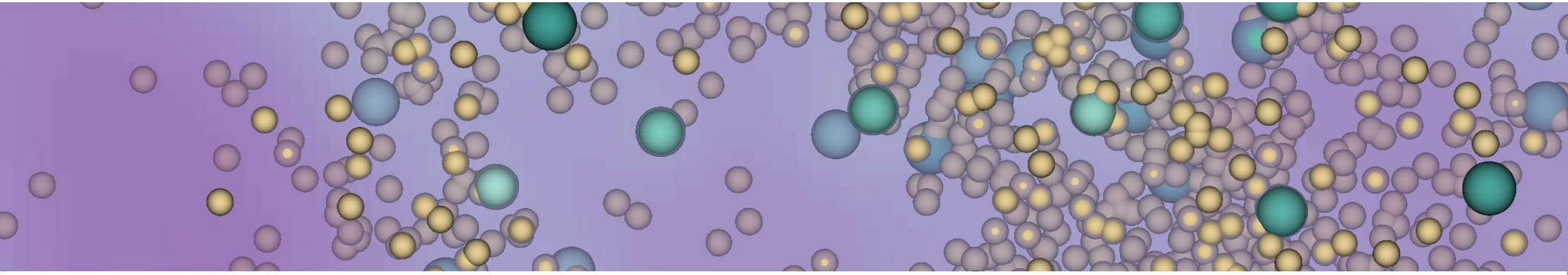
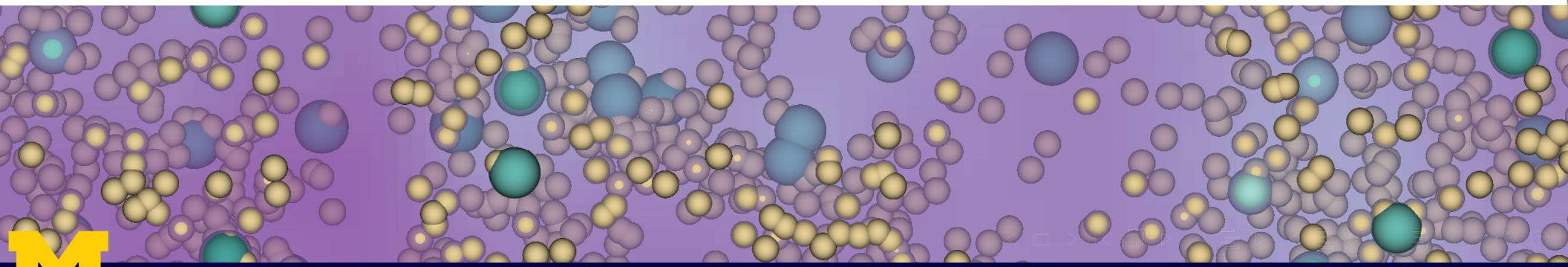
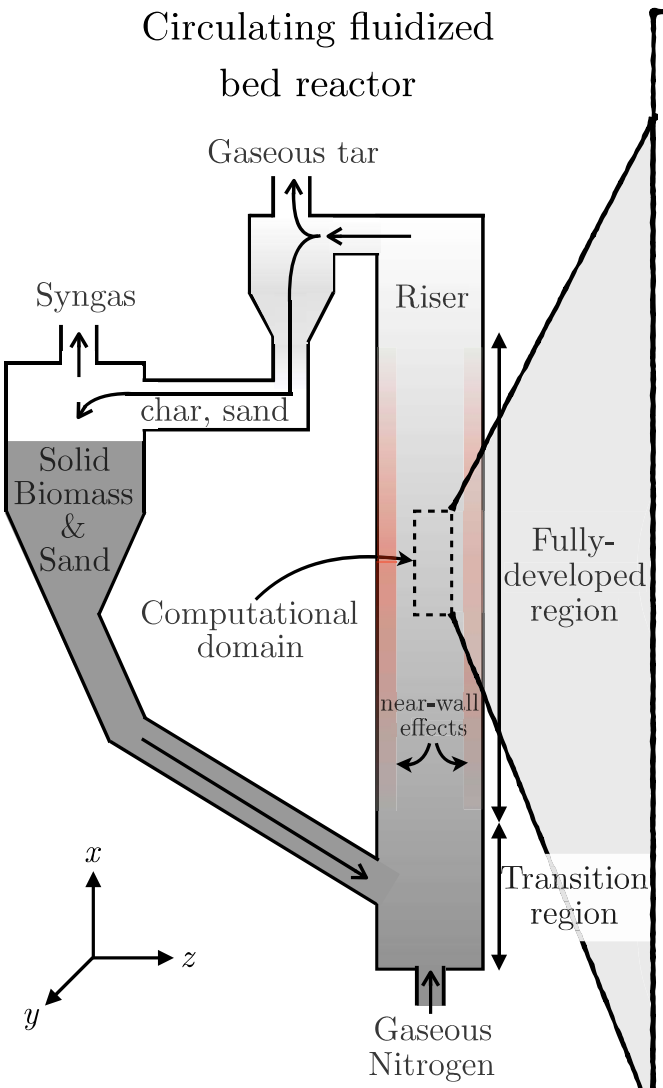


