An efficient data-driven approach for assessment and selection of Reynolds-stress-equation closure models

Ali Mani, Stanford University

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Closure Modeling Framework

- Reynolds stress transport equation and turbulent kinetic energy dissipation equation

$$\frac{\partial}{\partial t}\left(\overline{u_j' u_i'}\right) + \overline{u_k}\frac{\partial}{\partial x_k}\left(\overline{u_j' u_i'}\right) = -\overline{u_j' u_k'}\frac{\partial \overline{u_i}}{\partial x_k} - \overline{u_i' u_k'}\frac{\partial \overline{u_j}}{\partial x_k}$$
$$+\frac{\partial}{\partial x_k}\left(-\overline{u_k' u_j' u_i'} - \frac{1}{\rho}\left(\overline{p' u_j'}\delta_{ki} + \overline{p' u_i'}\delta_{kj}\right) + \nu\frac{\partial \overline{u_j' u_i'}}{\partial x_k}\right)$$
$$+\frac{2}{\rho}\overline{p' s_{ij}'} - 2\nu\left(\overline{\frac{\partial u_j'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}\right)$$

$$\frac{\partial \varepsilon}{dt} + \overline{u_k}\frac{\partial \varepsilon}{\partial x_k} = P^1 + P^2 + P^3 + P^4 + T + \Pi + D - Y$$

$$\varepsilon \equiv \nu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}$$

Closure Modeling Framework

- Compact representation

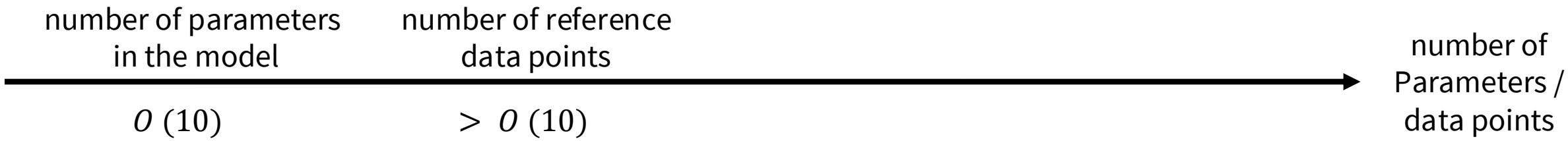
$$\frac{d}{dt}\left(\overline{u_j' u_i'}\right) + \text{closed terms} = f_{ij} + \frac{\partial}{\partial x_k}\left(g_{ijk}\right)$$

$$\frac{d\varepsilon}{dt} + \text{closed terms} = e + \frac{\partial}{\partial x_k}\left(h_k\right)$$

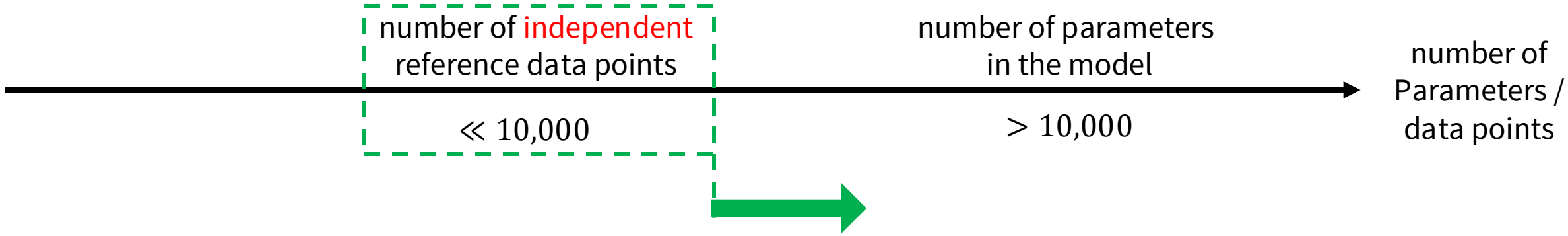
- Input space:
  - Primary variable (controlling anisotropy): $\tau_{ij} \equiv \frac{\overline{u_j' u_i'}}{\overline{u_k' u_k'}}$
  - Gradients (controlling transport): $\nabla \bar{u}_i, \nabla \overline{u_j' u_i'}, \nabla \varepsilon$
  - Parameters: y, ν
  - Scale variables: $k \equiv \frac{1}{2}\overline{u_j' u_i'}$, ε
- Dimension of the input space: **34** → many adjustable parameters (!)

Data Demand

- Traditional models



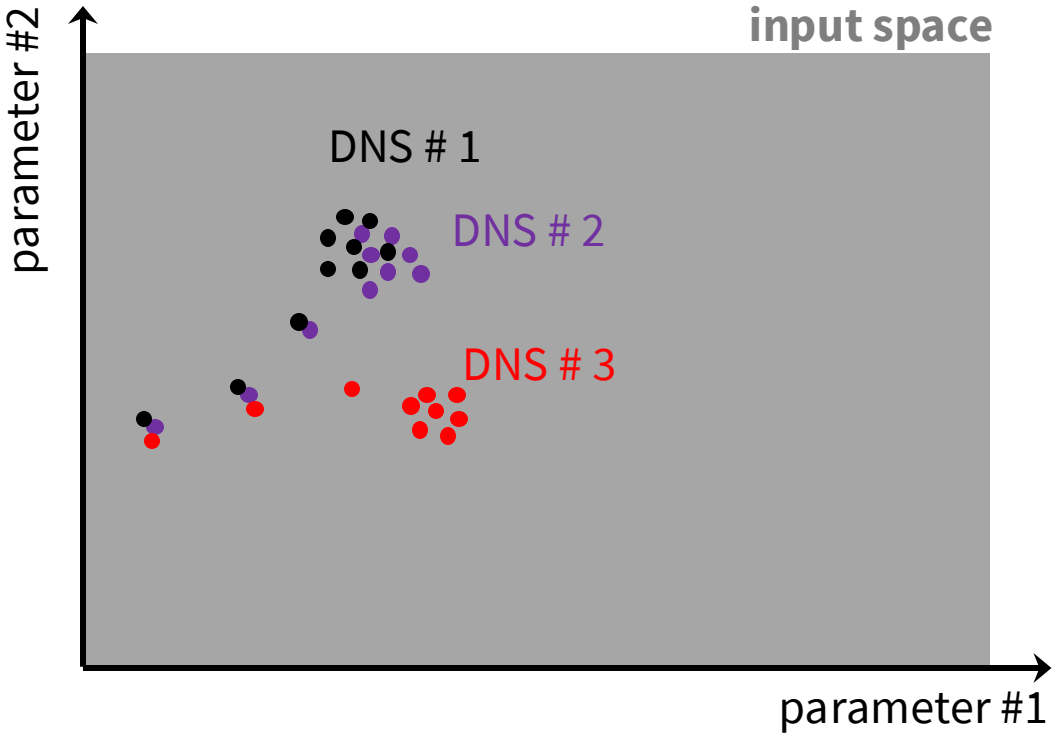
- ML-based models



- Research need: generate **diverse** data

Data Generation Challenge

- Standard DNS and experiments provide clusters of data points in the parameter space
  - Sparse coverage
  - Significant overlap in coverage
  - Limited "knob" for data diversification
    → change boundary conditions



- Desired data generation strategy:
  - Diverse coverage of the input space with minimal overlap

Our Data Generation Strategy

- Data generation via volumetrically forced simulations

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}\left(u_j u_i\right) = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu\frac{\partial^2 u_i}{\partial x_j \partial x_j} + s_i(x,y,z,t) + a_{ji}(x,y,z,t)u_j'$$

- s_i (macroscopic forcing[1]) controls $\overline{u_i}$, $\partial\overline{u_i}/\partial x_j$
- a_{ji} (linear forcing[2]) forces fluctuations → modifies $\overline{u_i'u_j'}$, $\partial\overline{u_i'u_j'}/\partial x_k$

  → On demand selection of diverse points in the input space

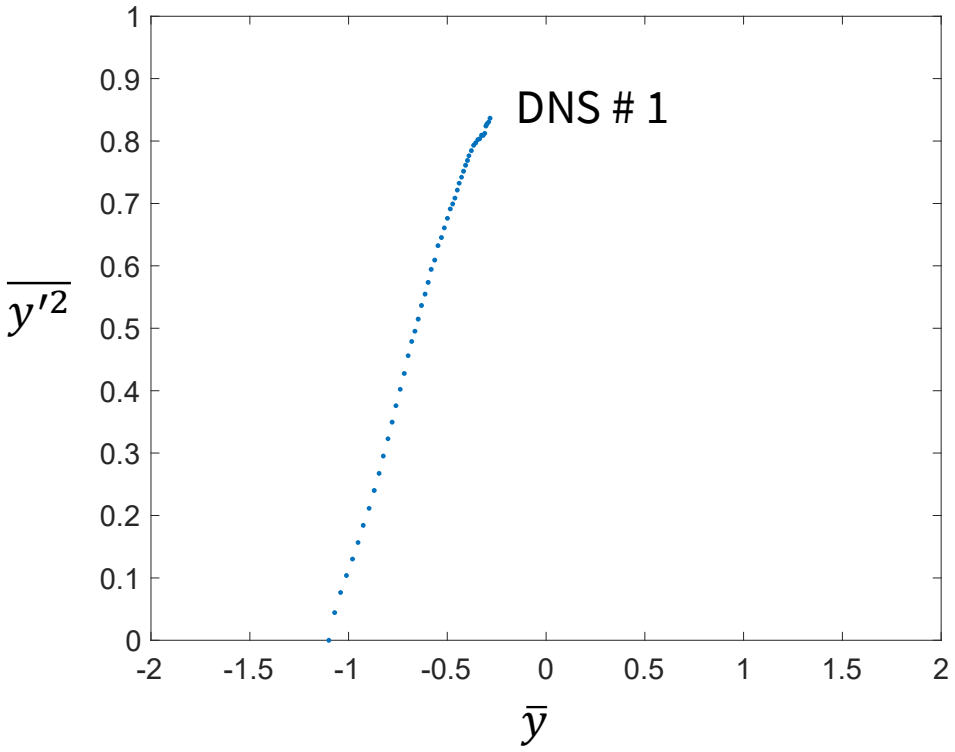
- Only need simple configurations
  - › Affordable simulations
  - › Homogeneous directions → fast statistical convergence

1: Mani and Park, PR-Fluids, 2021;
2: Homan, Shende, and Mani, PR-Fluids, 2024;

Example Demo: a First-order Stochastic ODE

$$dy = f(y)dt + g(y)dB$$

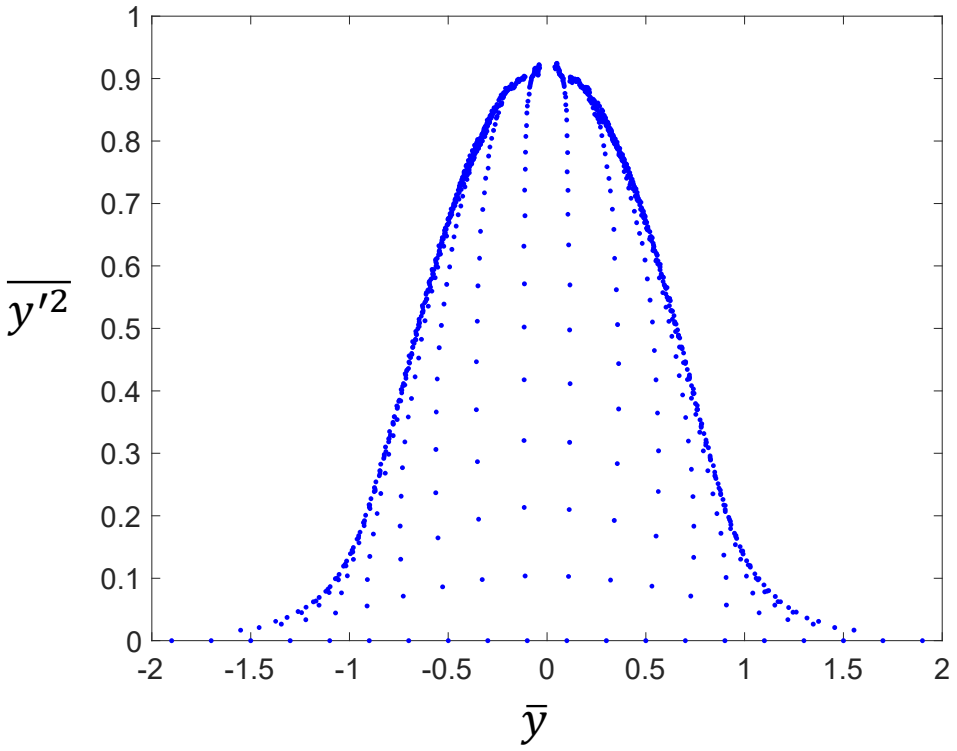
- Input space: first and second moments: $\bar{y}$, $\overline{y'^2}$



