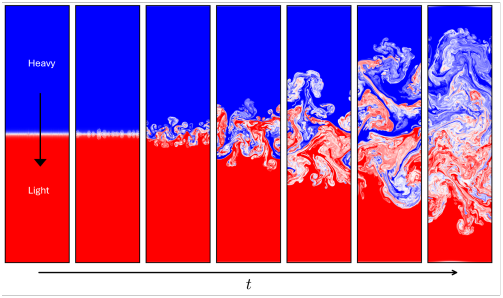
RT phenomenological results

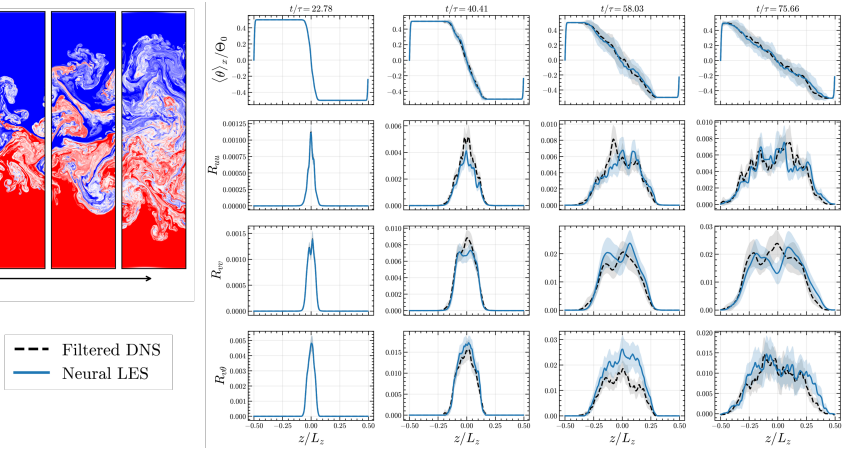




Conventional LES SGS models fail!

RT results


Heavy
Light
t


$t/\tau = 22.78$
$t/\tau = 40.41$
$t/\tau = 58.03$
$t/\tau = 75.66$
$\langle\hat{\theta}\rangle_z/\Theta_0$
R_{ww}
$R_{\theta\theta}$
$R_{w\theta}$
z/L_z
Filtered DNS
Neural LES

RT conclusions and ongoing work

Key Findings

- Able to reproduce large scale statistics
  - Mixing layer growth
  - Temperature profiles
  - Reynolds stresses and scalar fluxes

Open questions / ongoing work:

- Relevance of backscatter for large scale dynamics?
- Small scale statistics (structure functions)
- Optimal time-in-the-loop ($\tau_\eta \sim t^{-1}$)
- Generalization across the self-similar range
- IC optimization

detour into smart particles

How much can we control turbulence?

How much can we control turbulence?

- Can we alter the statistics of small scale turbulence? (Intermittency)

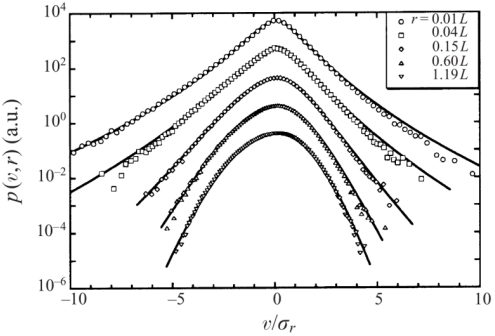


Figure: Renner et al., JFM (2001)

How much can we control turbulence?

- Can we alter the statistics of small scale turbulence? (Intermittency)
- How to affect the small scales?

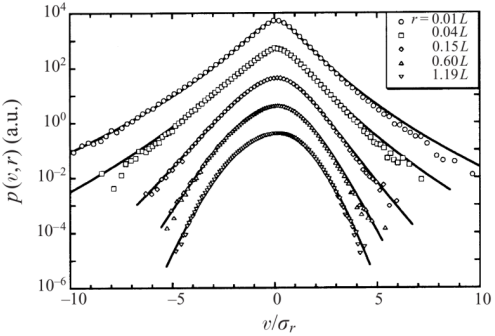


Figure: Renner et al., JFM (2001)

How much can we control turbulence?