Modeling multiphase turbulence using sparse regression with embedded invariance

Sarah Beetham, Jesse Capecelatro
University of Michigan, Ann Arbor



Motivation

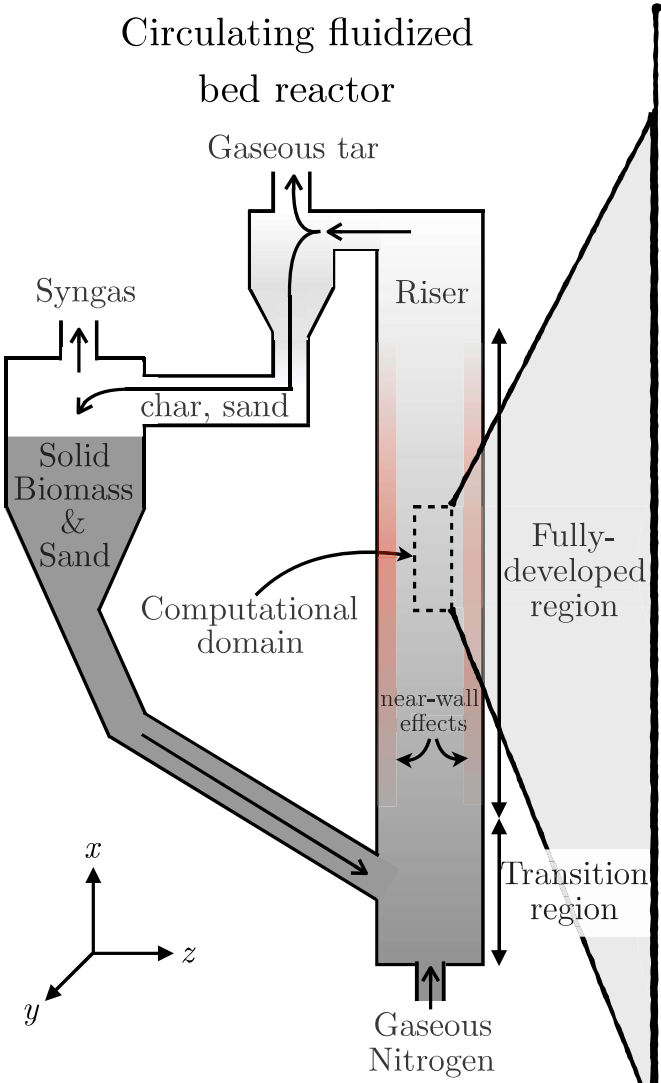


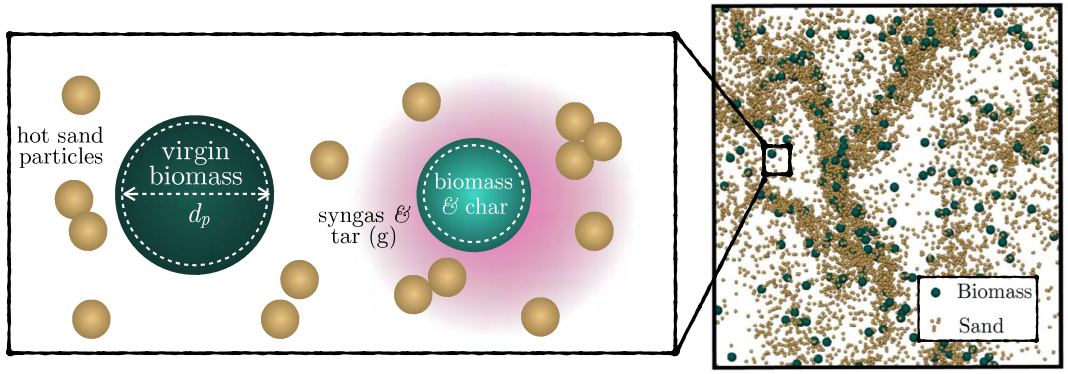
GOAL: Accurate, tractable RANS models for reactive, multiphase flows at industrial scales.

CHALLENGES:

- Strong coupling between phases drives turbulence.
- Turbulence impacts heat and mass transport.
- Turbulence models based on single-phase flow break down.