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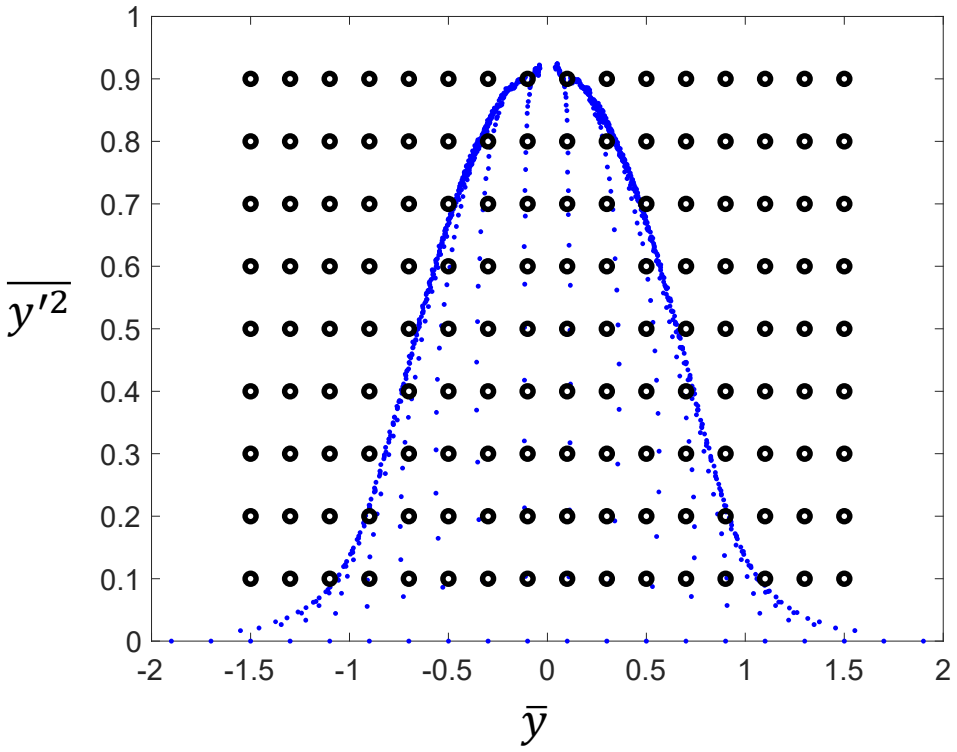


- Many DNSs → 20,000 data points
  each representing mean of 20,000 ensembles

Example Demo: a First-order Stochastic ODE

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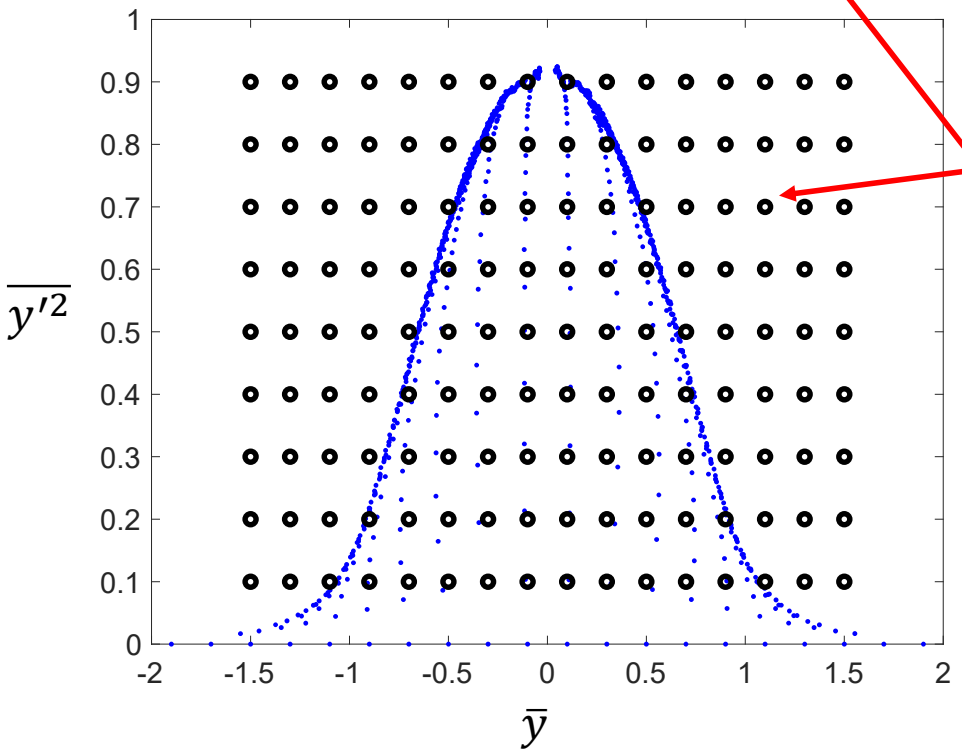


- Many DNSs → 20,000 data points
- Desired sampling: ~O(100) data points, no clusters

Example Demo: a First-order Stochastic ODE

$$dy = f(y)dt + g(y)dB + s(t) + a(t)y'$$

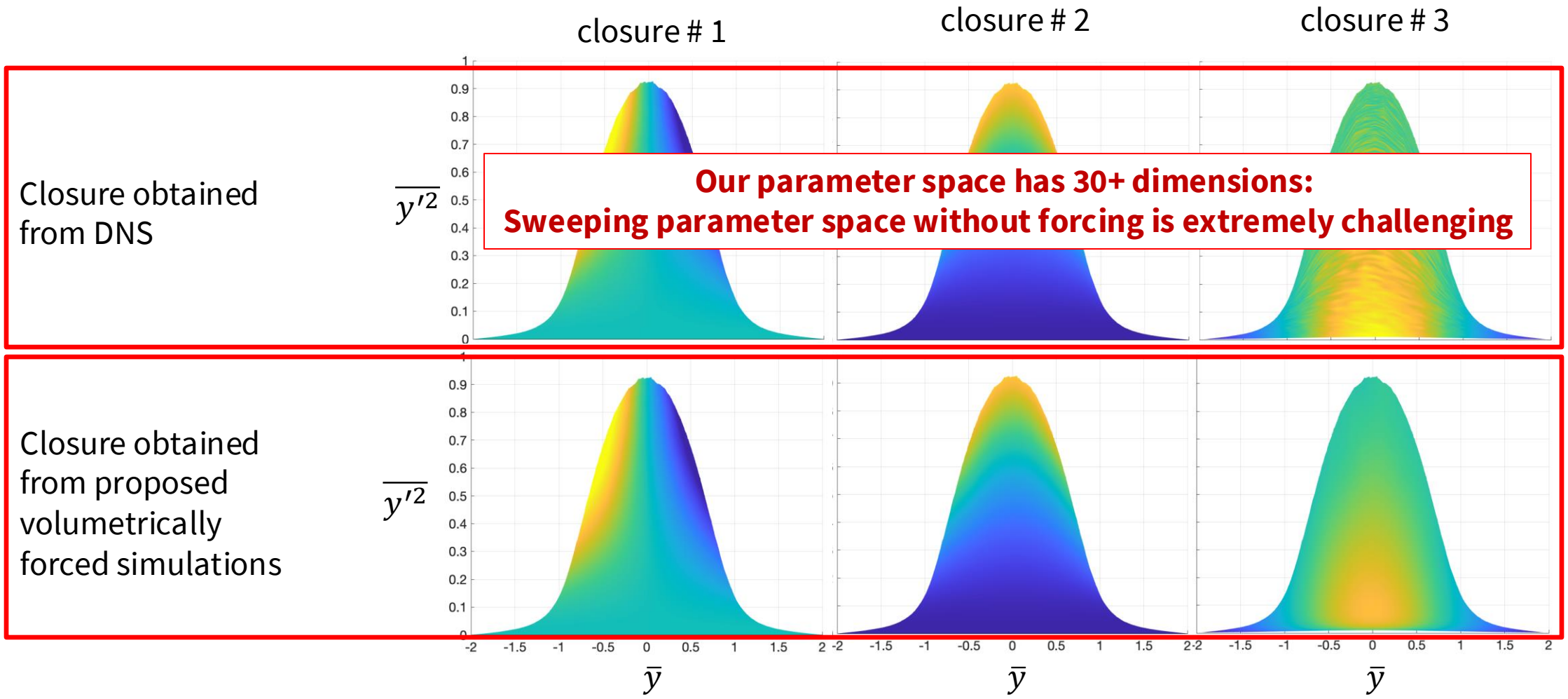
- Input space: first and second moments: $\bar{y}$, $\overline{y'^2}$



sampled using stationary forced simulations
~O(100) ensembles per simulations

- Many DNSs → 20,000 data points
- Desired sampling: ~O(100) data points, no clusters

Example Demo: Closure Results



- Proposed approach provides **more diverse** data, **~200 times faster**, and has **~twice smaller sampling error,** requires **~200 times less memory**

Application of the Method to the Navier Stokes Equation Part I: First Moment Closures

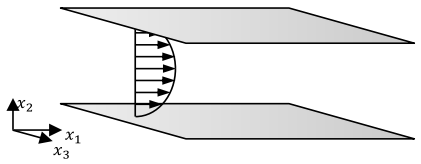
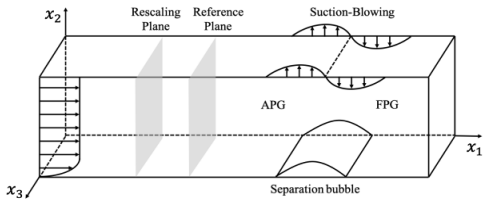
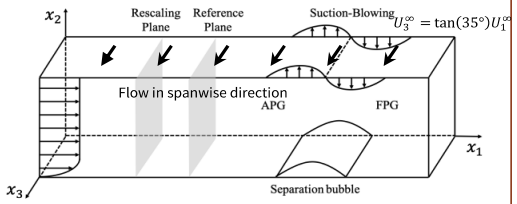
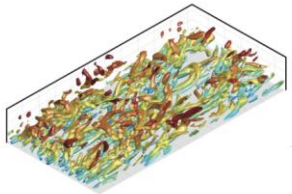
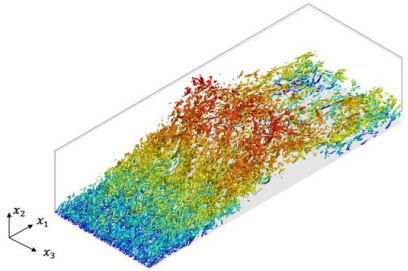
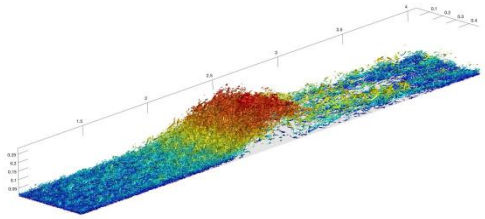
Analysis of First Moment Closures:

- A general (non-Boussinesq) eddy viscosity relates the Reynolds stresses to mean velocity gradients as (Kraichnan 1987, Hamba, JAS, 1995):

$$-\overline{u_i' u_j'}(\mathbf{x}) = \mathcal{D}\nabla\overline{\boldsymbol{u}} = \int D_{ijkl}(\mathbf{x},\mathbf{y}) \left.\frac{\partial \overline{u}_l}{\partial x_k}\right|_{\mathbf{y}} d\mathbf{y}$$

- How to measure D?

