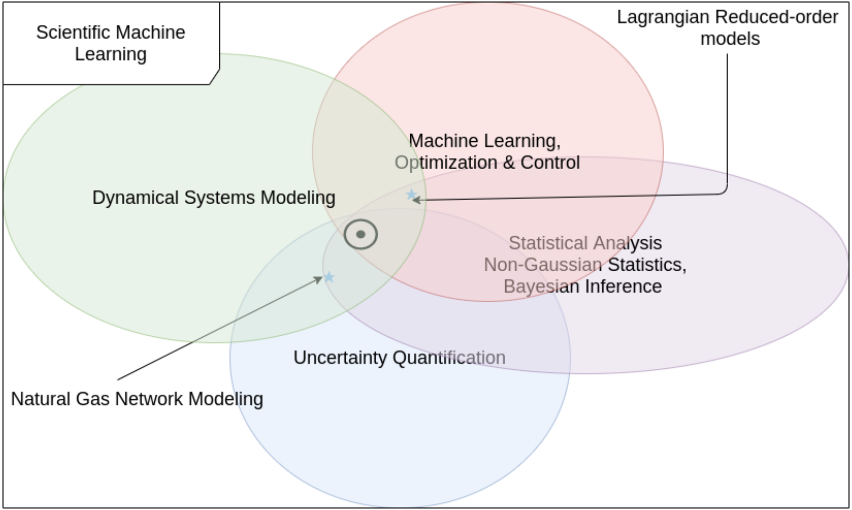
Comprehensive Exam

Criston Hyett

August 15, 2023

Overview


Scientific Machine Learning
Lagrangian Reduced-order models
Machine Learning, Optimization & Control
Dynamical Systems Modeling
Statistical Analysis Non-Gaussian Statistics, Bayesian Inference
Uncertainty Quantification
Natural Gas Network Modeling

Control of Line Pack in Natural Gas System of Israel: Balancing Limited Resources under Uncertainty

Criston Hyett, Laurent Pagnier, Jean Alisse, Lilah Saban, Igal Goldshtein, Misha Chertkov

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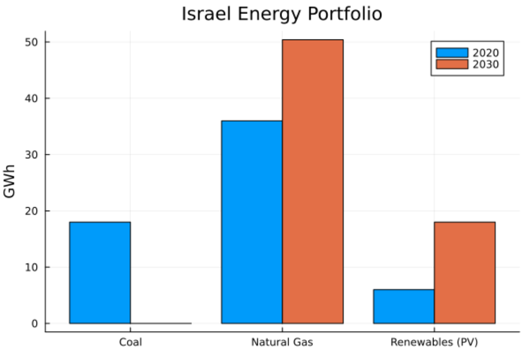
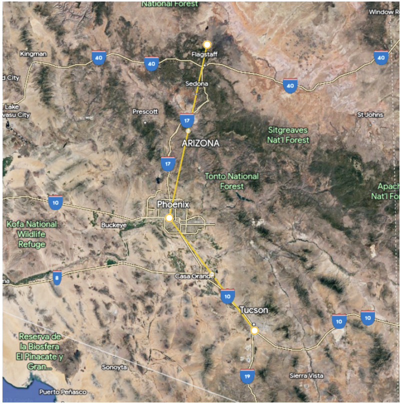
Context

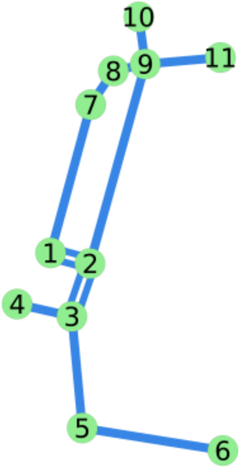

Israel Energy Portfolio
GWh
0
10
20
30
40
50
2020
2030
Coal
Natural Gas
Renewables (PV)


Kingman
Flagstaff
Sedona
Prescott
ARIZONA
Sitgreaves Nat'l Forest
Tonto National Forest
Phoenix
Buckeye
Kofa National Wildlife Refuge
Casa Grande
Tucson
Reserva de la Biosfera El Pinacate y Gran...
Sonoyta
Puerto Peñasco
Sierra Vista
St Johns

Project Goals

- Operations-aware modeling and simulation of a reduced model of Israel's natural gas network.
  - Flux control at inlet nodes
  - Realistic initial conditions
  - Assessing relevant challenges
    - Robustness in the case of uncertain PV generation
    - Robustness in the case of an insult to the system
- Model & open-source tool development
  - Solver suite specifically suited to the needs of natural gas networks
  - Advanced automatic controls
  - Monte-Carlo/Uncertainty Quantification