Motivation



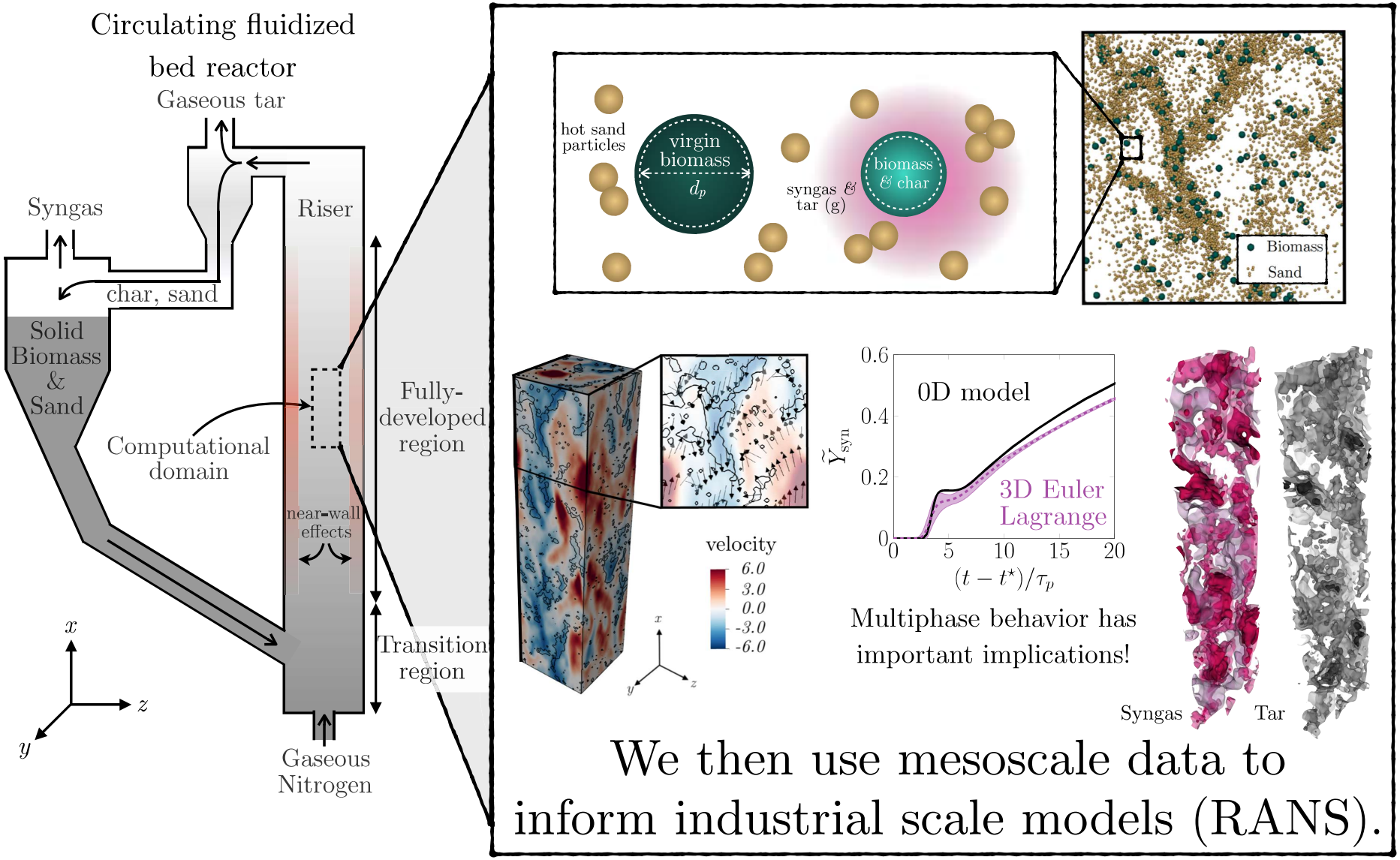


Micro-scale behavior (DNS) informs models for

- Chemical kinetics
- Drag
- Heat transfer

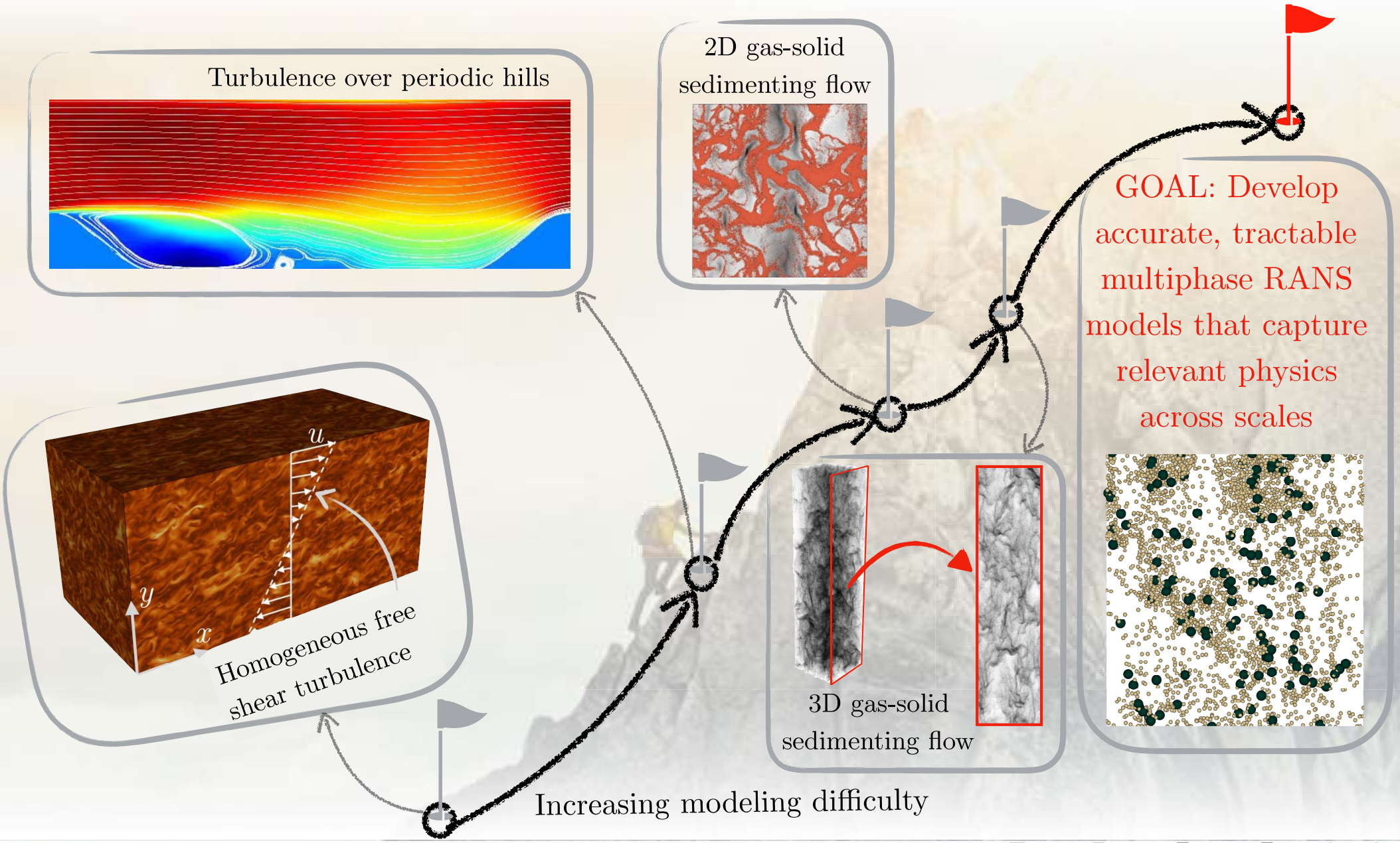
These models are then used to access mesoscale behavior (Euler-Lagrange).

Motivation



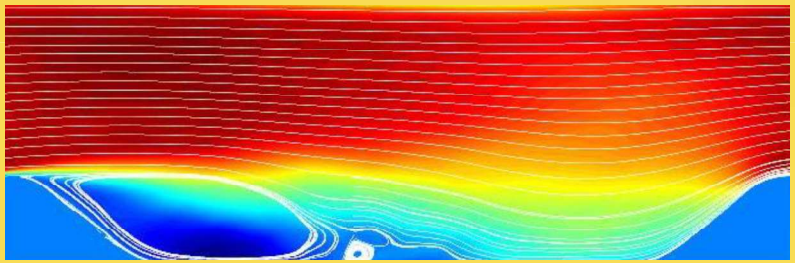
We then use mesoscale data to inform industrial scale models (RANS).

Toward improved multiphase models

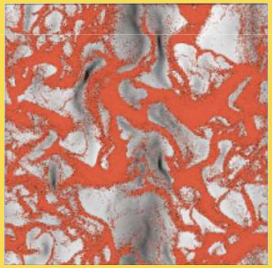


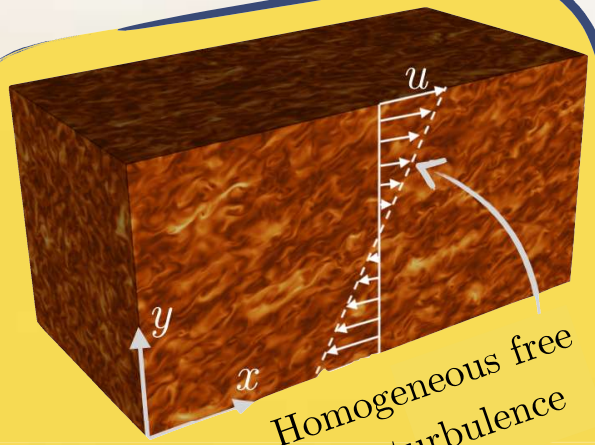
Agenda

Turbulence over periodic hills



2D gas-solid sedimenting flow



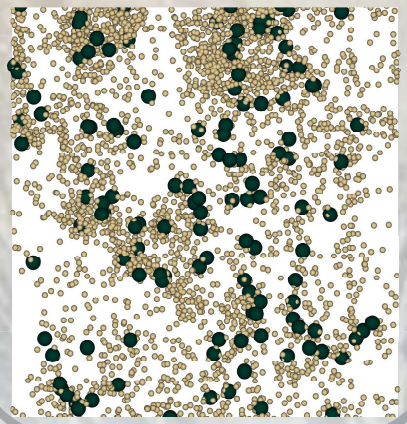


Homogeneous free shear turbulence

Today's agenda:

1. Modeling Methodology
2. Case studies
   i. Homogeneous free shear
   ii. Periodic hills
   iii. 2D gas-solid sedimenting flow

GOAL: Develop accurate, tractable multiphase RANS models that capture relevant physics across scales



Sparse regression with embedded form invariance

Postulate that a model for $\mathcal{D}_{ij}$ takes the form,

$$\mathcal{D}_{ij} = f\left(\beta^{(n)}, \mathcal{T}_{ij}^{(n)}\right) = \sum_n \beta^{(n)} \mathcal{T}_{ij}^{(n)}$$

where,

- f is a *linear* function of basis functions $\mathcal{T}_{ij}^{(n)}$ which may be *nonlinear*,
- $\mathcal{T}_{ij}^{(n)}$ are based upon knowledge of physics,
- β_k are coefficients that at most depend (nonlinearly) on the principal invariants of $\mathcal{T}_{ij}^{(n)}$.

In contrast to Neural Networks, this methodology results in a model in compact, algebraic form.