Quantified Eddy Viscosity for Attached and Separated Flows (Summary)

	Channel Flow	Separated Boundary Layer (SBL)	Separated Boundary Layer with Spanwise Sweep (SBLS)
Schematics	 $\mathrm{Re}_\tau = 180$	 $\mathrm{Re}_\theta = 350$	 $\mathrm{Re}_\theta = 350$
MFM measurement	Nonlocal and anisotropic D^0_{ijkl}, D_{ij21}	Local and anisotropic D^0_{ij1l}, D^0_{ij2l}	Local and anisotropic D^0_{ij1l}, D^0_{ij2l}
DNS snapshot			
	Park and Mani, JFM 998, A33, 2024	Park, Liu, Mani, AIAA 0940, 2022	Park and Mani, AIAA 3268, 2023

Measured eddy viscosities: proven accurate

Input space insufficient (too small) to build local closures

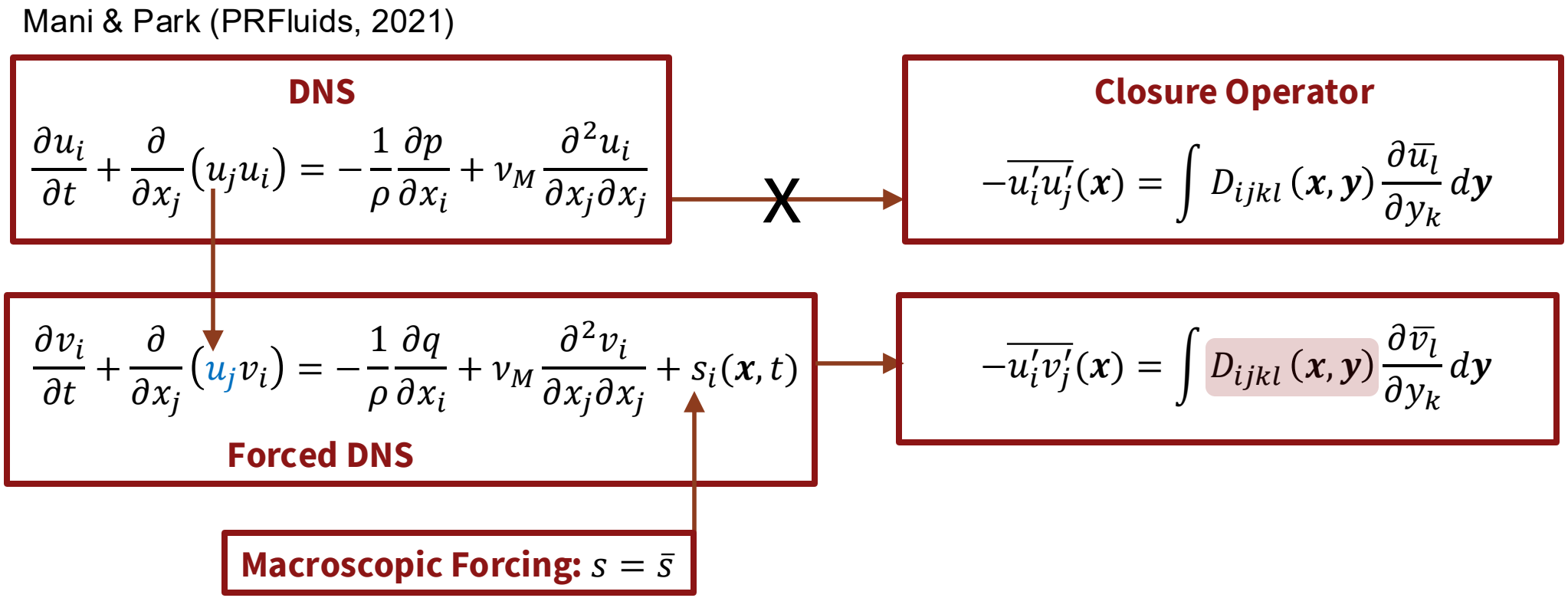
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- How to measure D?

Macroscopic Forcing Method (MFM)



- Dirac delta forcing → Green's function approach (Liu et al. PRFluids, 2023)
- MFM exploits the smoothness of closure operators
  → Substantial reduction in computing cost

Eddy Diffusivity Operator as a Series Expansion

- Inspired by the Kramers-Moyal expansion (in the context of gas dynamics)

$$-\overline{u_i' c'}(\boldsymbol{x}) = \int_y D_{ij}(\boldsymbol{x}, \boldsymbol{y}) \frac{\partial \bar{c}}{\partial x_j}\Big|_{\boldsymbol{y}} \mathbf{d}\boldsymbol{y}$$

$$= \int_y D_{ij}(\boldsymbol{x}, \boldsymbol{y}) \left(\frac{\partial \bar{c}}{\partial x_j}\Big|_{\boldsymbol{x}} + (y_m - x_m) \frac{\partial^2 \bar{c}}{\partial x_j \partial x_m}\Big|_{\boldsymbol{x}} + \cdots \right) \mathbf{d}\boldsymbol{y}$$

$$= D_{ij}^0(\boldsymbol{x}) \frac{\partial \bar{c}}{\partial x_j} + D_{ijm}^1(\boldsymbol{x}) \frac{\partial^2 \bar{c}}{\partial x_j \partial x_m} + \cdots$$

leading term characterizes local effects

higher-order terms characterize non-local effects

Eddy Diffusivity Operator as a Series Expansion

- Inspired by the Kramers-Moyal expansion (in the context of gas dynamics)

spatial moments of the eddy diffusivity kernel

$$-\overline{u_i' c'}(\boldsymbol{x}) = \int_y D_{ij}(\boldsymbol{x}, \boldsymbol{y}) \left. \frac{\partial \bar{c}}{\partial x_j} \right|_y \mathbf{dy}$$

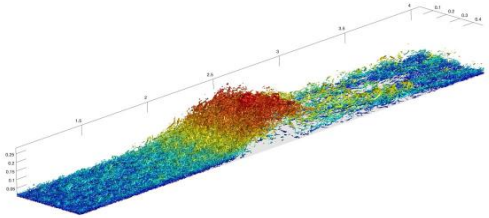
$$= \int_y D_{ij}(\boldsymbol{x}, \boldsymbol{y}) \left(\left. \frac{\partial \bar{c}}{\partial x_j} \right|_x + (y_m - x_m) \left. \frac{\partial^2 \bar{c}}{\partial x_j \partial x_m} \right|_x + \cdots \right) \mathbf{dy}$$

$$= D_{ij}^0(\boldsymbol{x}) \frac{\partial \bar{c}}{\partial x_j} + D_{ijm}^1(\boldsymbol{x}) \frac{\partial^2 \bar{c}}{\partial x_j \partial x_m} + \cdots$$

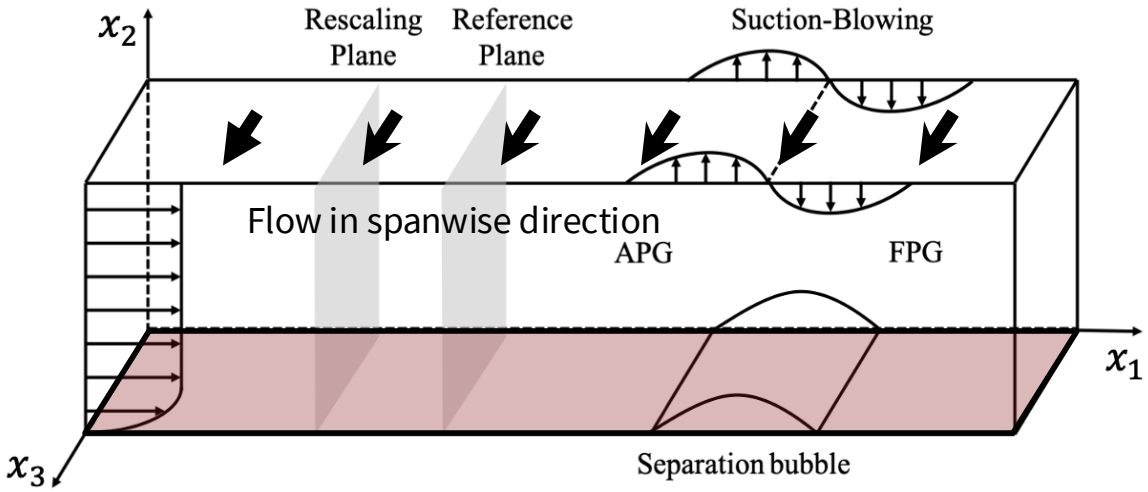
- For a given j, $D_{ij}^0(\boldsymbol{x})$ can be measured with one DNS simulation
- Ansatz: set the forcing such that $\frac{\partial \bar{c}}{\partial x_j} = 1$
- Forcing in the form of higher order polynomials can reveal higher order terms

Example: Quantification of Eddy Viscosity Components in a Separated Boundary Layer with Spanwise Sweep