Reduced Model of Israel's Gas Network



[0]https://www.gov.il/he/departments/guides/distribution_area

Effective Gas Flow Equations

Under reasonable assumptions, the system of PDEs governing gas flow is

$$\partial_t \rho + \partial_x \phi = 0 \tag{1}$$

$$\partial_t \phi + \partial_x P = -\beta \frac{\phi|\phi|}{\rho} \tag{2}$$

These, supplemented with initial

$$\rho(x,0) = \rho_0(x) \tag{3}$$

$$\phi(x,0) = \phi_0(x) \tag{4}$$

and boundary conditions at each node

$$\rho_i(t) \ or \ \phi_i(t) \tag{5}$$

and an equation of state relating pressure and density

$$P(\rho) = \dots \quad \rho(P) = \dots \tag{6}$$

Staggered Grid Method

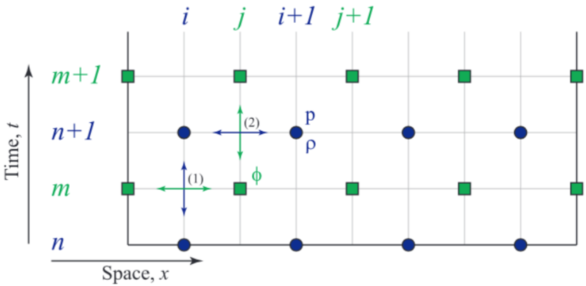


Figure taken from Gyrya,Zlotnik: "An explicit staggered-grid method for numerical simulation of large-scale natural gas pipeline networks"

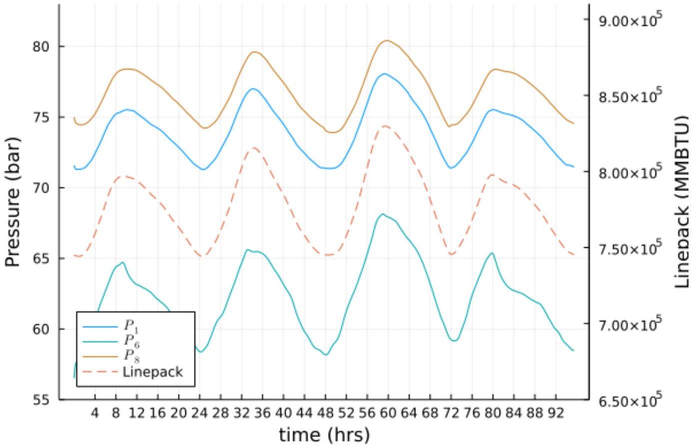
$$\partial_t \rho + \partial_x \phi = 0$$

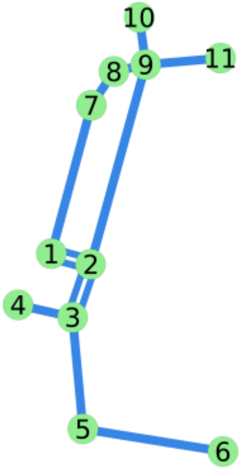
$$\partial_t \phi + \partial_x P = -\beta \frac{\phi|\phi|}{\rho}$$

CFL stability condition:

$$\sqrt{P'(\rho)}\frac{\Delta t}{\Delta x} \leq 1$$

Results: Scenario 1





Nominal week in August.

Uncertainty

Moderate uncertainty at demand nodes is represented through addition of a random noise at the consumption site