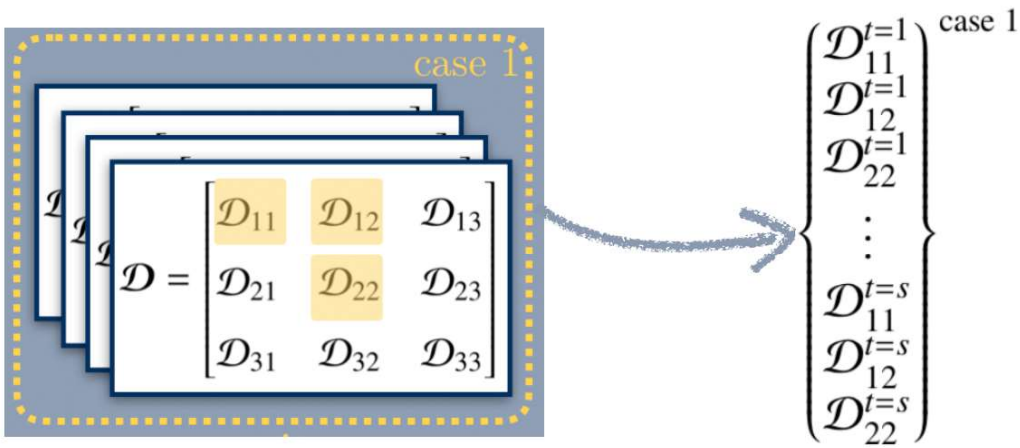
Sparse regression with embedded form invariance

We can ensure form invariance due to

1. Linearity in the basis functions. This guarantees invariance upon Galilean rotation, $\mathbf{Q}$

$$\mathbf{Q} f(\beta_1 \mathcal{T}_{ij}^{(1)}, \beta_2 \mathcal{T}_{ij}^{(2)}, \ldots) \mathbf{Q}^{\mathrm{T}} = f(\beta_1 \mathbf{Q} \mathcal{T}_{ij}^{(1)} \mathbf{Q}^{\mathrm{T}}, \beta_2 \mathbf{Q} \mathcal{T}_{ij}^{(2)} \mathbf{Q}^{\mathrm{T}}, \ldots)$$

2. Formulating the problem as tall and skinny vectors. This ensures that β does not vary based on orientation.



Sparse regression with embedded form invariance

$$\mathbb{D} = \mathbb{T}\,\hat{\boldsymbol{\beta}}$$

A *sparse* vector of coefficients

Vertically concatenate n unique components over c cases, each containing s snapshots.

case 1

$$\mathcal{D} = \begin{bmatrix} \mathcal{D}_{11} & \mathcal{D}_{12} & \mathcal{D}_{13} \\ \mathcal{D}_{21} & \mathcal{D}_{22} & \mathcal{D}_{23} \\ \mathcal{D}_{31} & \mathcal{D}_{32} & \mathcal{D}_{33} \end{bmatrix}$$

case c

$$\mathcal{D} = \begin{bmatrix} \mathcal{D}_{11} & \mathcal{D}_{12} & \mathcal{D}_{13} \\ \mathcal{D}_{21} & \mathcal{D}_{22} & \mathcal{D}_{23} \\ \mathcal{D}_{31} & \mathcal{D}_{32} & \mathcal{D}_{33} \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} \left\{\begin{matrix} \mathcal{D}_{11}^{t=1} \\ \mathcal{D}_{12}^{t=1} \\ \mathcal{D}_{22}^{t=1} \\ \vdots \\ \mathcal{D}_{11}^{t=s} \\ \mathcal{D}_{12}^{t=s} \\ \mathcal{D}_{22}^{t=s} \end{matrix}\right\} \text{case 1} \\ \vdots \\ \left\{\begin{matrix} \mathcal{D}_{11}^{t=1} \\ \mathcal{D}_{12}^{t=1} \\ \mathcal{D}_{22}^{t=1} \\ \vdots \\ \mathcal{D}_{11}^{t=s} \\ \mathcal{D}_{12}^{t=s} \\ \mathcal{D}_{22}^{t=s} \end{matrix}\right\} \text{case } c \end{bmatrix}}_{\mathbb{D}\in\mathbb{R}^{(n\cdot s\cdot c)\times 1}}$$

Vertically concatenate each of the tensors in a minimal integrity basis.

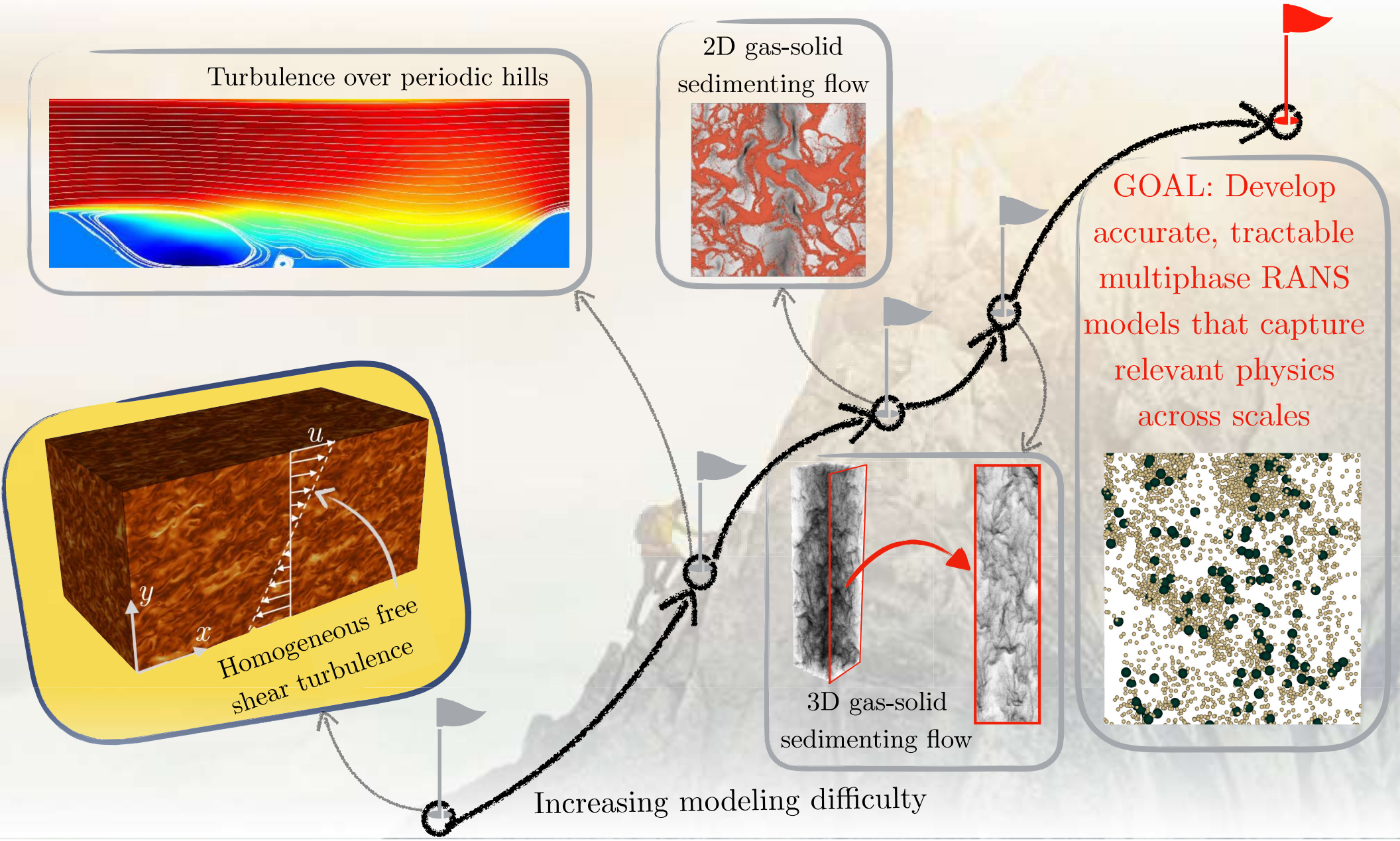
$$\underbrace{\begin{bmatrix} \left\{\begin{matrix} \mathcal{T}_{11}^{(1),\,t=1} & \mathcal{T}_{11}^{(2),\,t=1} & \cdots & \mathcal{T}_{11}^{(g),\,t=1} \\ \mathcal{T}_{12}^{(1),\,t=1} & \mathcal{T}_{12}^{(2),\,t=1} & \cdots & \mathcal{T}_{12}^{(g),\,t=1} \\ \mathcal{T}_{22}^{(1),\,t=1} & \mathcal{T}_{22}^{(2),\,t=1} & \cdots & \mathcal{T}_{22}^{(g),\,t=1} \\ \vdots & \vdots & & \vdots \\ \mathcal{T}_{11}^{(1),\,t=s} & \mathcal{T}_{11}^{(2),\,t=s} & \cdots & \mathcal{T}_{11}^{(g),\,t=s} \\ \mathcal{T}_{12}^{(1),\,t=s} & \mathcal{T}_{12}^{(2),\,t=s} & \cdots & \mathcal{T}_{12}^{(g),\,t=s} \\ \mathcal{T}_{22}^{(1),\,t=s} & \mathcal{T}_{22}^{(2),\,t=s} & \cdots & \mathcal{T}_{22}^{(g),\,t=s} \end{matrix}\right\} \text{case 1} \\ \vdots \\ \left\{\begin{matrix} \mathcal{T}_{11}^{(1),\,t=1} & \mathcal{T}_{11}^{(2),\,t=1} & \cdots & \mathcal{T}_{11}^{(g),\,t=1} \\ \mathcal{T}_{12}^{(1),\,t=1} & \mathcal{T}_{12}^{(2),\,t=1} & \cdots & \mathcal{T}_{12}^{(g),\,t=1} \\ \mathcal{T}_{22}^{(1),\,t=1} & \mathcal{T}_{22}^{(2),\,t=1} & \cdots & \mathcal{T}_{22}^{(g),\,t=1} \\ \vdots & \vdots & & \vdots \\ \mathcal{T}_{11}^{(1),\,t=s} & \mathcal{T}_{11}^{(2),\,t=s} & \cdots & \mathcal{T}_{11}^{(g),\,t=s} \\ \mathcal{T}_{12}^{(1),\,t=s} & \mathcal{T}_{12}^{(2),\,t=s} & \cdots & \mathcal{T}_{12}^{(g),\,t=s} \\ \mathcal{T}_{22}^{(1),\,t=s} & \mathcal{T}_{22}^{(2),\,t=s} & \cdots & \mathcal{T}_{22}^{(g),\,t=s} \end{matrix}\right\} \text{case } c \end{bmatrix}}_{\mathbb{T}\in\mathbb{R}^{(n\cdot s\cdot c)\times g}}$$