- Identified important components of D^0_{ijkl}

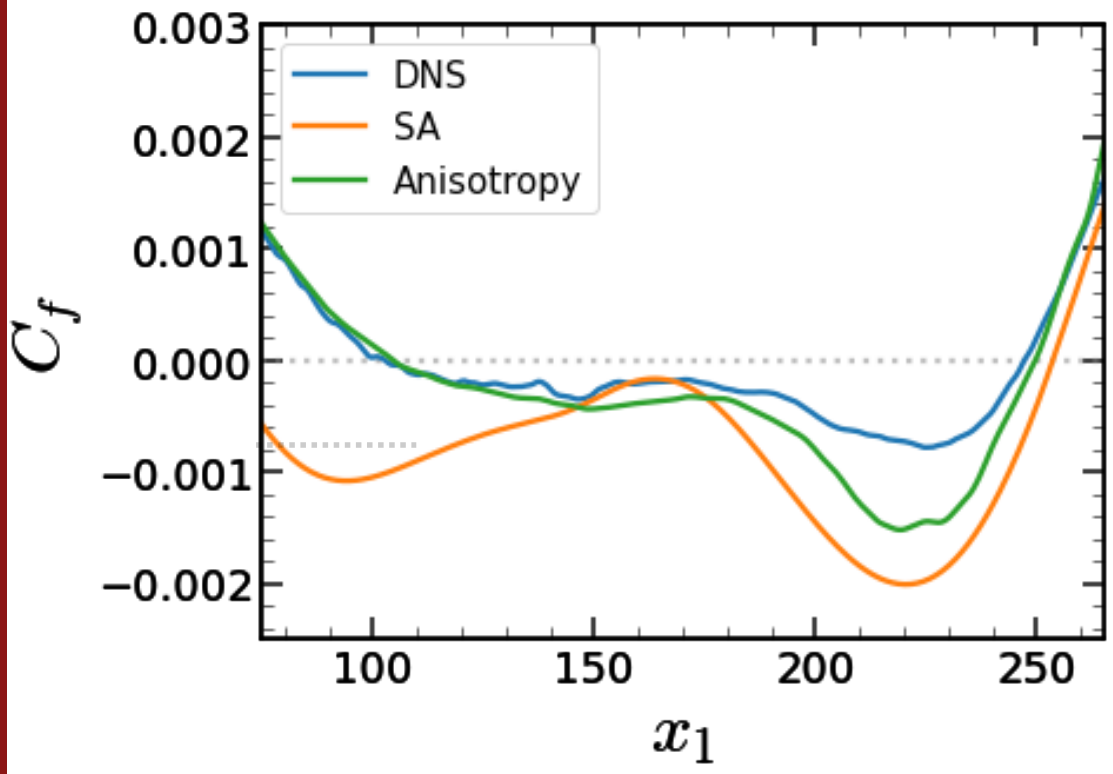


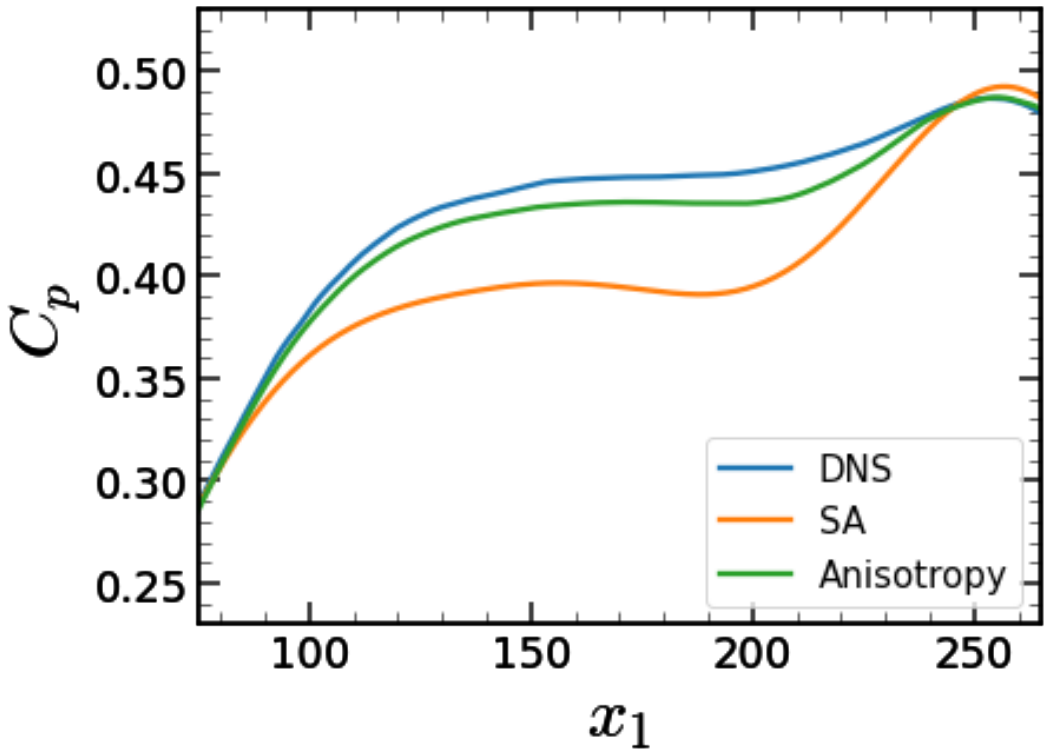
$$\begin{bmatrix} D^0_{1111} & D^0_{1112} & D^0_{1113} & D^0_{1121} & D^0_{1122} & D^0_{1123} \\ D^0_{1211} & D^0_{1212} & D^0_{1213} & D^0_{1221} & D^0_{1222} & D^0_{1223} \\ D^0_{1311} & D^0_{1312} & D^0_{1313} & D^0_{1321} & D^0_{1322} & D^0_{1323} \\ D^0_{2111} & D^0_{2112} & D^0_{2113} & D^0_{2121} & D^0_{2122} & D^0_{2123} \\ D^0_{2211} & D^0_{2212} & D^0_{2213} & D^0_{2221} & D^0_{2222} & D^0_{2223} \\ D^0_{2311} & D^0_{2312} & D^0_{2313} & D^0_{2321} & D^0_{2322} & D^0_{2323} \end{bmatrix}$$



- Anisotropic extensions of existing first moment closures (eddy viscosity closures) do not capture correct ratios among these components
  - Some components are not even represented

Impact of Anisotropy on Prediction



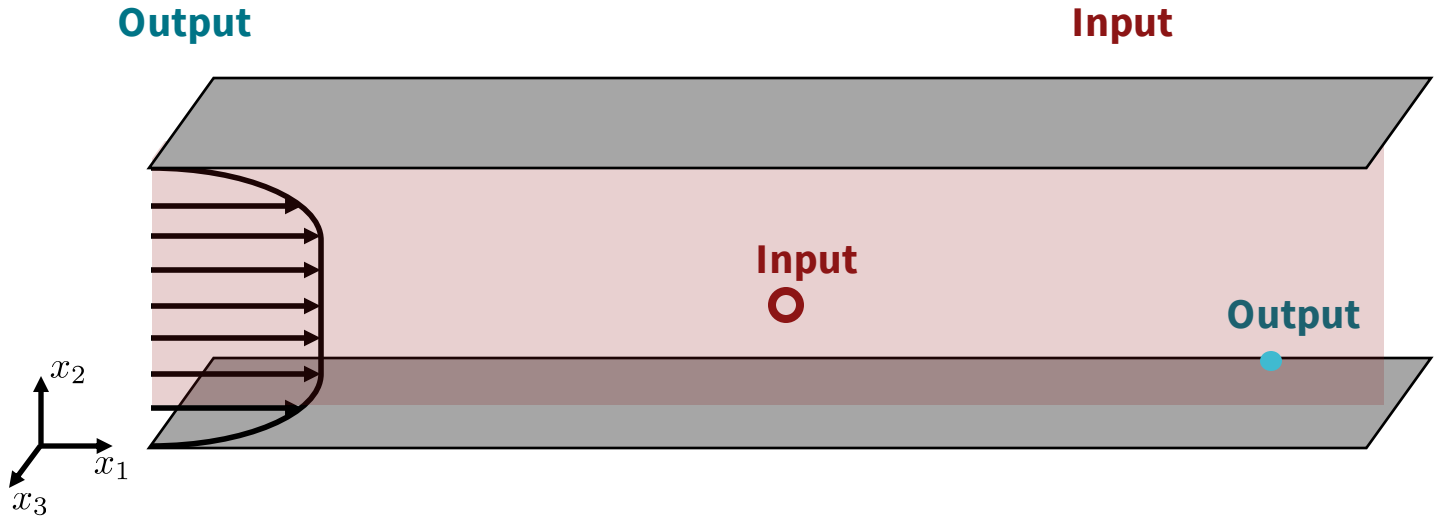


- Significant improvement especially in the separation zone
- Remaining gap with DNS is due to local approximation

Assessment of Nonlocality in Eddy Viscosity

- Example: 2D non-local eddy viscosity in turbulent channel flow

$$-\overline{u_i' v_j'}(x_1, x_2) = \int_{y_1, y_2} D_{ij21}(x_1, x_2, y_1 - x_1, y_2) \left.\frac{\partial V_1}{\partial x_2}\right|_{y_1, y_2} dy_1 dy_2$$

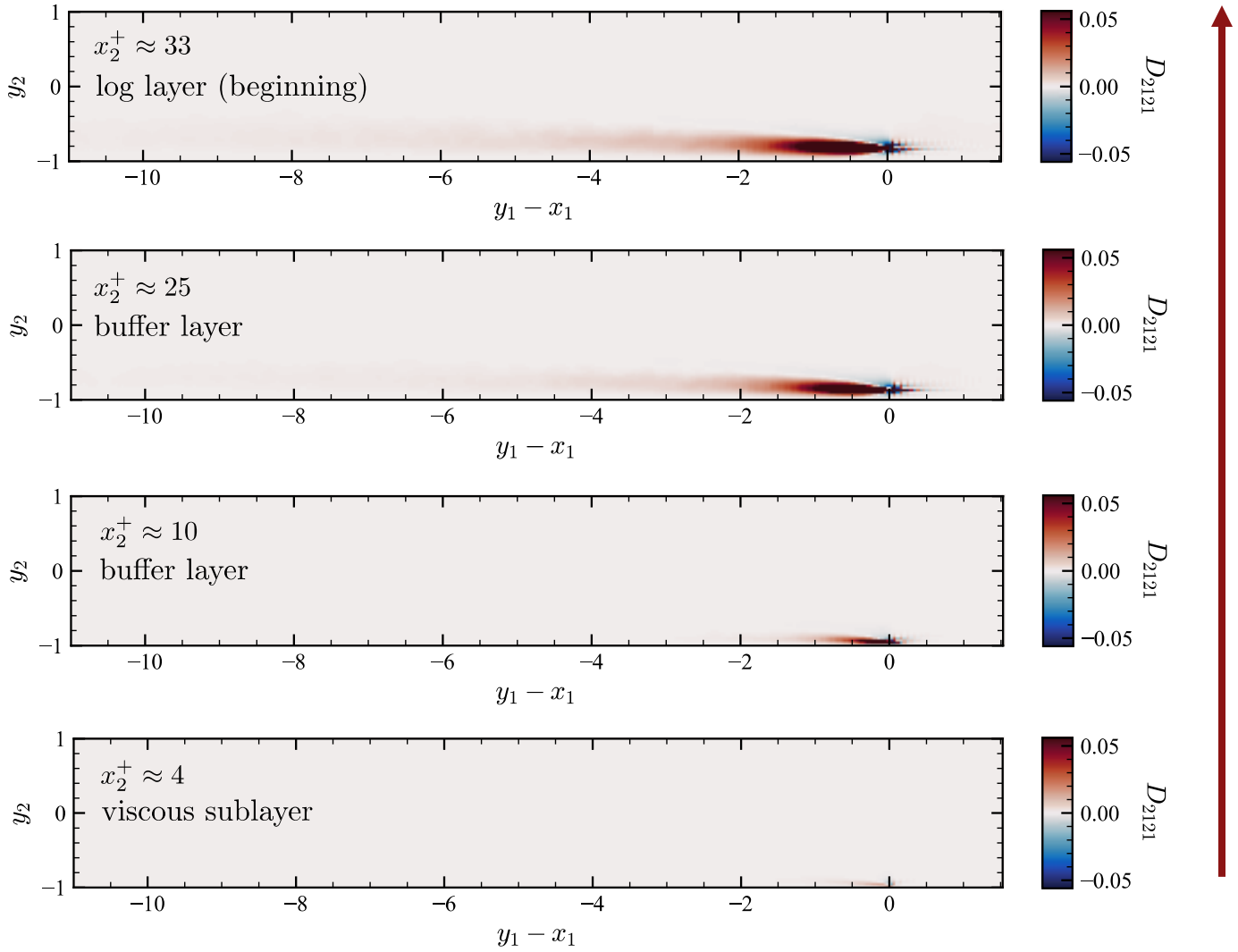


- For a given coordinate (x_1, x_2) we can quantify D using one simulation. Requires combining MFM with adjoint methods.