$$d_i(t) \rightarrow X_i(t) \tag{7}$$

where

$$dX_i(t) = \alpha(d_i(t) - X_i(t))dt + \gamma dW \tag{8}$$

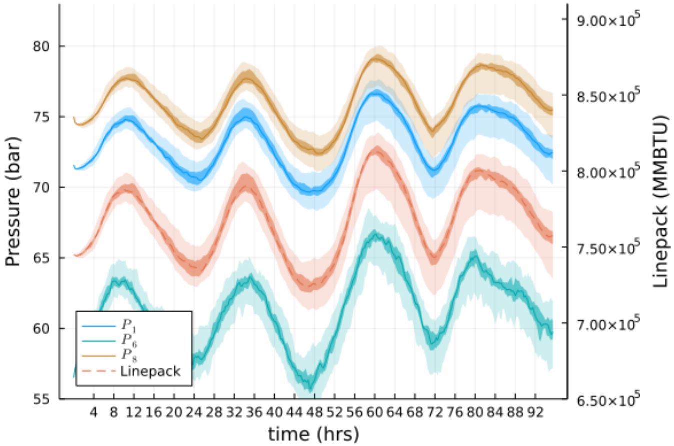
is a Ornstein–Uhlenbeck process

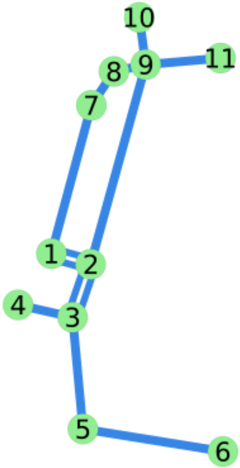
- $\mathbb{E}[X_i(t)] = d_i(t)$
- $\mathrm{Var}(X_i(t)) = \frac{\gamma}{2\alpha}(1 - e^{-2\alpha t})$
- The parameters were tuned heuristically to ensure the mean was respected, and the variance approaches

$$\mathrm{Var}(X_i(t)) \approx 0.01\mu_i^2 \tag{9}$$

With μ_i being the mean withdrawal of node i.

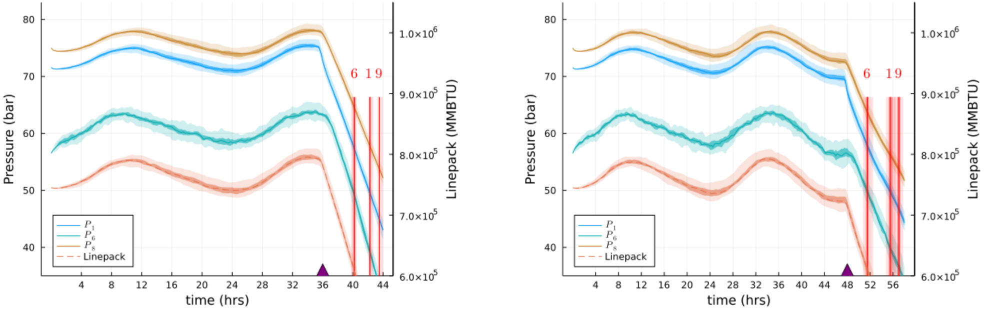
Results: Scenario 2





Linepack and pressures for random perturbation on top of nominal August days.

Results: Scenario 3 & 4

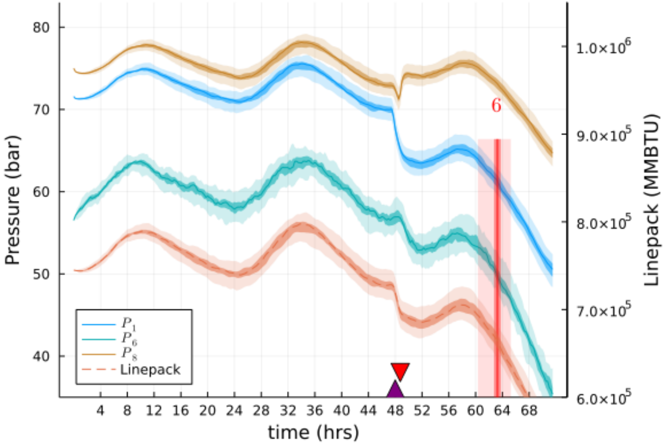


Linepack and pressures responding to loss of supply at node 1. (Left) shows the insult at a peak of intraday linepack, and (right) shows the same insult at the trough.

$\tau = 4.13 \pm 0.38$ hrs

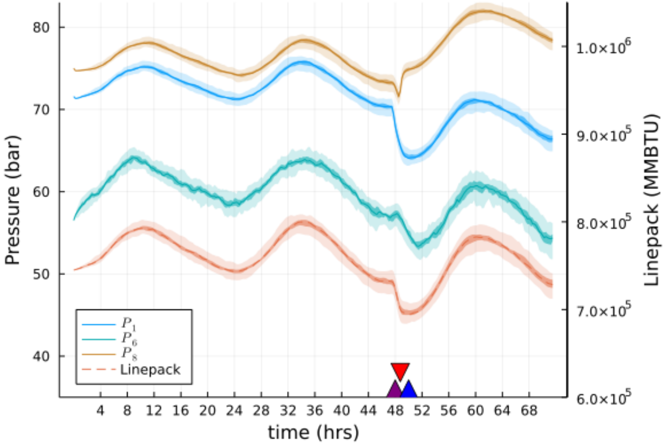
$\tau = 3.58 \pm 0.89$ hrs

Results: Scenario 5



Linepack and pressures for insult at hour 48, implementing a max-flow control on the remaining supply at node 8. $\tau = 14.17 \pm 4.07$ hrs