- Can we alter the statistics of small scale turbulence? (Intermittency)
- How to affect the small scales?
- Small scale universality ... how to avoid this?

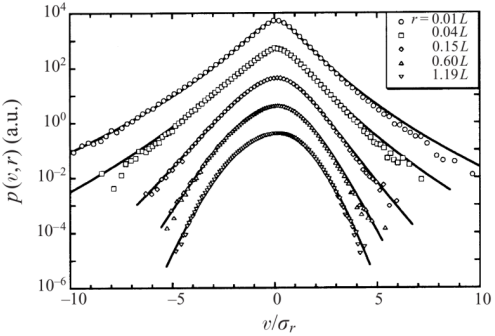


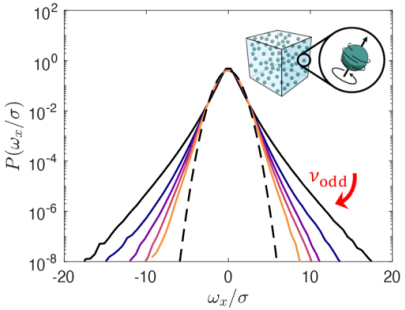
Figure: Renner et al., JFM (2001)

How much can we control turbulence?

How much can we control turbulence?

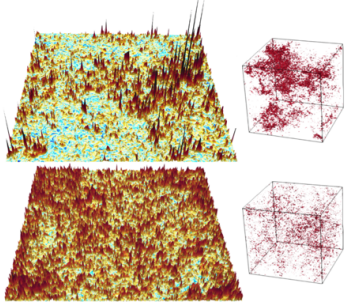
- Directly modify the small scales. How? (odd viscosity? Artificial tweaking of NSE?)

Chen, PRL (2024)



$$D_t \boldsymbol{u} = -\nabla P + \nu \Delta \boldsymbol{u} + \nu_{\rm odd} \hat{\boldsymbol{e}}_z \times \Delta \boldsymbol{u} + \boldsymbol{f}$$

Buzzicotti, PRL (2020)

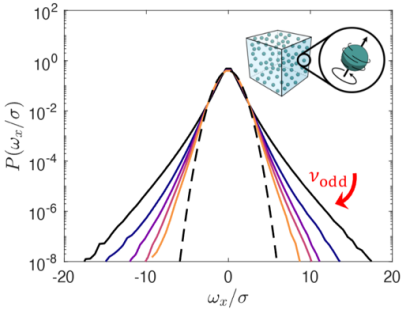


$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} P + \nu \Delta \boldsymbol{u} + \mathbf{F} - \boldsymbol{f}_c$$

How much can we control turbulence?

- Directly modify the small scales. How? (odd viscosity? Artificial tweaking of NSE?)
- We need Lagrangian agents that preferentially sample important degrees of freedom: in the case of intermittency, vortex filaments!

Chen, PRL (2024)



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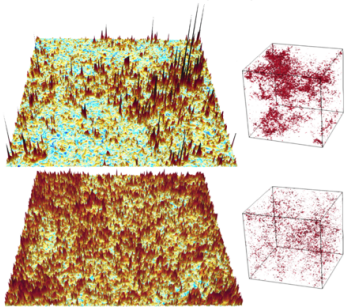

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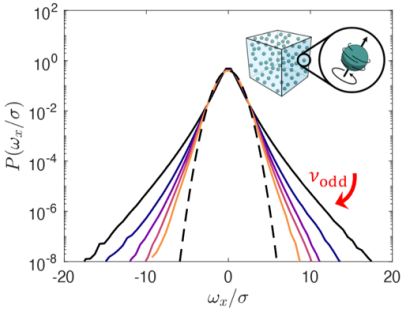
How much can we control turbulence?

- Directly modify the small scales. How? (odd viscosity? Artificial tweaking of NSE?)
- We need Lagrangian agents that preferentially sample important degrees of freedom: in the case of intermittency, vortex filaments!
- Light particles!