Liu, J., Schäfer, F., Bryngelson, S. H., Zaki, T. A., and Mani, A. "Adjoint-based computation of nonlocal eddy viscosity in turbulent channel flow," *Phys. Rev. Fluids* 9(9) 094606, 2024

2D nonlocal eddy viscosity using adjoint MFM

- Comparison of eddy viscosity for different locations

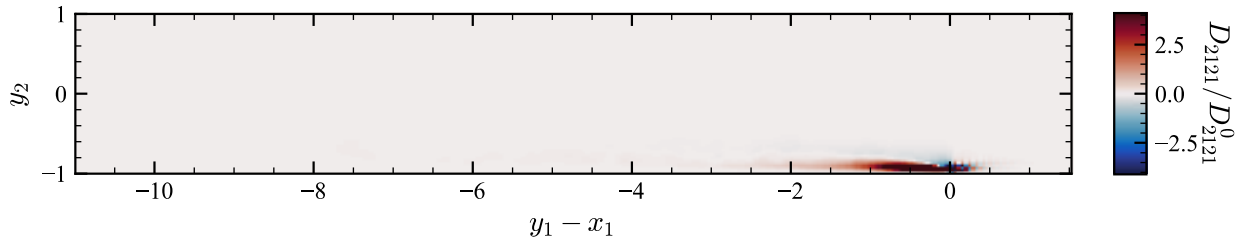


Streamwise nonlocality increases with wall distance

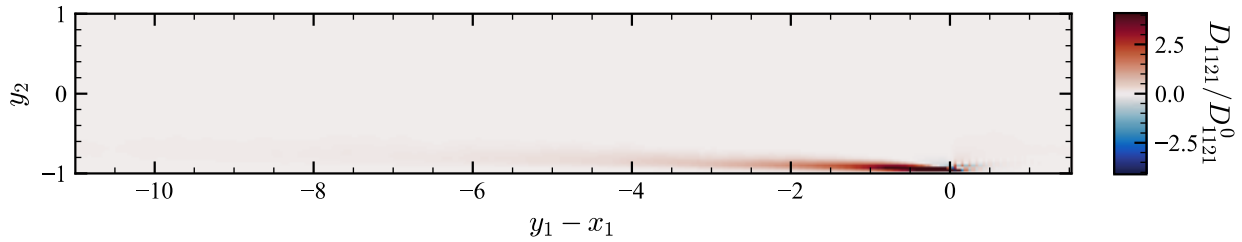
Normal Reynolds stress components

- Comparison of other Reynolds stress components

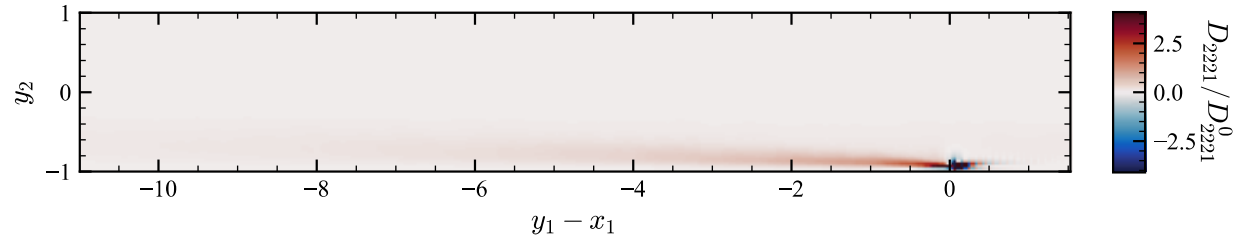
$\overline{u_2' v_1'}$



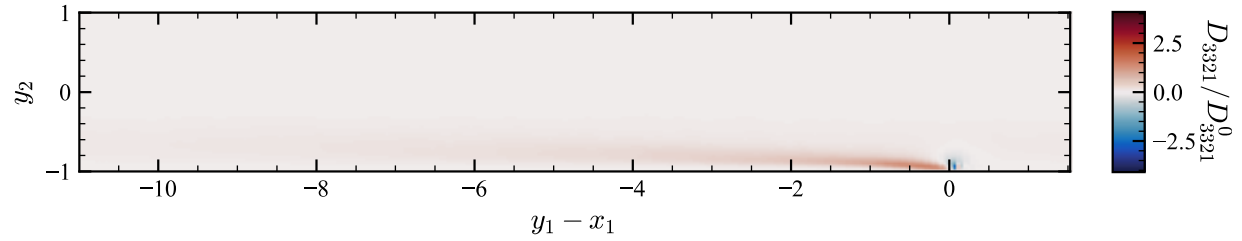
$\overline{u_1' v_1'}$



$\overline{u_2' v_2'}$



$\overline{u_3' v_3'}$



Longer for normal components

$$T \frac{D}{Dt} \overline{u_i' u_j'} = \dots$$

Implies tensorial decay timescale

2D nonlocal eddy viscosity summary

- Longer streamwise nonlocality than wall-normal nonlocality
  - Increases with distance from the wall
- Normal components of the Reynolds stress have longer streamwise nonlocality than $\overline{u_2' v_1'}$

Modeling implications:

- Intuitively expected, but now quantified
- Tensorial decay time scale

Observed trends in nonlocality and anisotropy render the eddy viscosity framework over-complicated for modeling (while useful for diagnostics)
→ The trends are capturable with proper closure models for the Reynolds stress transport equation

Application of the Method to the Navier Stokes Equation Part II: Second Moment Closures

Second Moment Closure

- Compact representation

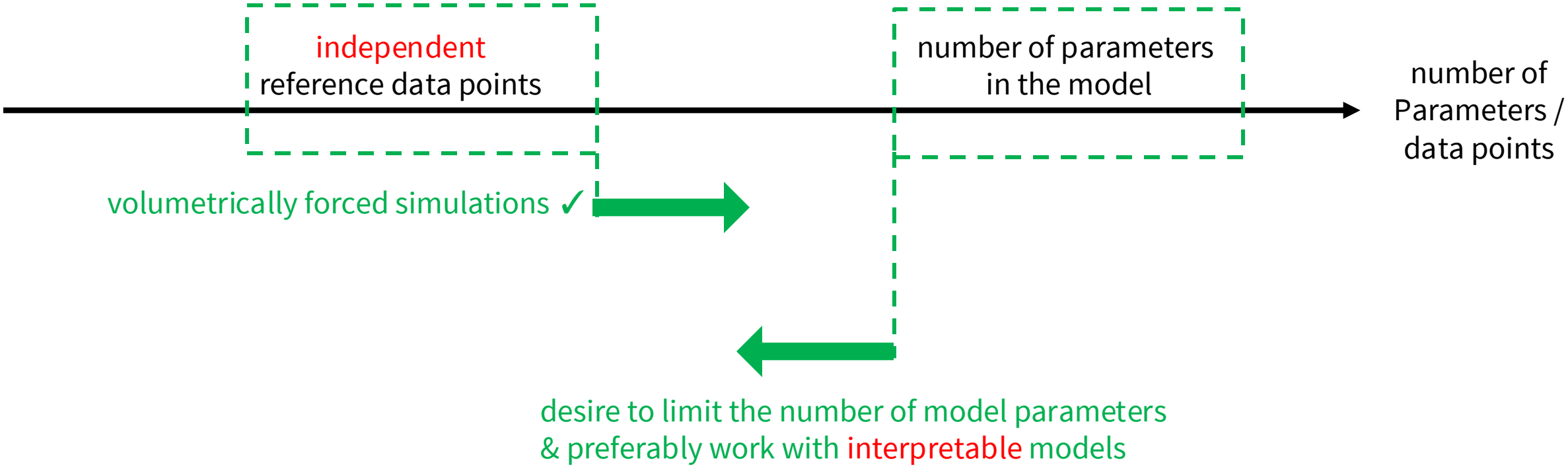
$$\frac{d}{dt}\left(\overline{u_j' u_i'}\right) + \text{closed terms} = f_{ij} + \frac{\partial}{\partial x_k}\left(g_{ijk}\right)$$

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- Input space:
  - Primary variable (controlling anisotropy): $\tau_{ij} \equiv \frac{\overline{u_j' u_i'}}{\overline{u_k' u_k'}}$
  - Gradients (controlling transport): $\nabla \bar{u}_i, \nabla \overline{u_j' u_i'}, \nabla \varepsilon$
  - Parameters: y, ν
  - Scale variables: $k \equiv \frac{1}{2}\overline{u_j' u_i'}, \varepsilon$
- Dimension of the input space: **34** → many adjustable parameters (!)

Data Demand

- Proposed data-driven approach



Closure Model Form

$$\frac{d}{dt}\left(\overline{u_j' u_i'}\right) + \text{closed terms} = f_{ij} + \frac{\partial}{\partial x_k}\left(g_{ijk}\right)$$

- Our "minimal" model: Cubic dependence on τ_{ij}, leading order expansion with respect to other inputs
- Apply rotational invariance analysis

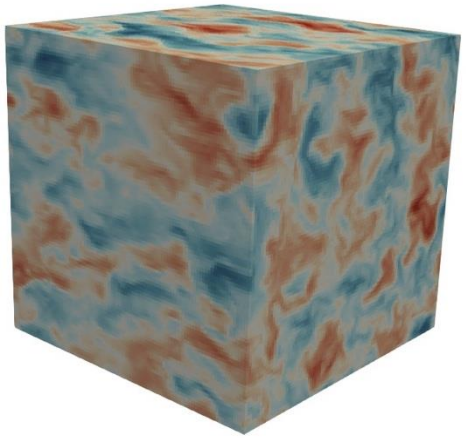
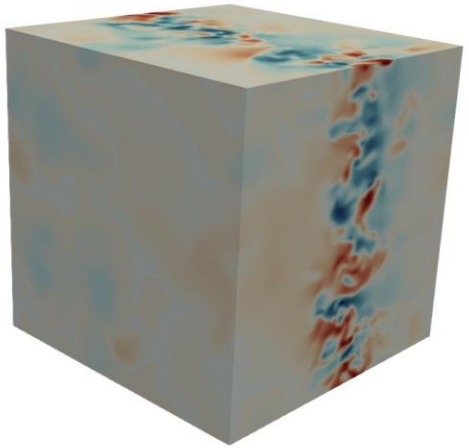
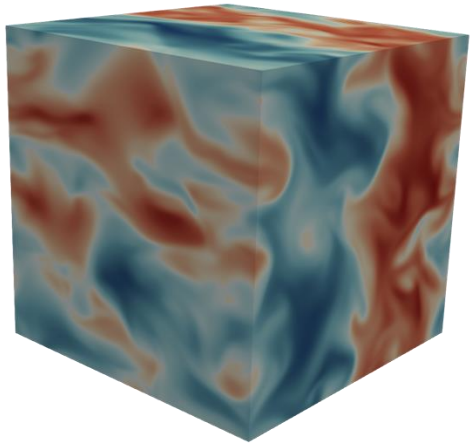
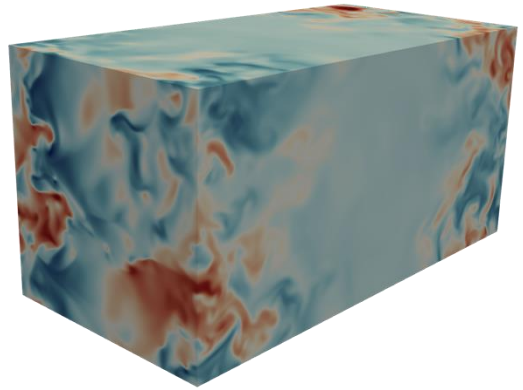
- $f_{ij} = 2\varepsilon f_{ij}^{0}\left(\underline{\tau}\right) + k\frac{\partial \overline{u_m}}{\partial x_l} f_{ijlm}^{u}\left(\underline{\tau}\right) + \left(\frac{k^{\frac{3}{2}}}{y}\right) n_l n_m f_{ijlm}^{y}\left(\underline{\tau}\right) + \left(\frac{\varepsilon^2 \nu}{k^2}\right) f_{ij}^{\nu}\left(\underline{\tau}\right) + \cdots$
- $g_{ijk} = \left(\frac{k^2}{\varepsilon}\right) \overline{\frac{\partial u_m' u_n'}{\partial x_l}}\, g_{ijklmn}^{0}\left(\underline{\tau}\right) + \cdots$

Earlier less comprehensive model forms in:
Speziale (1995)
Younis et al (1999)

Data Generation using Canonical settings

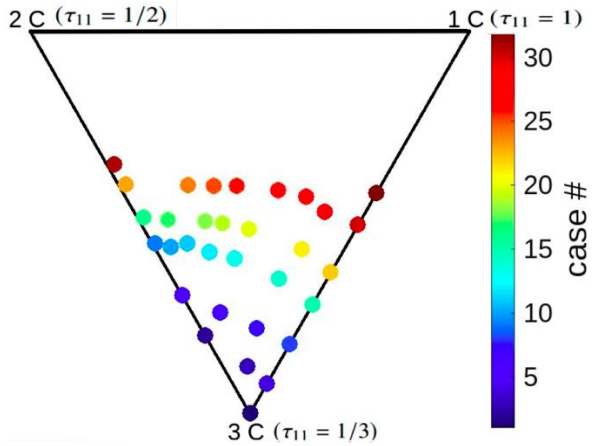
$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_j u_i) = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + s_i + a_{ji} u_j'$$