Results: Scenario 6



Linepack and pressures for insult at hour 48, implementing a max-flow control on the remaining supply at node 8, and curtailing demand 2 hours after the insult.

Next Steps

- Better UQ: Stochastic Finite Volumes(?)
- Higher order method and efficient implementation to allow for parallelization and acceleration.
- Advanced automatic controls
    - This would mimick some actual protocol, and allow you to make statements such as, "with 95% confidence, using protocol A, the natural gas system is robust to an insult of type B"
- Simulation and optimization of the joint power and gas grids, under uncertainty.

Questions/Comments/Suggestions?

- cmhyett@math.arizona.edu
- https://arxiv.org/abs/2304.01955
- https://github.com/cmhyett/FluxControlLinepack

Velocity gradient prediction using parameterized Lagrangian deformation models

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August 15, 2023

Motivation

- The **velocity gradient tensor** (VGT) describes many important aspects of turbulence. It displays characteristic **non-Gaussian statistics** including **intermittency**, describes the **deformation of a fluid volume**, and encapsulates **alignment between strain and vorticity**.
- Similar to velocity in the Eularian frame, the VGT is the natural object of study in the **Lagrangian frame**.
- We combine **phenomenological models** of the VGT with **physics-informed machine learning** to create efficient (and interpretable?) **reduced-order models of the VGT**.

Governing Equations for the Velocity Gradient Tensor

- The **velocity gradient tensor** (VGT) is defined by $A_{ij} = \frac{\partial u_i}{\partial x_j}$, so from Navier Stokes

$$\frac{\partial u_i}{\partial t} + u_k \frac{\partial u_i}{\partial x_k} = -\frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_k \partial x_k} \tag{10}$$

- We apply spatial derivatives, and use incompressibility to find the governing equations for the VGT:

$$\frac{dA_{ij}}{dt} = -\boxed{\left(A_{ik}A_{kj} + \frac{1}{3}A_{mn}A_{nm}\delta_{ij}\right)} - \boxed{\left(\frac{\partial^2 P}{\partial x_i \partial x_j} - \frac{1}{3}\frac{\partial^2 P}{\partial x_k \partial x_k}\delta_{ij}\right)} + \boxed{\nu \frac{\partial^2 A_{ij}}{\partial x_k \partial x_k}} \tag{11}$$

- The main challenge is to predict the nonlocal **deviatoric** part of the pressure hessian, defined as

$$H_{ij} = -\left(\frac{\partial^2 P}{\partial x_i \partial x_j} - \frac{1}{3}\frac{\partial P}{\partial x_k \partial x_k}\delta_{ij}\right) \tag{12}$$

Previous Work

- (a) Restricted Euler
- (b) Deviatoric Pressure Hessian
- (c) Viscous Term
- (d) Combined

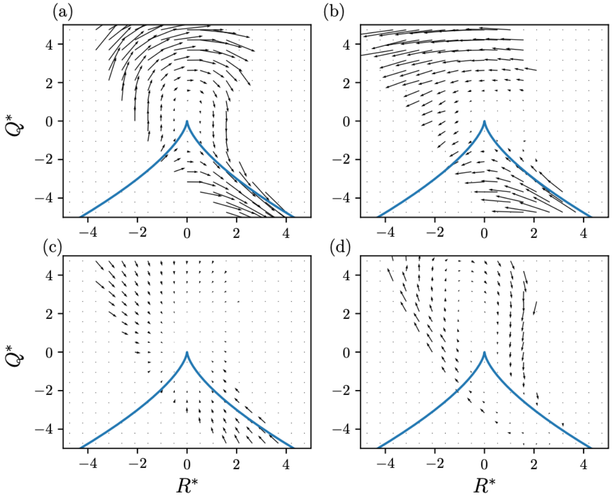


Figure taken from Tian et.al 2021

Tensor Basis Neural Network

- We can write the formal solution for the deviatoric pressure hessian as[1]

$$H_{ij}(\mathbf{x}) = \iiint \frac{\delta_{ij} - \hat{r}_i \hat{r}_j}{2\pi r^3} Q(\mathbf{x} + \mathbf{r}) d\mathbf{r} \tag{13}$$