Chen, PRL (2024)



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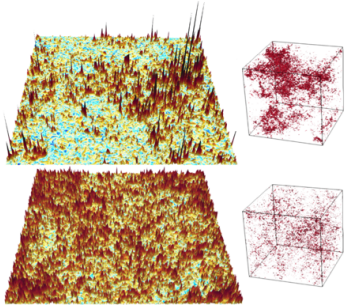

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$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} P + \nu \Delta \boldsymbol{u} + \mathbf{F} - \boldsymbol{f}_c$$

Governing equations

NSE:

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{f} + \mathbf{f}_p\,, \qquad \nabla\cdot\mathbf{u} = 0\,, \tag{3}$$

Particle phase (Maxey-Riley):

$$\frac{d\mathbf{X}}{dt} = \mathbf{V} + (\text{collisions}), \tag{4}$$

$$\frac{d\mathbf{V}}{dt} = \beta\frac{D\mathbf{u}}{Dt} - \frac{1}{\tau_p}(\mathbf{V}-\mathbf{u}) + \boldsymbol{f}_E, \tag{5}$$

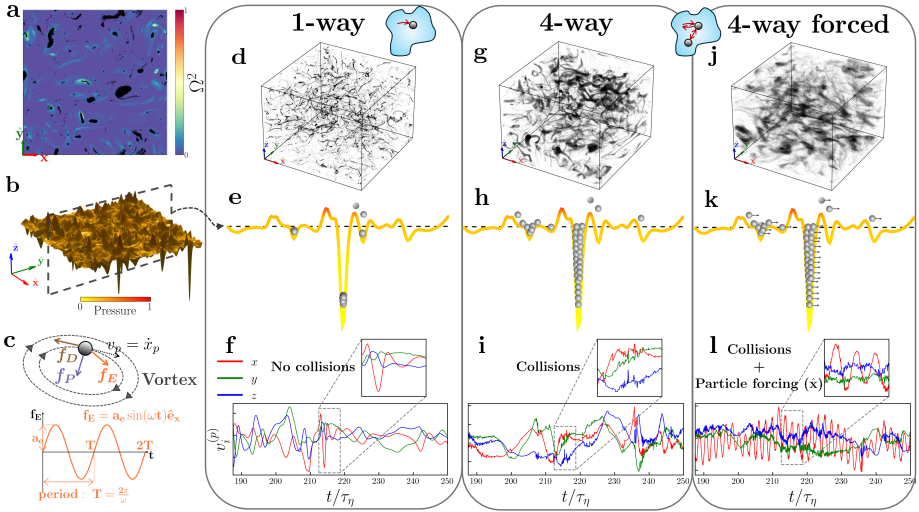
where $\beta = 3/(1+2\rho_p/\rho_f)$ (we take $\beta = 3$).
Particle feedback on the fluid:

$$\mathbf{f}_p(\mathbf{x},t) = \sum_i \left[\frac{D\mathbf{u}}{Dt} - \frac{\rho_p}{\rho_f}\frac{d\mathbf{V}_i}{dt} + \frac{3}{2\beta}f_E\right] \mathscr{V}_p\delta(\mathbf{x}-\mathbf{X}_i(t)), \tag{6}$$

External forcing acting on the particle:

$$f_E = a_e\sin(\omega t)\hat{\mathbf{e}}_x\,. \tag{7}$$

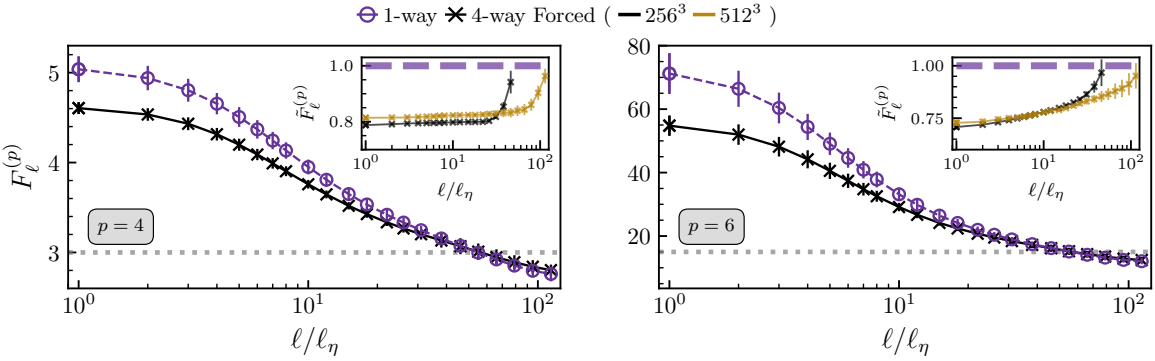
Problem setup



Intermittency reduction

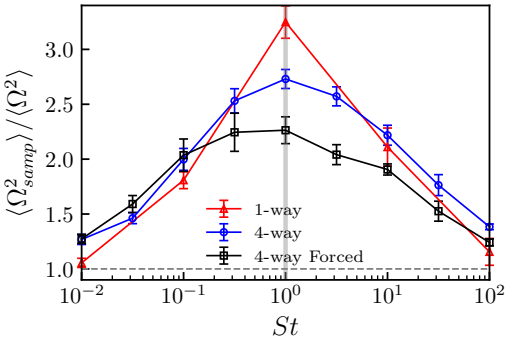
$$S_\ell^{(p)} \equiv \langle (\delta_\ell u)^p \rangle \qquad (8)$$

$$F_\ell^{(p)} = \frac{S_\ell^{(p)}}{\left(S_\ell^{(2)}\right)^{p/2}} \qquad (9)$$



$Re_\lambda = 87$ and $Re_\lambda = 168$, $\phi = 1\%$.

Differentiable control of turbulence



Not passive tracers:
smart agents embedded in the cascade.

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f} + \mathbf{f}_p$$

$$\dot{\mathbf{X}}_i = \mathbf{V}_i, \qquad \dot{\mathbf{V}}_i = \mathcal{F}_{\mathrm{MR}}(\mathbf{u}, \mathbf{X}_i, \mathbf{V}_i) + \pi_\theta(\mathbf{X}_i, \mathbf{V}_i, t)$$

$$\theta^\star = \arg\min_\theta \ \mathcal{L}\Big(\text{statistics of } \mathbf{u}_\theta\Big)$$

Backpropagate through the flow, then let particles modify it.

Lagrangian closure

Motivation – why Lagrangian turbulent transport?

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nu \nabla^2 \boldsymbol{u} + \boldsymbol{f},$$
$$\nabla \cdot \boldsymbol{u} = 0.$$

Passive tracers are the zero-inertia limit of particle dynamics:

$$\frac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{v}_i, \qquad \boldsymbol{v}_i(t) = \boldsymbol{u}(\boldsymbol{x}_i(t), t).$$

Classical route

Decades of Lagrangian turbulence modelling use phenomenological stochastic equations, e.g.

$$\mathrm{d}\boldsymbol{v} = \boldsymbol{A}(\boldsymbol{v}, t)\,\mathrm{d}t + \mathsf{B}(\boldsymbol{v}, t)\,\mathrm{d}\boldsymbol{W}_t,$$

with drift and noise chosen to reproduce selected statistics.

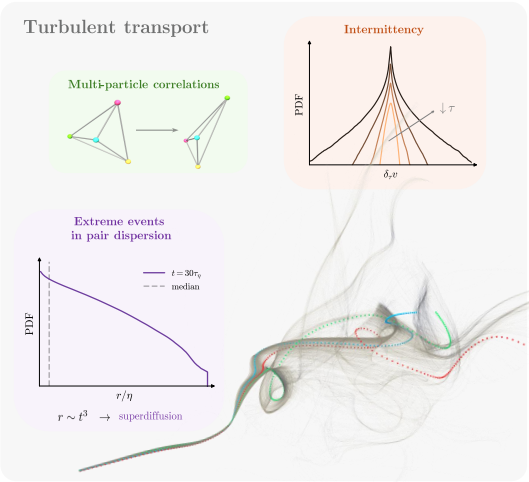
- Ocean drifters
- Pollutant dispersion
- Cloud droplets
- Sprays and combustion
- Microplastics / plankton

Problem setup

Particle trajectories are driven by a flow that is

- chaotic and multiscale,
- intermittent, with extreme acceleration events,
- spatially correlated, with non-trivial multi-particle statistics,
- expensive to resolve by DNS at large Reynolds numbers.