Sparse regression with embedded form invariance

$$\hat{\boldsymbol{\beta}} = \min_{\boldsymbol{\beta}} \boxed{||\mathbb{D} - \mathbb{T}\boldsymbol{\beta}||_2^2} + \boxed{\lambda||\boldsymbol{\beta}||_1}$$

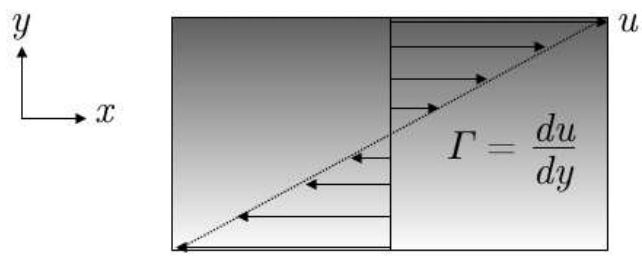
The *l-2* norm regresses the coefficients to the data (OLS).

The *l-1* norm induces sparsity in the coefficients with increasing the tuning parameter, λ.


Turbulence over periodic hills
2D gas-solid sedimenting flow
GOAL: Develop accurate, tractable multiphase RANS models that capture relevant physics across scales
u
y
x
Homogeneous free shear turbulence
3D gas-solid sedimenting flow
Increasing modeling difficulty

Sparse identification of single-phase free shear turbulence

System under consideration:



Mean flow quantities:

$\langle u_i \rangle$	Mean velocity
$\langle u_i' u_j' \rangle$	Mean Reynolds stresses
$k = \frac{1}{2}\langle u_k' u_k' \rangle$	Turbulent kinetic energy
$\Gamma_{ij} = \frac{\partial \langle u_i \rangle}{\partial x_j}$	Shear rate tensor

$$\frac{d}{dt}\langle u_i' u_j' \rangle = \mathcal{P}_{ij} + \mathcal{R}_{ij} - \varepsilon_{ij}$$

$\mathcal{P}_{ij} = -\left[\langle u_j' u_k' \rangle \frac{\partial \langle u_i \rangle}{\partial x_k} + \langle u_i' u_k' \rangle \frac{\partial \langle u_j \rangle}{\partial x_k}\right]$	Production, Closed
$\mathcal{R}_{ij} = \left\langle \frac{p}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right\rangle$	Redistribution, Unclosed
$\varepsilon_{ij} = 2\nu \left\langle \frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}\right\rangle$	Dissipation, Unclosed

Sparse identification of single-phase free shear turbulence

Formulation of the invariant tensor basis:

$$\frac{\mathcal{R}_{ij}}{\varepsilon} = \sum_{n=1}^{\infty} \beta^{(n)} \mathcal{T}_{ij}^{(n)} \left(b_{ij}, \hat{R}_{ij}, \hat{S}_{ij} \right)$$

Anisotropy tensor: $b_{ij} = \frac{\langle u_i' u_j' \rangle}{2k} - \frac{1}{3}\delta_{ij}$

Mean rotation rate tensor: $\hat{R}_{ij} = \frac{1}{2}\frac{k}{\varepsilon}\left(\frac{\partial \langle u_i \rangle}{\partial x_j} - \frac{\partial \langle u_j \rangle}{\partial x_i} \right)$

Mean shear rate tensor: $\hat{S}_{ij} = \frac{1}{2}\frac{k}{\varepsilon}\left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right)$

Since $\mathcal{R}_{ij}$ is symmetric, deviatoric and traceless, each of the bases must also satisfy these properties.