- Using a Taylor expansion, Cayley-Hamilton Theorem, and Tensor Basis expansion[2], we can write

$$\hat{H} = \sum_{i=1}^{10} g^{(i)}(\lambda_1, \ldots, \lambda_5) \cdot \hat{T}^{(i)}(\hat{A}) \tag{14}$$

$$\lambda_1 = \mathrm{tr}(\hat{S}^2) \quad \lambda_2 = \mathrm{tr}(\hat{W}^2) \quad \lambda_3 = \mathrm{tr}(\hat{S}^3) \quad \lambda_4 = \mathrm{tr}(\hat{W}^2 \hat{S}) \quad \lambda_5 = \mathrm{tr}(\hat{W}^2 \hat{S}^2)$$

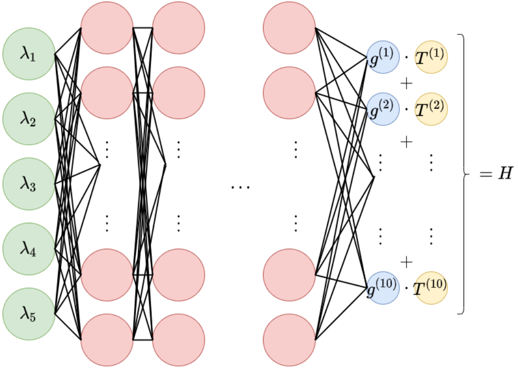
- We use the natural timescale $\tau = \langle \|S^2\|_2 \rangle^{-1}$ to normalize our VGT, and thus all of the λ_i, $T^{(j)}$.

[1] Ohkitani, K. & Kishiba, S. *Physics of Fluids* 1995.
[2] Pope, S. B. *Journal of Fluid Mechanics* 1975.

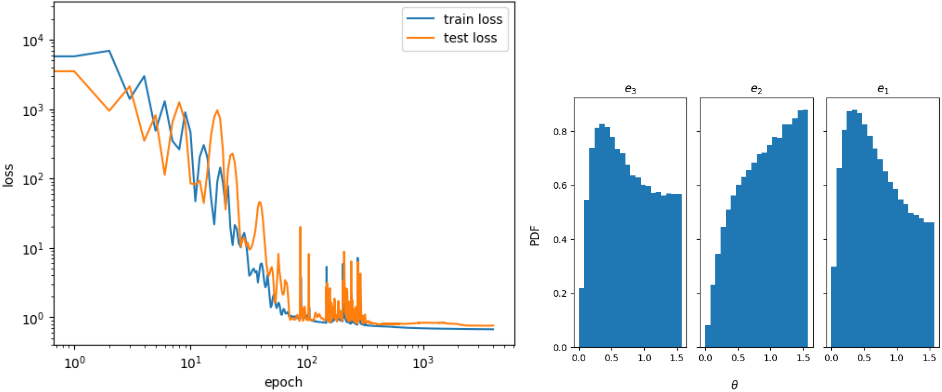
Tensor Basis Neural Network

$$\hat{H} = \sum_{i=1}^{10} {g_{\theta}}^{(i)}(\lambda_1, \ldots, \lambda_5) \cdot \hat{T}^{(i)}(\hat{A}) \tag{15}$$

$$\lambda_1 = \mathrm{tr}(\hat{S}^2) \quad \lambda_2 = \mathrm{tr}(\hat{W}^2) \quad \lambda_3 = \mathrm{tr}(\hat{S}^3) \quad \lambda_4 = \mathrm{tr}(\hat{W}^2\hat{S}) \quad \lambda_5 = \mathrm{tr}(\hat{W}^2\hat{S}^2)$$