$\#_{\mathrm{DOF}}^{\mathrm{Eulerian}} \sim \mathrm{Re}^{9/4}$ in 3D turbulence $\Rightarrow$ need for reduced models of particle dynamics.



A compact puff is stretched, folded and dispersed by turbulence.

Problem setup – learning reduced particle dynamics

Given DNS trajectories of passive tracers,

$$\{\boldsymbol{x}_i^n, \boldsymbol{v}_i^n, \boldsymbol{a}_i^n\}_{i=1}^{N_p},$$

we want to learn a closed autoregressive model for the acceleration:

$$\widehat{\boldsymbol{a}}_i^n = \mathcal{K}_\theta\left(\{\boldsymbol{x}_j^n, \boldsymbol{v}_j^n\}_{j=1}^{N_p}, \text{history}\right)_i.$$

The learned acceleration is then rolled out as

$$\boldsymbol{v}_i^{n+1} = \boldsymbol{v}_i^n + \Delta t\, \widehat{\boldsymbol{a}}_i^n, \qquad \boldsymbol{x}_i^{n+1} = \boldsymbol{x}_i^n + \Delta t\, \boldsymbol{v}_i^n.$$



Key challenge

The model must capture temporal memory and multi-particle spatial correlations while preserving the symmetries of homogeneous isotropic turbulence.

Method – Mori–Zwanzig formalism

Given a high-dimensional state $\boldsymbol{p} \in \mathbb{R}^N$, we retain only a reduced set of observables

$$\boldsymbol{g}(\boldsymbol{p}) \in \mathbb{R}^M, \qquad M \ll N.$$

The Mori–Zwanzig formalism gives an exact non-Markovian Langevin equation:

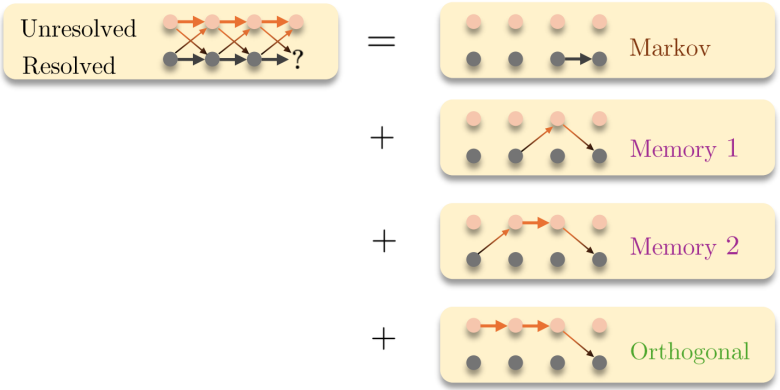
$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{g}(t) = \underbrace{\boldsymbol{M}(\boldsymbol{g}(t))}_{\text{Markovian}} - \underbrace{\int_0^t \boldsymbol{K}(t-s, \boldsymbol{g}(s))\,\mathrm{d}s}_{\text{memory}} + \underbrace{\boldsymbol{F}(t)}_{\text{orthogonal dynamics}} . \tag{10}$$

Projecting out unresolved degrees of freedom produces memory and residual forcing.

Method – discrete GLE

In discrete time, the generalized Langevin equation (GLE) motivates

$$\boldsymbol{g}_{n+1} = \boldsymbol{\Omega}_0(\boldsymbol{g}_n) + \sum_{k=1}^{n} \boldsymbol{\Omega}_k(\boldsymbol{g}_{n-k}) + \boldsymbol{W}_n. \tag{11}$$



Method – MZ applied to Lagrangian turbulence

$$\boldsymbol{g}_n = \{(\boldsymbol{x}_i^n, \boldsymbol{v}_i^n)\}_{i=1}^{N_p}\,. \tag{12}$$

$$\boldsymbol{a}_i^n = \sum_{k=0}^{K} \boldsymbol{\Omega}_\theta^{(k)} \left(\mathcal{G}^{\,n-ks}, \boldsymbol{v}^{\,n-ks}\right)_i, \tag{13}$$

$$\boldsymbol{v}_i^{n+1} = \boldsymbol{v}_i^n + \Delta t\, \boldsymbol{a}_i^n, \tag{14a}$$

$$\boldsymbol{x}_i^{n+1} = \boldsymbol{x}_i^n + \Delta t\, \boldsymbol{v}_i^n. \tag{14b}$$

Can we learn the memory kernels $\boldsymbol{\Omega}_\theta^{(k)}$ from data? And if so, what is the ideal architecture to do so applied to Lagrangian turbulence?