Sparse identification of single-phase free shear turbulence

Validating the methodology with 'synthetic data'

$$\frac{d}{dt}\langle u_i u_j \rangle = \mathcal{P}_{ij} + \mathcal{R}_{ij} - \frac{2}{3}\varepsilon\delta_{ij}$$

$$\mathcal{R}_{ij}^{\text{LRR-IP}} = -C_R\frac{\varepsilon}{k}\left(\langle u_i u_j - \frac{2}{3}k\delta_{ij}\right) - C_2\left(\mathcal{P}_{Ij} - \frac{2}{3}\mathcal{P}\delta_{ij}\right)$$

$$\frac{d\varepsilon}{dt} = -C_{\varepsilon 1}\mathcal{P}\frac{\varepsilon}{k} - C_{\varepsilon 2}\frac{\varepsilon^2}{k}$$

Collect data for shear rates: $S = (3.2,\ 16.1,\ 30.7)$

with $C_R = 1.8$, $C_2 = 0.6$, $C_{\varepsilon 1} = 1.44$ and $C_{\varepsilon 1} = 1.92$

[7] Pope, S. (2012)

Sparse identification of single-phase free shear turbulence

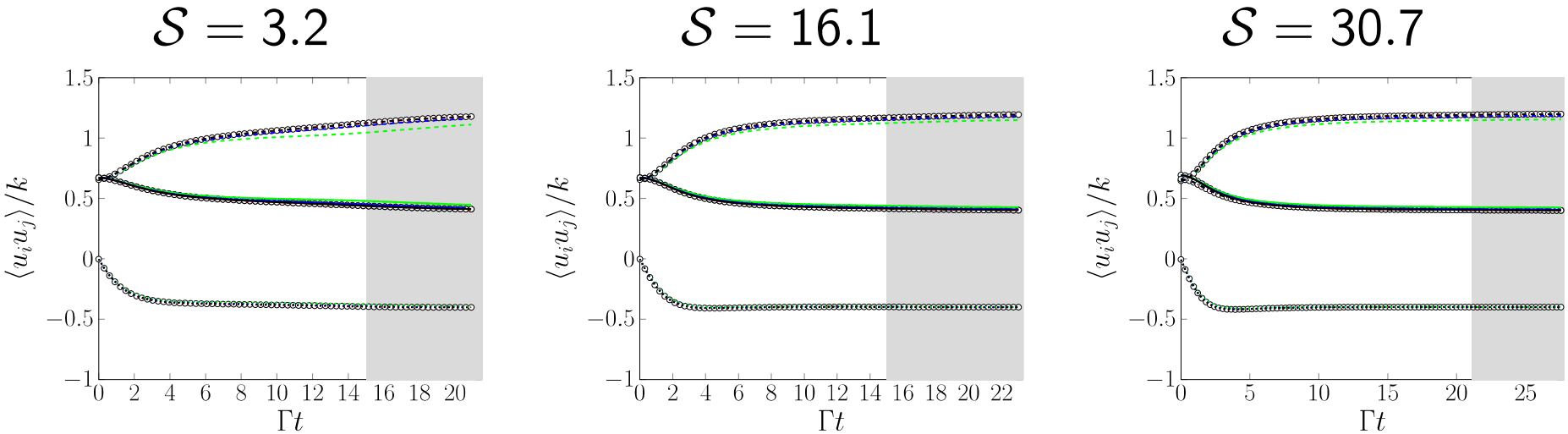
Validating the methodology with 'synthetic data'

Order	$\mathcal{T}^{(n)}$	LRR-IP	Sparse Regression $\lambda = 0.1$ $\mathcal{N} = 0$	$\lambda = 0.1$ $\mathcal{N} = 0.01$	$\lambda = 0.1$ $\mathcal{N} = 0.05$	$\lambda = 0.5$ $\mathcal{N} = 0.1$
0						
	S_{ij}	0.8	0.8	0.8007	0.8121	0.8394
1						
	b_{ij}	-3.6	-3.6	-3.5984	-3.5617	-3.4715
	$R_{il}b_{lj} + R_{jl}b_{li}$	1.2	1.2	1.2010	1.2187	1.2608
	$S_{il}b_{lj} + S_{jl}b_{li} - \frac{2}{3}S_{lm}b_{ml}\delta_{ij}$	1.2	1.2	1.2011	1.2213	1.2700
2						
	$b^2_{ij} - \frac{1}{3}b^2_{ll}\delta_{ij}$	0	0	0	0	0
	$S_{il}b^2_{lj} + S_{jl}b^2_{li} - \frac{2}{3}S_{lm}b^2_{ml}\delta_{ij}$	0	0	0	0	0
	$R_{il}b^2_{lj} + R_{jl}b^2_{li}$	0	0	0	0	0
3						
	$b^2_{ik}R_{kp}b_{pj} - b_{il}R_{lk}b^2_{kj}$	0	0	0	0	0
	mean error	–	*0.0*	*7.1e-4*	*0.013*	*0.044*

Sparse regression correctly returns the model, even when artificial noise is added.

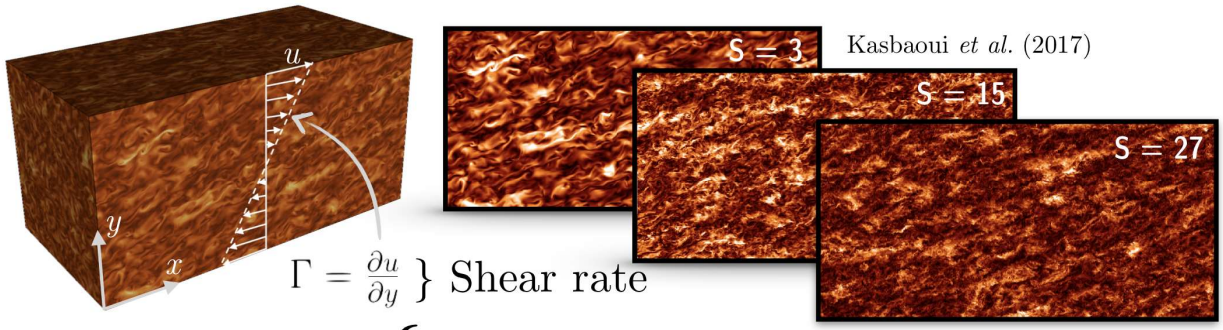
Sparse identification of single-phase free shear turbulence

Validating the methodology with 'synthetic data'



Sparse regression correctly returns the model, even when artificial Gaussian noise is added with standard deviations of: 0 (——), 0.01 (- - -), 0.05 (·····) and 0.15 (·····).

Sparse identification of single-phase free shear turbulence



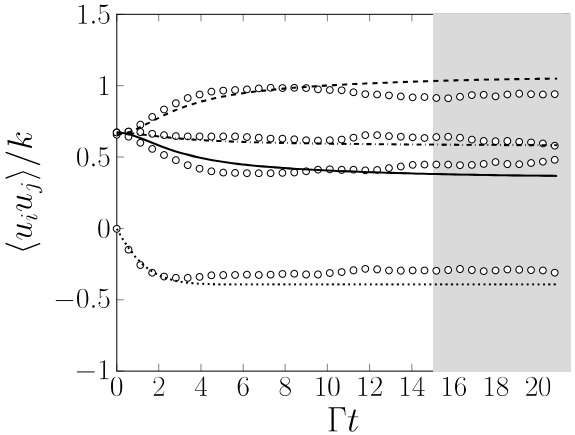
Kasbaoui *et al.* (2017)

$\Gamma = \frac{\partial u}{\partial y}$ } Shear rate

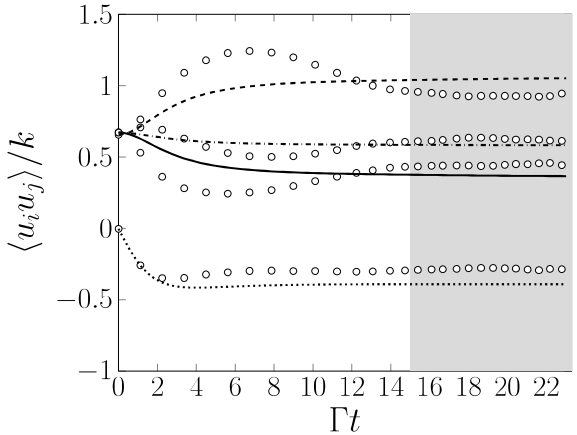
Non-dimensional shear rate $\left\{ S = \frac{2\Gamma k_0}{\varepsilon_0} \right.$