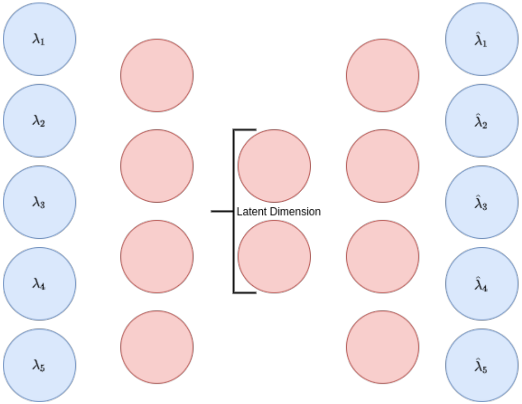


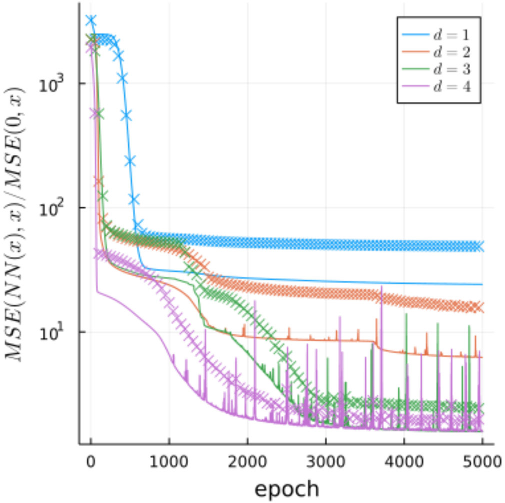
Reproducing Results



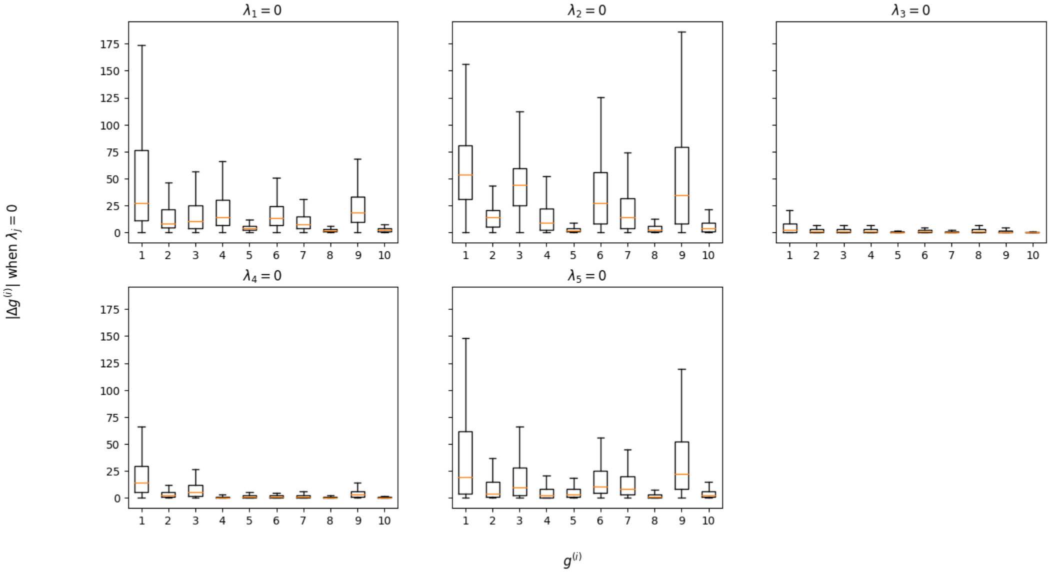
Implementing the architecture described, I show ability to train and reproduce loss plots (left) and eigenvector alignment PDFs (right)

Poking at Interpretability?





Poking at Interpretability?



Future Work

- Work currently being done to enrich TBNN using history of the VGT
  - Temporal convolutions? LSTM?
- This work was originally inspired by the Tetrad model, and the coarse-grained velocity gradient tensor
  - Particle-based coarse-graining and the opportunities/nuances/challenges is another challenge entirely
- Can we learn physics?
  - Interpretability
  - Data-driven hypothesis testing

References I

- Ohkitani, K. & Kishiba, S. Nonlocal nature of vortex stretching in an inviscid fluid. *Physics of Fluids* **7,** 411–421 (1995).
- Pope, S. B. A more general effective-viscosity hypothesis. *Journal of Fluid Mechanics* **72,** 331–340 (1975).
- Tian, Y., Livescu, D. & Chertkov, M. Physics-informed machine learning of the Lagrangian dynamics of velocity gradient tensor. *Physical Review Fluids* **6,** 094607 (2021).
- Chertkov, M., Pumir, A. & Shraiman, B. I. Lagrangian tetrad dynamics and the phenomenology of turbulence. *Physics of Fluids* **11,** 2394–2410 (1999).