Symmetries to preserve in HIT

Let the learned MZ kernel map the particle state to accelerations,

$$\mathcal{K}_\theta : \{(\boldsymbol{x}_i, \boldsymbol{v}_i)\}_{i=1}^{N_p} \longmapsto \{\boldsymbol{a}_i\}_{i=1}^{N_p} .$$

Symmetry	**Transformation**	**Kernel response**
Translational invariance	$\boldsymbol{x}_i \mapsto \boldsymbol{x}_i + \boldsymbol{X}$	$\boldsymbol{a}_i \mapsto \boldsymbol{a}_i$
Galilean invariance	$\boldsymbol{v}_i \mapsto \boldsymbol{v}_i + \boldsymbol{V}$	$\boldsymbol{a}_i \mapsto \boldsymbol{a}_i$
$O(3)$-equivariance	$\boldsymbol{x}_i \mapsto \mathsf{Q}\boldsymbol{x}_i, \quad \boldsymbol{v}_i \mapsto \mathsf{Q}\boldsymbol{v}_i,$ $\mathsf{Q}^\top\mathsf{Q} = I, \ \det \mathsf{Q} = \pm 1$	$\boldsymbol{a}_i \mapsto \mathsf{Q}\boldsymbol{a}_i$
Permutation equivariance	$(\boldsymbol{x}_i, \boldsymbol{v}_i) \mapsto \left(\boldsymbol{x}_{\pi(i)}, \boldsymbol{v}_{\pi(i)}\right)$	$\boldsymbol{a}_i \mapsto \boldsymbol{a}_{\pi(i)}$

Consequence

The kernels should depend only on relative particle configurations and velocities, while their vector outputs must transform as physical accelerations.

Method – Message passing graph neural networks

A graph is defined as

$$\mathcal{G} = (\mathcal{V}, \mathcal{E}),$$

where nodes $i \in \mathcal{V}$ carry features $\boldsymbol{h}_i$, and edges $(i, j) \in \mathcal{E}$ encode local neighbourhoods.
A message-passing layer has the generic form

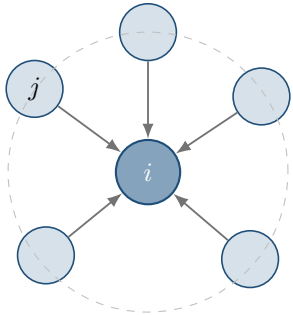
$$\boldsymbol{m}_{ij}^{(\ell)} = \phi_m^{(\ell)} \left(\boldsymbol{h}_i^{(\ell)}, \boldsymbol{h}_j^{(\ell)}, \boldsymbol{e}_{ij} \right),$$

$$\boldsymbol{M}_i^{(\ell)} = \underset{j \in \mathcal{N}(i)}{\mathrm{AGG}} \, \boldsymbol{m}_{ij}^{(\ell)},$$

$$\boldsymbol{h}_i^{(\ell+1)} = \phi_h^{(\ell)} \left(\boldsymbol{h}_i^{(\ell)}, \boldsymbol{M}_i^{(\ell)} \right).$$

After N_{MP} layers, a readout map gives the node prediction:

$$\widehat{\boldsymbol{y}}_i = \phi_{\mathrm{out}} \left(\boldsymbol{h}_i^{(N_{\mathrm{MP}})} \right).$$



local neighbourhood $\mathcal{N}(i)$

same message function on every edge
$\Rightarrow$ permutation equivariance

Method – Message passing graph neural networks: our approach

We model acceleration as a finite-memory sum of equivariant graph operators:

$$\boldsymbol{a}_i^n = \sum_{k=0}^{K} \boldsymbol{\Omega}_\theta^{(k)} \left(\mathcal{G}^{\,n-ks}, \boldsymbol{v}^{\,n-ks} \right)_i .$$