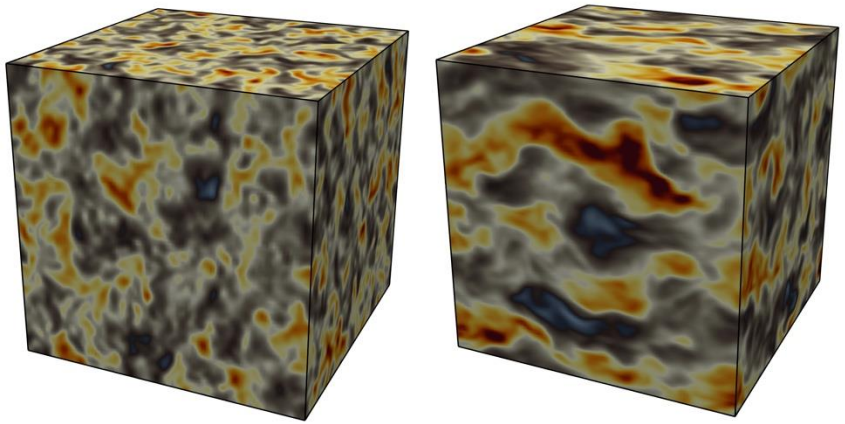
increasing complexity →

$a_{ij} \neq 0$ $s_i = 0$	$a_{ij} = a_{ij}(y)$ $s_i = 0$	$a_{ij} = a_{ij}(y)$ $s_i = s_i(y)$	$a_{ij} = a_{ij}(y)$ + walls
			
⇩	⇩	⇩	⇩
f_{ij}^0, f_{ij}^ν	g_{ijklmn}^0	f_{ijlm}^u	f_{ijlm}^y

First Model: f_{ij}^0

- Forced homogeneous anisotropic turbulence:
  - $\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_j u_i) = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + a_{ji} u_j'$
- 32 simulations with diversified a_{ij}
- Numerical convergence to:
  mesh, Reynolds, domain, orientation
- Allowed full characterization and fitting of f^0

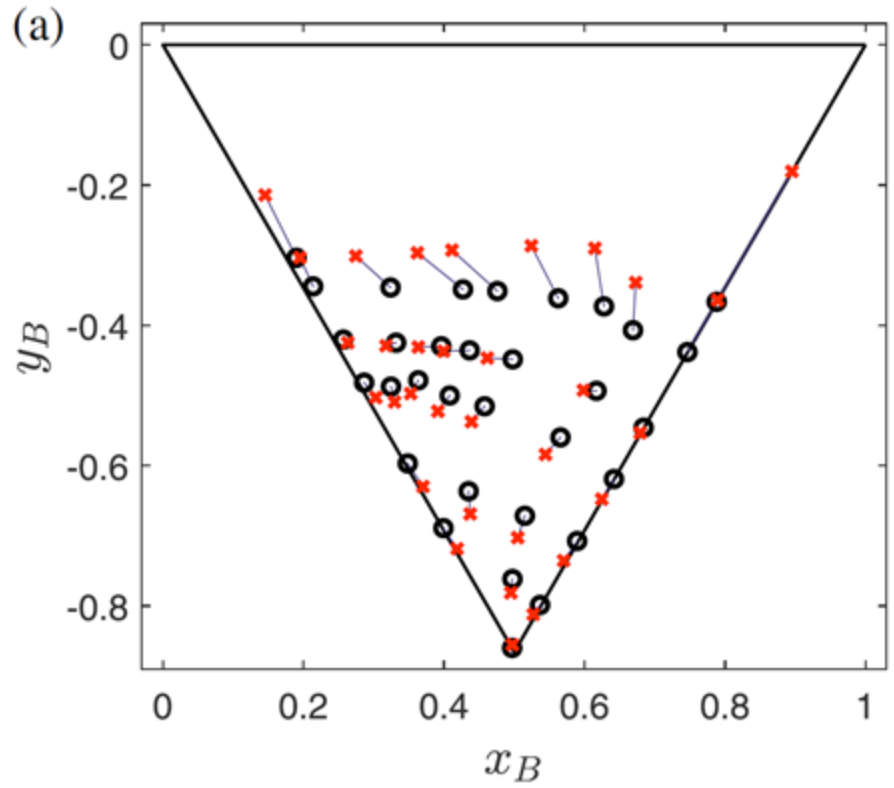




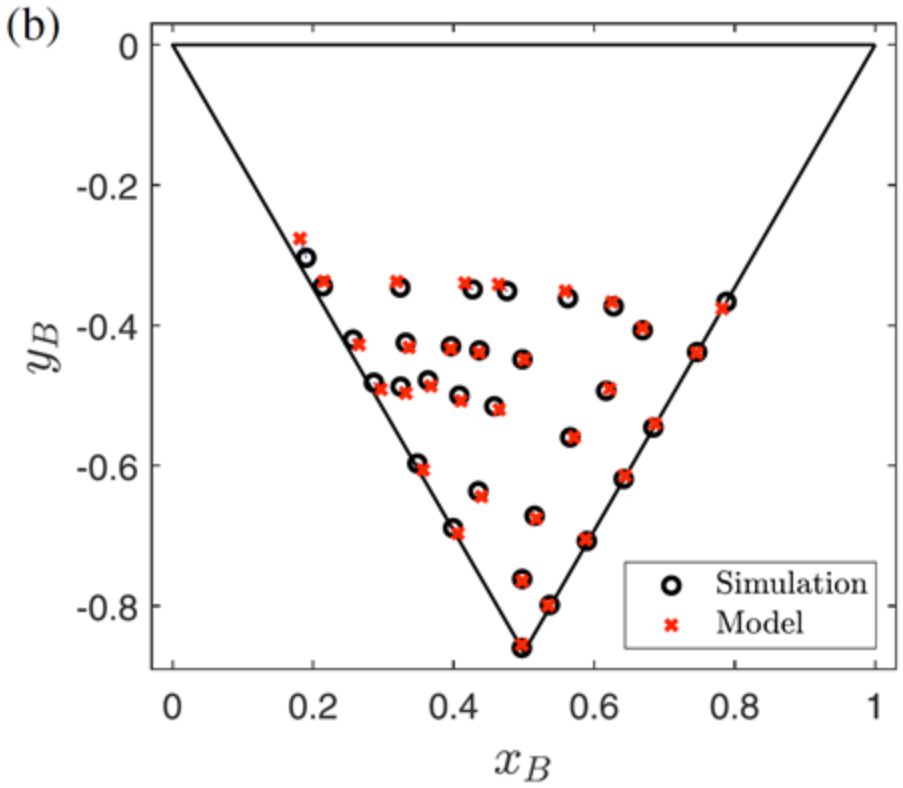
- $f_{11}^0 = -2\varepsilon[C_1 T_{11} + C_2(T_{22} + T_{33}) + C_3 T_{11}^2 + C4(T_{22}^2 + T_{33}^2) + C_5 T_{11}^3 + C_6(T_{22}^3 + T_{33}^3)]$
- $(C_1, C_2, C_3, C_4, C_5, C_6) = (8.2, -3.6, -14.9, 7.5, 11.3, -5.7)$

Homan, Shende, Mani (Phys. Rev. Fluids 9, 094608, 2024)