DNS simulated on Flux Domain: 1024x512x512 , (2π× π× π)

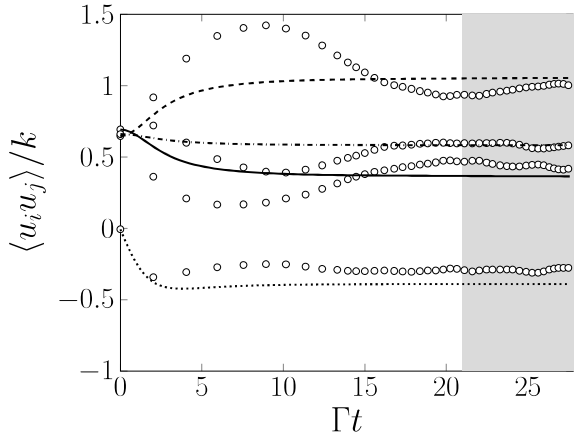
$\mathcal{S} = 3.2$



$\mathcal{S} = 16.1$



$\mathcal{S} = 30.7$

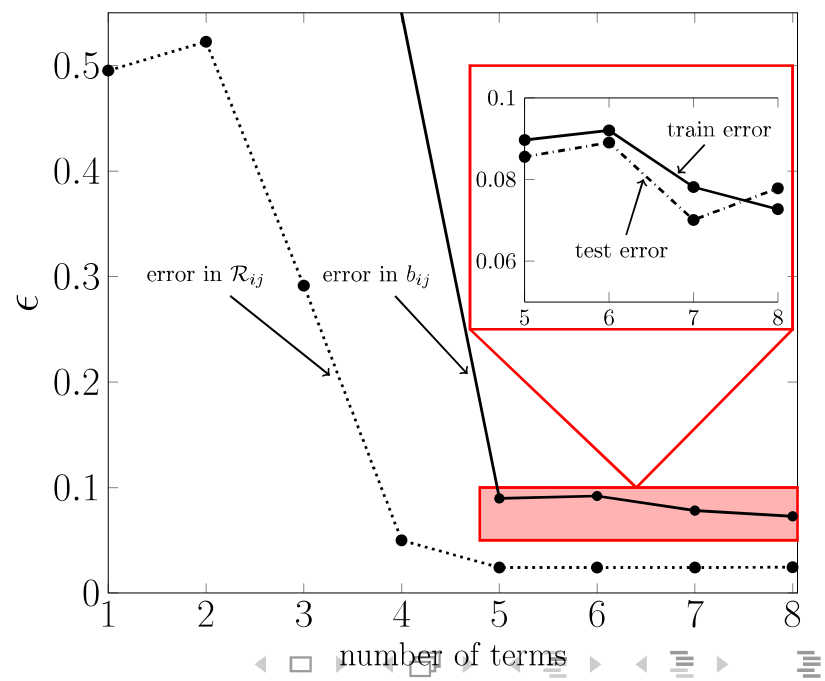


Can sparse regression uncover a better model than LRR-IP?

Sparse identification of single-phase free shear turbulence

order in b_{ij}	$\mathcal{T}^{(n)}$	LRR-IP	Sparse Regression $\lambda = 0.75$	$\lambda = 0.6$	$\lambda = 0.5$	$\lambda = 0$
0	S_{ij}	0.8	1.01	1.01	0.98	0.98
	b_{ij}	-3.6	1.27	1.31	1.45	1.46
1	$R_{il}b_{lj} + R_{jl}b_{li}$	1.2	1.53	1.56	1.49	1.48
	$S_{il}b_{lj} + S_{jl}b_{li} - \frac{2}{3}S_{lm}b_{ml}\delta_{ij}$	1.2	1.73	1.71	1.79	1.78
	$b_{ij}^2 - \frac{1}{3}b_{ll}^2\delta_{ij}$	0	5.22	4.64	7.02	6.71
2	$S_{il}b_{lj}^2 + S_{jl}b_{li}^2 - \frac{2}{3}S_{lm}b_{ml}^2\delta_{ij}$	0	0	0	0.57	0.56
	$R_{il}b_{lj}^2 + R_{jl}b_{li}^2$	0	0	0	0	0.13
3	$b_{ik}^2R_{kp}b_{pj} - b_{il}R_{lk}b_{kj}^2$	0	0	-0.65	2.08	2.45
	mean training error	0.26	0.090	0.092	0.078	0.073
	mean testing error		0.086	0.089	0.070	0.078

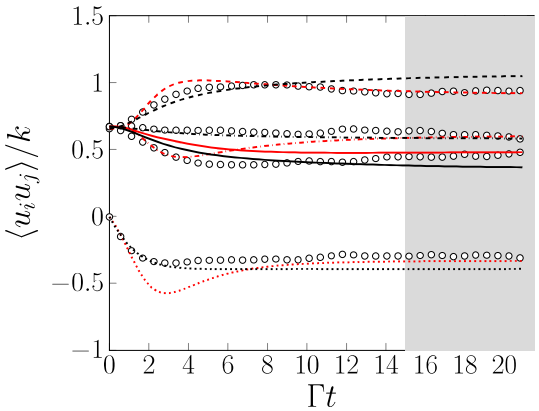
Yes! Sparse regression identifies a model that reduces error in the Reynolds stresses by more than a factor of 3 compared with LRR-IP.



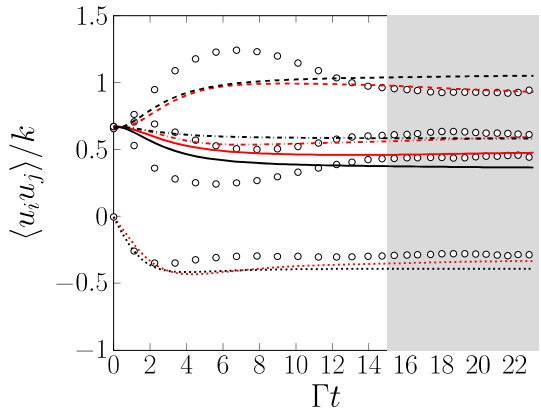
Sparse identification of single-phase free shear turbulence