Radius graph

For each memory lag k, particles are nodes:

$$\mathcal{V} = \{1, \dots, N_p\}.$$

Edges are built by radius search:

$$(i,j) \in \mathcal{E}^{\,n-ks} \quad \Longleftrightarrow \quad 0 < \|\boldsymbol{r}_{ij}^{\,n-ks}\| < r_c,$$

with relative features

$$\boldsymbol{r}_{ij} = \boldsymbol{x}_j - \boldsymbol{x}_i, \qquad \boldsymbol{v}_{ij} = \boldsymbol{v}_j - \boldsymbol{v}_i.$$

Node update

$$\boldsymbol{h}_i^{(\ell+1)} = \boldsymbol{h}_i^{(\ell)} + \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} \boldsymbol{m}_{ij}^{(\ell)}.$$

$O(3)$-equivariant message

Define

$$\boldsymbol{h}_{ij}^{(\ell)} = \boldsymbol{h}_j^{(\ell)} - \boldsymbol{h}_i^{(\ell)}, \qquad \boldsymbol{h}_i^{(0)} = \mathbf{0}.$$

Scalar invariants:

$$s_{ij}^{(\ell)} = \big(\|\boldsymbol{r}_{ij}\|^2,\ \boldsymbol{r}_{ij}\cdot\boldsymbol{v}_{ij},\ \|\boldsymbol{v}_{ij}\|^2,\ \boldsymbol{r}_{ij}\cdot\boldsymbol{h}_{ij}^{(\ell)},\ \boldsymbol{v}_{ij}\cdot\boldsymbol{h}_{ij}^{(\ell)},\ \|\boldsymbol{h}_{ij}^{(\ell)}\|^2 \big).$$

Shared MLP:

$$\left(\alpha_{ij}^{(\ell)}, \beta_{ij}^{(\ell)}, \gamma_{ij}^{(\ell)} \right) = \phi_\ell \left(s_{ij}^{(\ell)} \right).$$

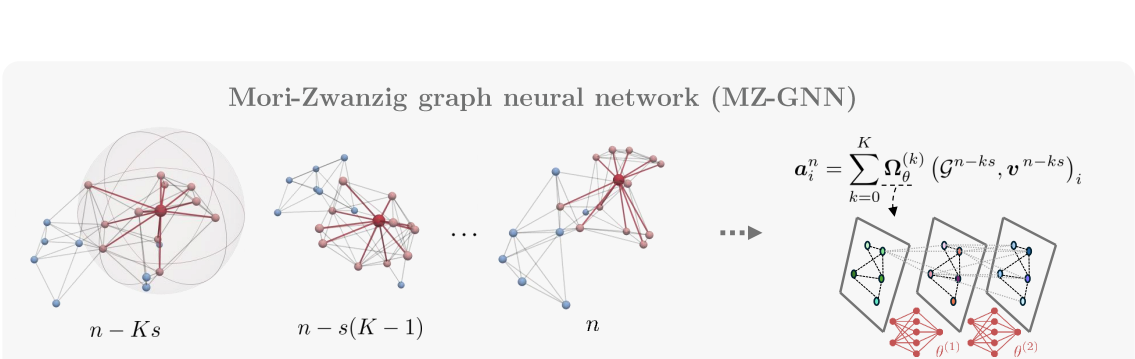
Vector message:

$$\boldsymbol{m}_{ij}^{(\ell)} = \alpha_{ij}^{(\ell)} \boldsymbol{r}_{ij} + \beta_{ij}^{(\ell)} \boldsymbol{v}_{ij} + \gamma_{ij}^{(\ell)} \boldsymbol{h}_{ij}^{(\ell)}.$$

$$\boldsymbol{a}_i^{(k)} = \boldsymbol{h}_i^{(N_{\mathrm{MP}})}.$$

Relative features give translation/Galilean invariance; scalar coefficients with vector bases give $O(3)$-equivariance.