Assessment of Fitting Error



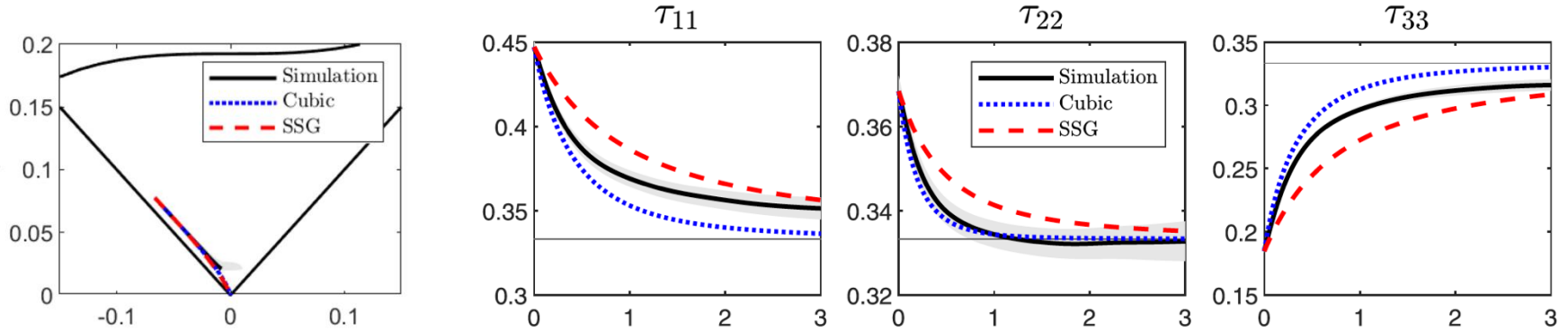
Quadratic fit



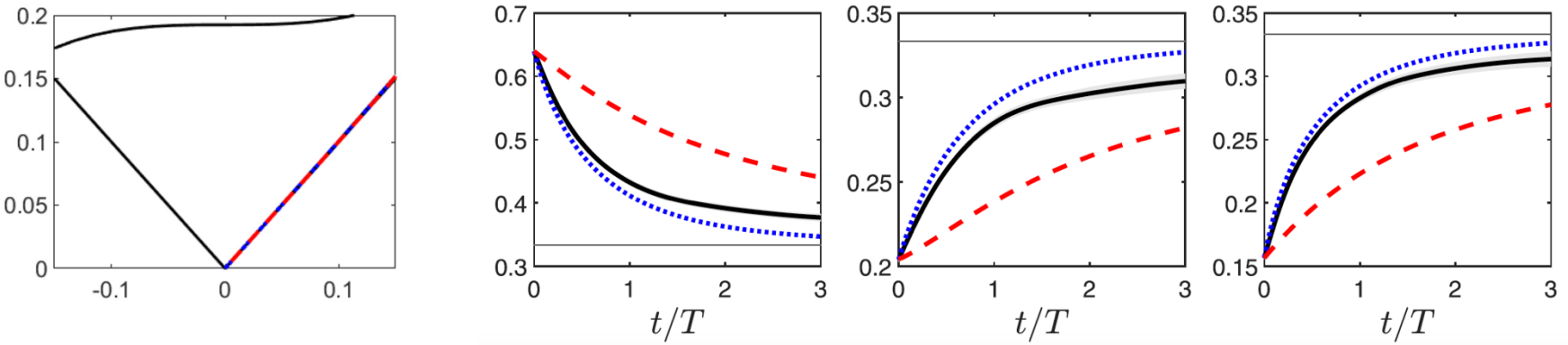
Cubic fit

Model Assessment: Decay of Homogeneous Turbulence

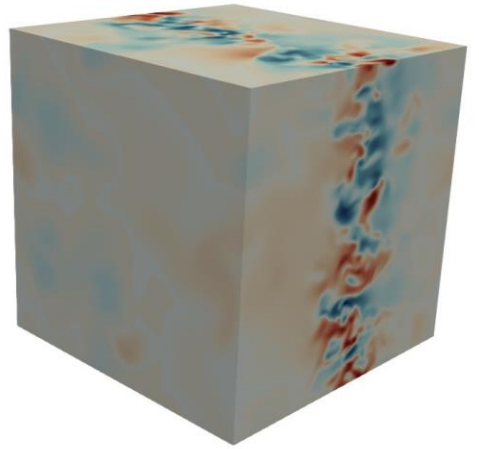
Decay trajectory # 1



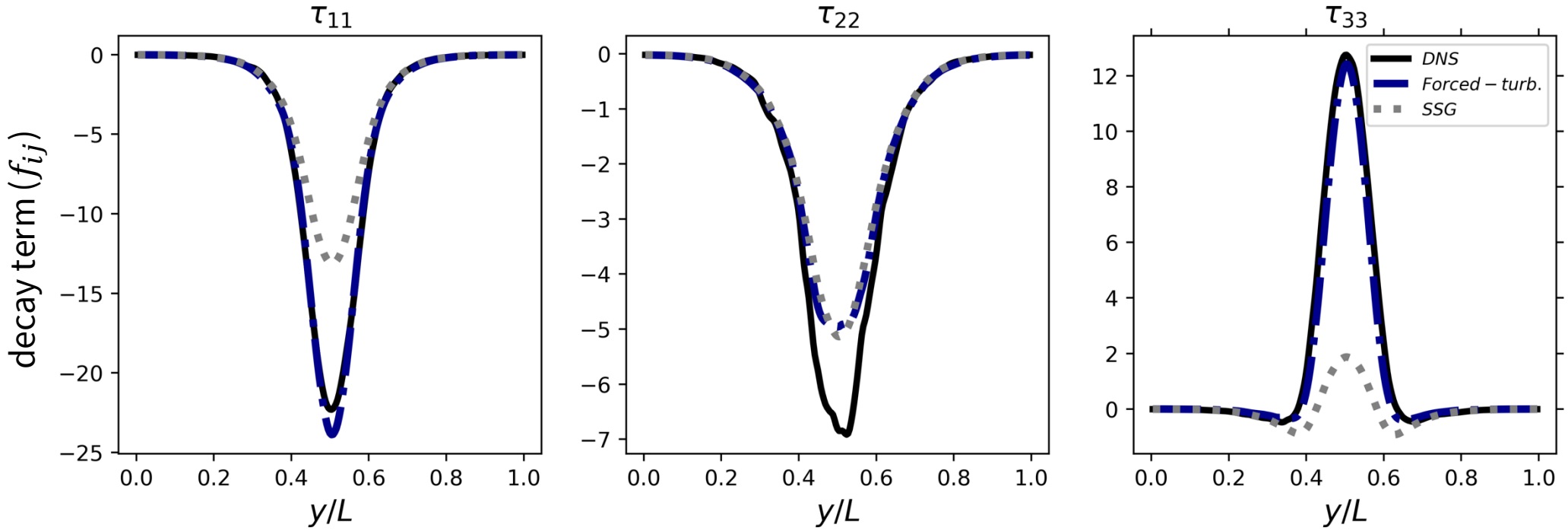
Decay trajectory # 2



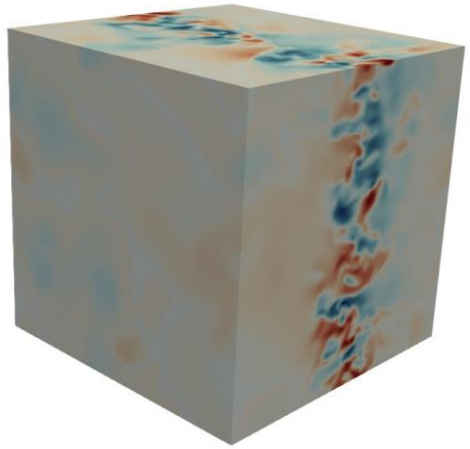
Additional Verification



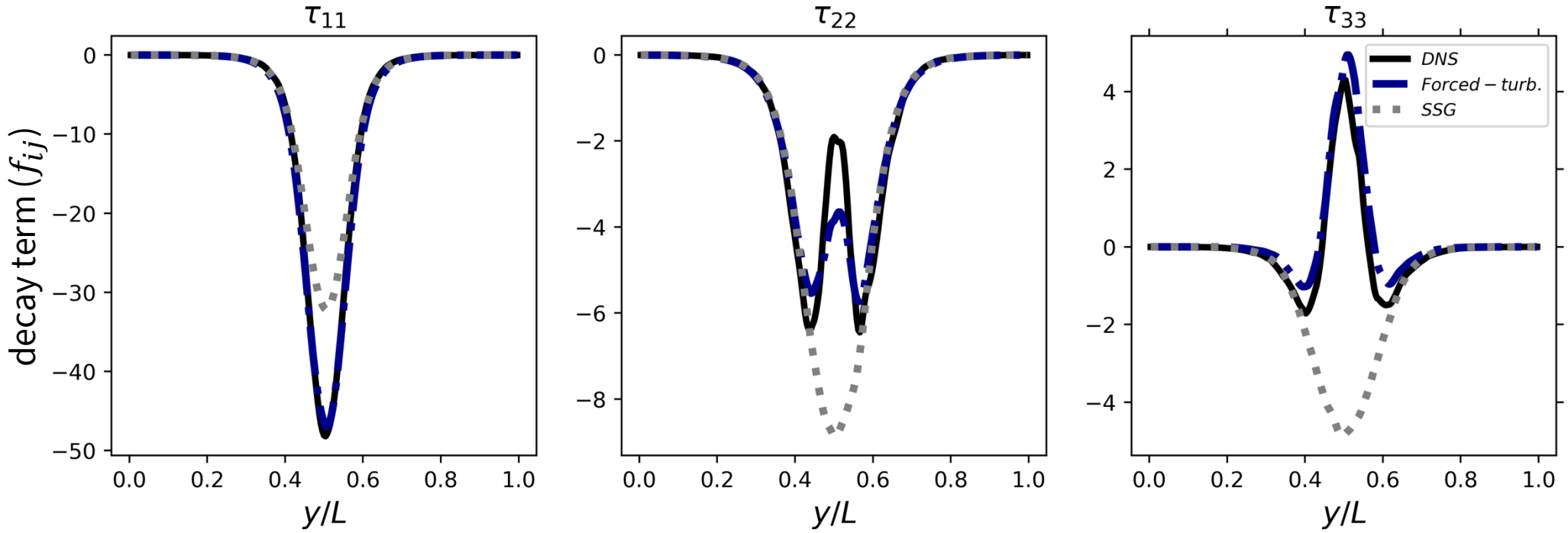
- Decay models developed using homogeneous flows
- Assess model performance in inhomogeneous systems
- Reynolds stress decay (case 31)



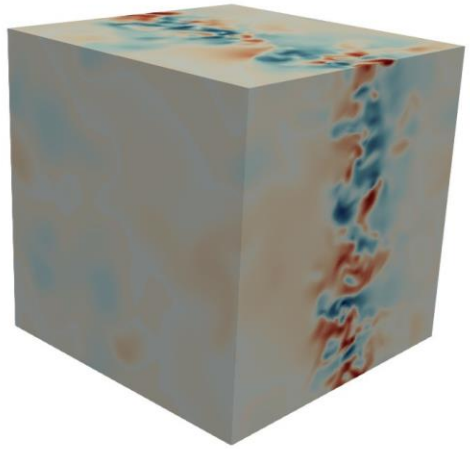
Additional Verification



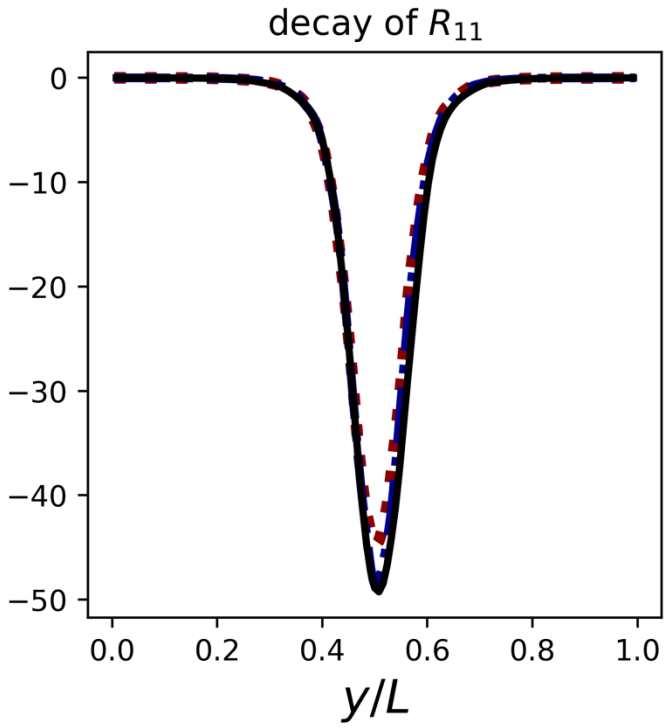
- Decay models developed using homogeneous flows
- Assess model performance in inhomogeneous systems
- Reynolds stress decay (case 14)

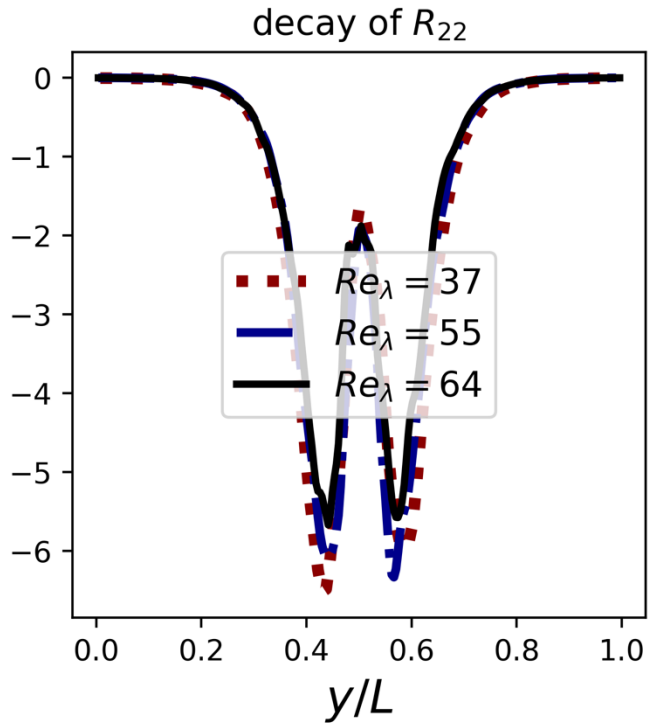


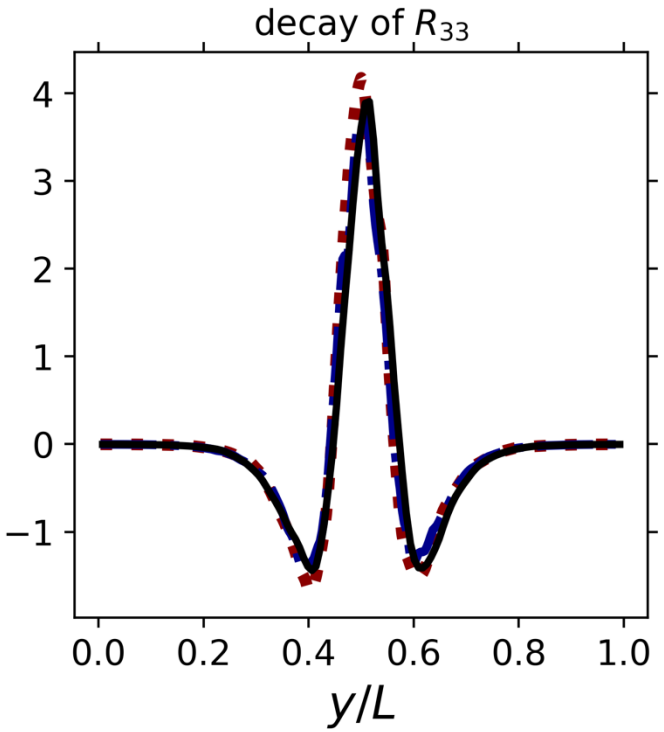
Convergence with respect to Reynolds Number