Methodology sketch



Results – rollout diagnostics

After training, the model is rolled out autoregressively:

$$\boldsymbol{v}_i^{n+1} = \boldsymbol{v}_i^n + \Delta t\, \widehat{\boldsymbol{a}}_i^n, \qquad \boldsymbol{x}_i^{n+1} = \boldsymbol{x}_i^n + \Delta t\, \boldsymbol{v}_i^n.$$

We evaluate observables that are **not imposed during training**:

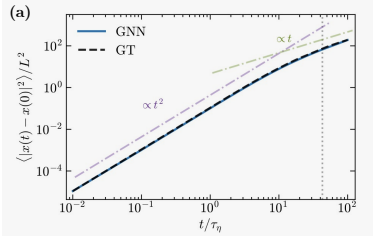
- Single particle — absolute dispersion and acceleration intermittency
- Pair — relative dispersion and separation PDFs
-  Tetrad — multi-particle deformation, size growth and shape statistics

Question

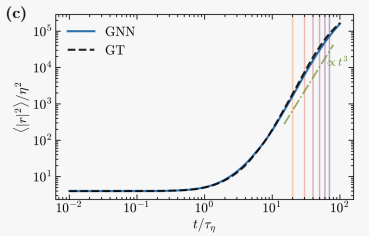
Does the learned model reproduce long-time Lagrangian statistics from short-time acceleration training?

Results

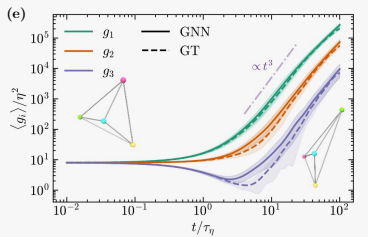
single particle



particle pairs

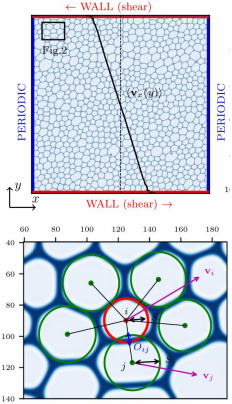


particle tetrads

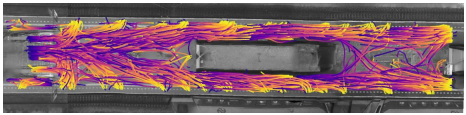


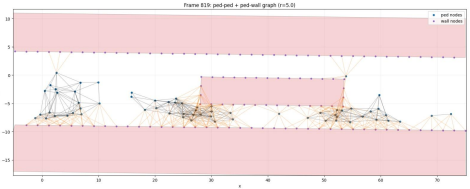
Ongoing and future work

DROPLET DYNAMICS IN EMULSIONS



ACTIVE MATTER





Current status: powerful models, weak understanding

What we can now do

- accurate function approximation
- hard-code symmetries and constraints
- learn closures and memory kernels
- train through numerical solvers
- represent stochastic reduced dynamics

What remains hard

- reliable extrapolation
- interpretable mechanisms
- extracting new terms/equations
- knowing when the model is wrong (UQ)

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F. Toschi


D. Livescu


M. Woodward


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- **AF**, K. Um, M. Desbrun, M. Buzzicotti, L. Biferale. *Solver-in-the-loop approach to closure of shell models of turbulence*. **Phys. Rev. Fluids** 10, 044602 (2025).
- **AF**, L. Biferale, M. Desbrun, G. Eyink, A. A. Mailybaev, K. Um. *On the importance of stochasticity in closures of turbulence*. **EPL** 154, 23002 (2026).
- **AF**, K. Um, M. Desbrun, M. Buzzicotti, L. Biferale. *A posteriori closure of turbulence models: Are symmetries preserved?* **Eur. J. Mech. B/Fluids** 119, 204496 (2026).
- **AF**, K. Um, M. Desbrun, D. Livescu, L. Biferale. *Learning a subgrid model for buoyancy-driven turbulence*. Manuscript in preparation.
- **AF**, X. de Wit, Z. Wang, L. Biferale, F. Toschi. *Intermittency suppression in turbulence via forced light particles*. **EPL** 155, 23002 (2026).
- **AF**, X. M. de Wit, A. Gabbana, M. Woodward, F. Toschi, Y. Ting Lin, D. Livescu. *Learning turbulent transport via Mori–Zwanzig graph neural networks*. **Communications Physics** (2026).