- Case 14

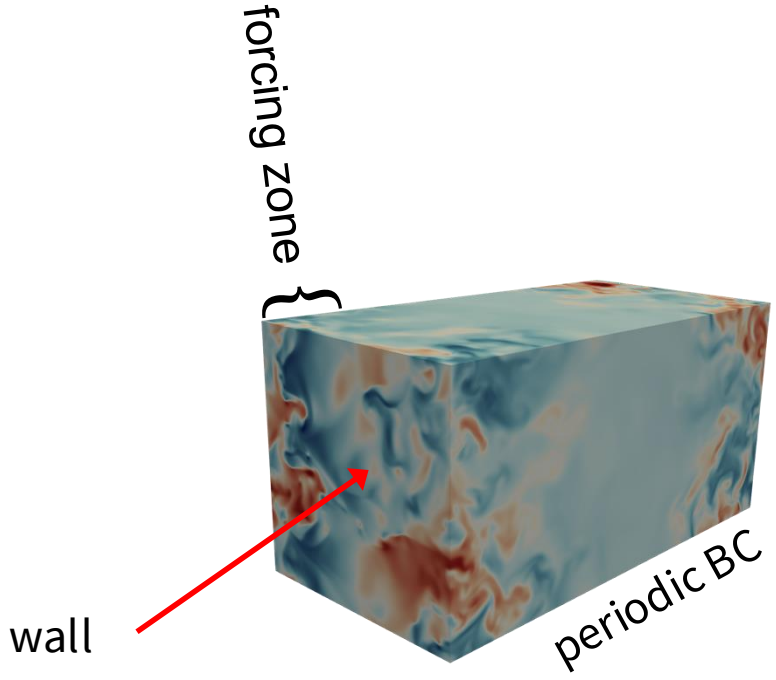






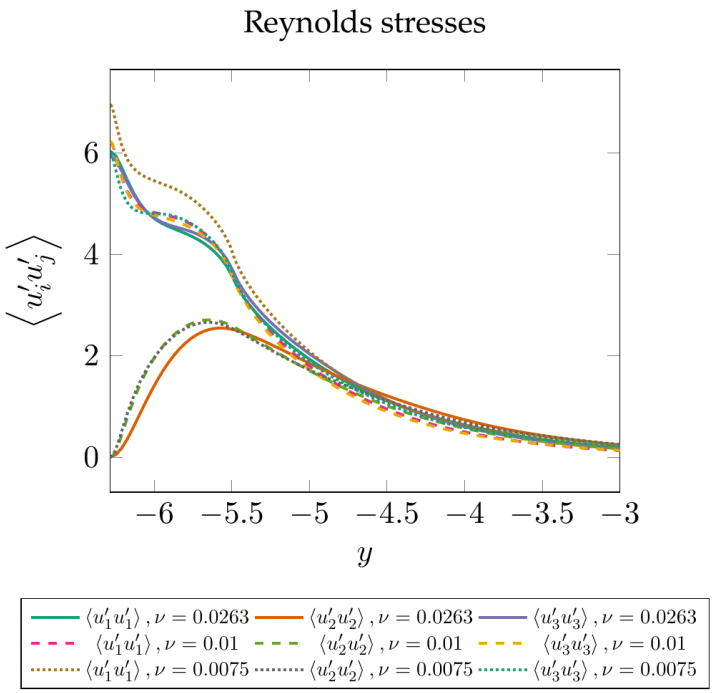
Ongoing Work: Modeling Wall Effects

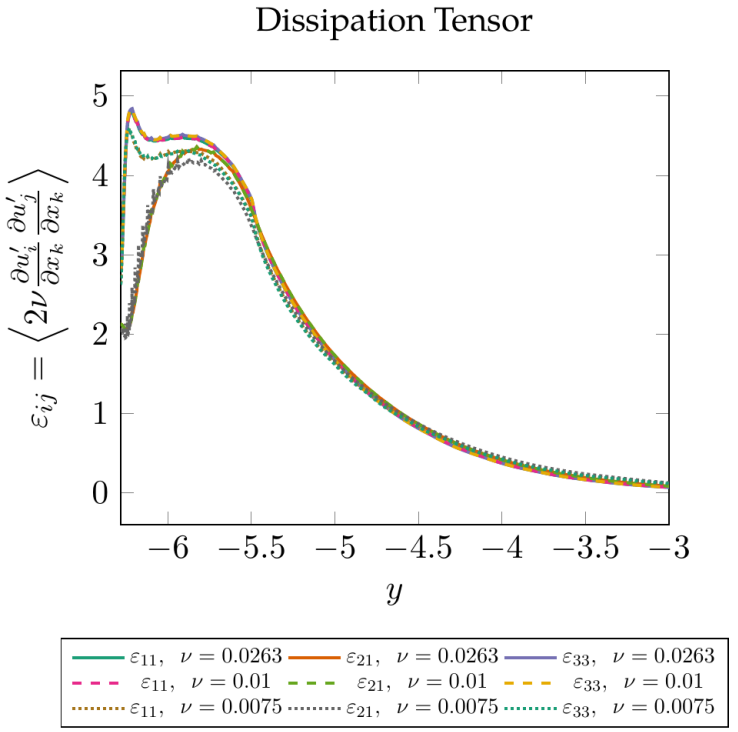
- Decay model should be corrected using wall reflection terms
- $f_{ij} = 2\varepsilon f_{ij}^{0}\left(\underline{\tau}\right) + \left(\frac{k^{\frac{3}{2}}}{y}\right) n_l n_m f_{ijlm}^{y}\left(\underline{\tau}\right) + \cdots$
- Setup: Linearly forced turbulence near a wall
  - Zero mean flow
  - Wide range of anisotropy due to forcing
- Convergence parameters:
  box size, mesh, Re
- Reynolds stress and dissipation budgets closed
- Data to be used for fitting f_{ijlm}^{y}

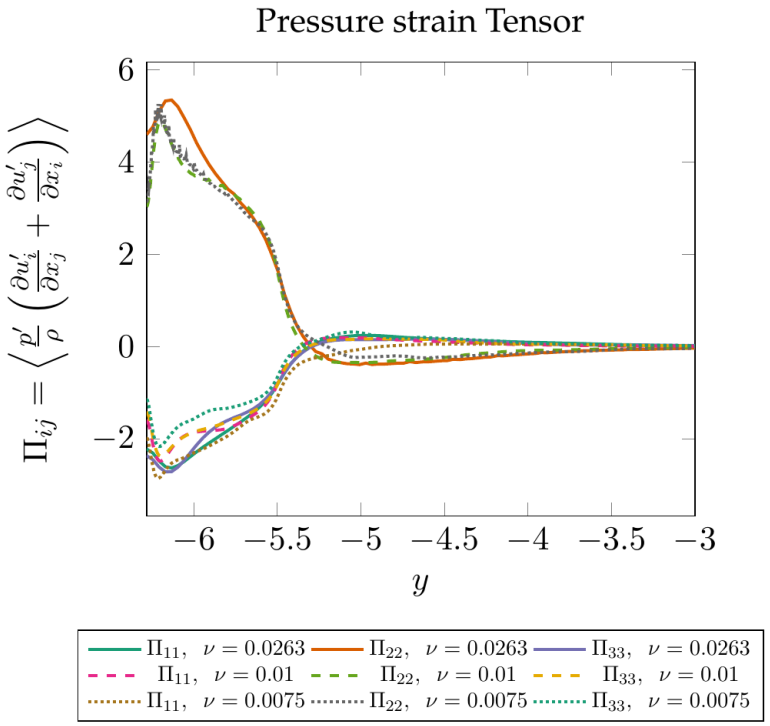


Convergence with respect to Reynolds Number

- In this setup wall boundary condition is a slip condition
- We are investigating walls with no-slip (simulations in progress)
- Sample preliminary results

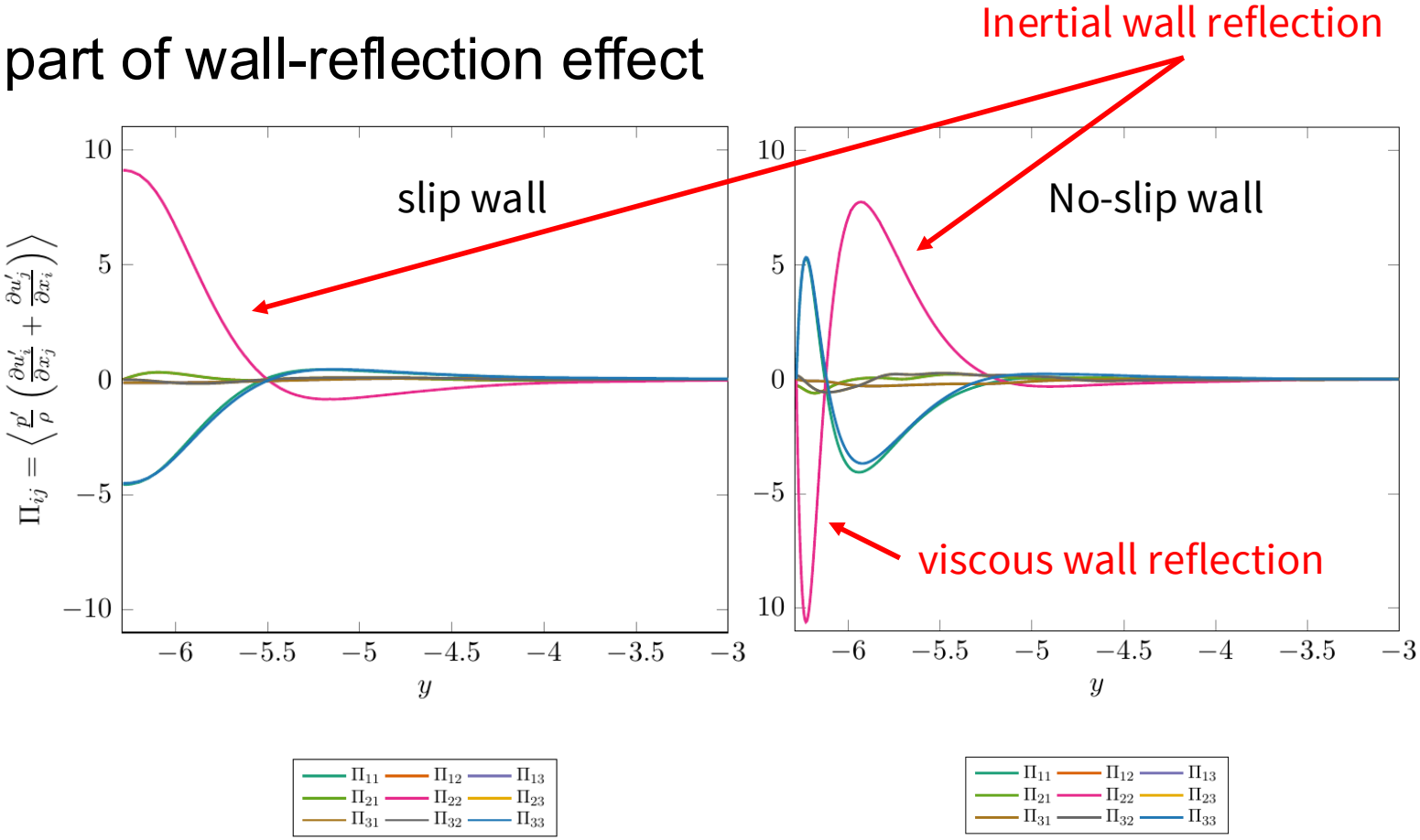






Physics Learning

- Slow pressure strain term near the wall
  - Traditionally modeled as part of wall-reflection effect
- No mean flow
  - Slow term isolated
- Pink curve:
  Wall normal component



- Two regimes of behavior: inertial and viscous

Ref: HIT near wall studied in similar fashion by Perot and Moin (1995)

Summary

- Developed an efficient framework for data generation for assessment and selection of closure models

  → Fast convergence, affordable, provides diverse data

- Smooth closures allow Taylor series expansion with respect to input parameters
  → closure problem divided into subproblems
  → each involving smaller input space dimension
  → substantial reduction in number of adjustable parameters
  → data driven approach crucial for a comprehensive expansion-based modeling

- Identified wide range of canonical setups using volumetrically forced DNS
  → Tailored for piece-by-piece probing of the closure terms

- Dat generation strategy compatible with ML-based approaches if needed