Training dataset

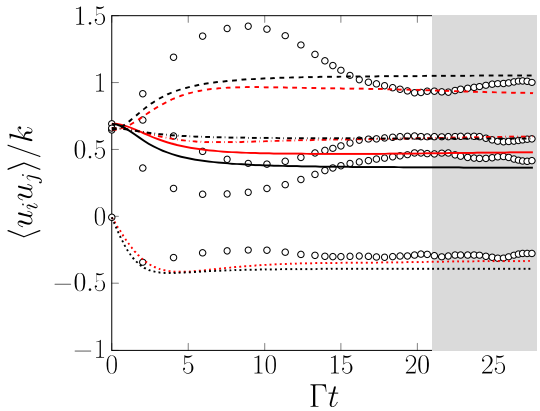
$\mathcal{S} = 3.2$



$\mathcal{S} = 16.1$

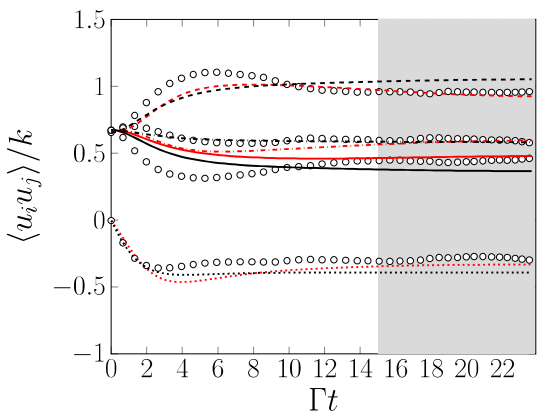


$\mathcal{S} = 30.7$

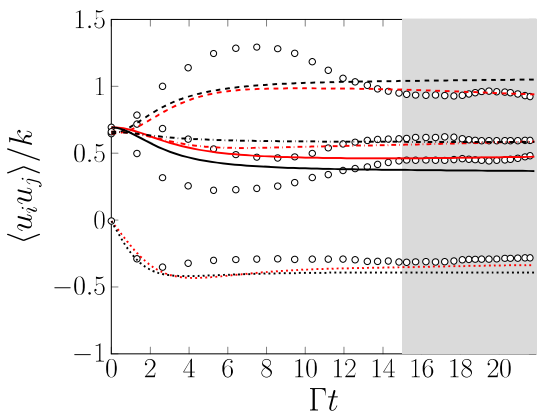


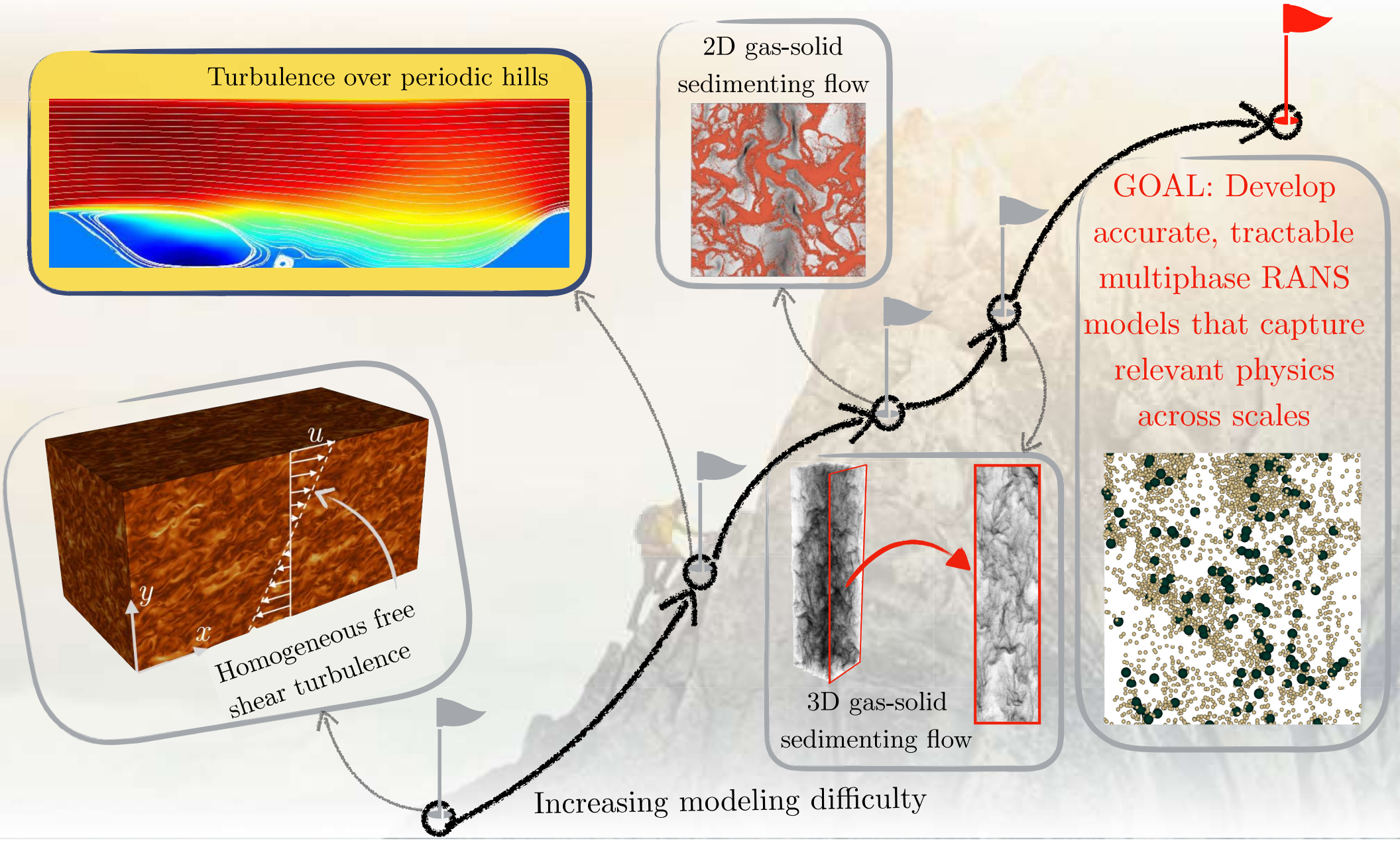
Testing dataset

$\mathcal{S} = 10.0$



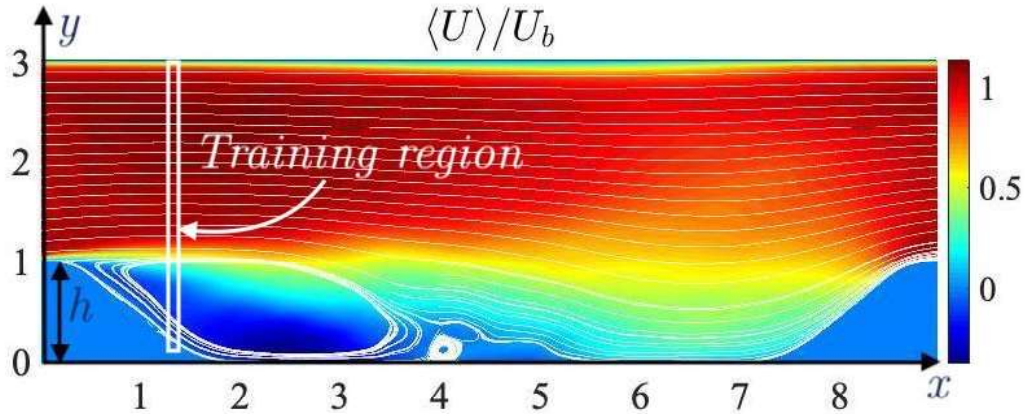
$\mathcal{S} = 20.1$




Turbulence over periodic hills
2D gas-solid sedimenting flow
GOAL: Develop accurate, tractable multiphase RANS models that capture relevant physics across scales
u
y
x
Homogeneous free shear turbulence
3D gas-solid sedimenting flow
Increasing modeling difficulty

Configuration under study

Flow through a periodically constricted channel.



Boundary conditions:

- No slip at walls
- Periodic in z-direction and inlet/outlet

Velocity is forced to maintain Re= 2800 at the hill crest.

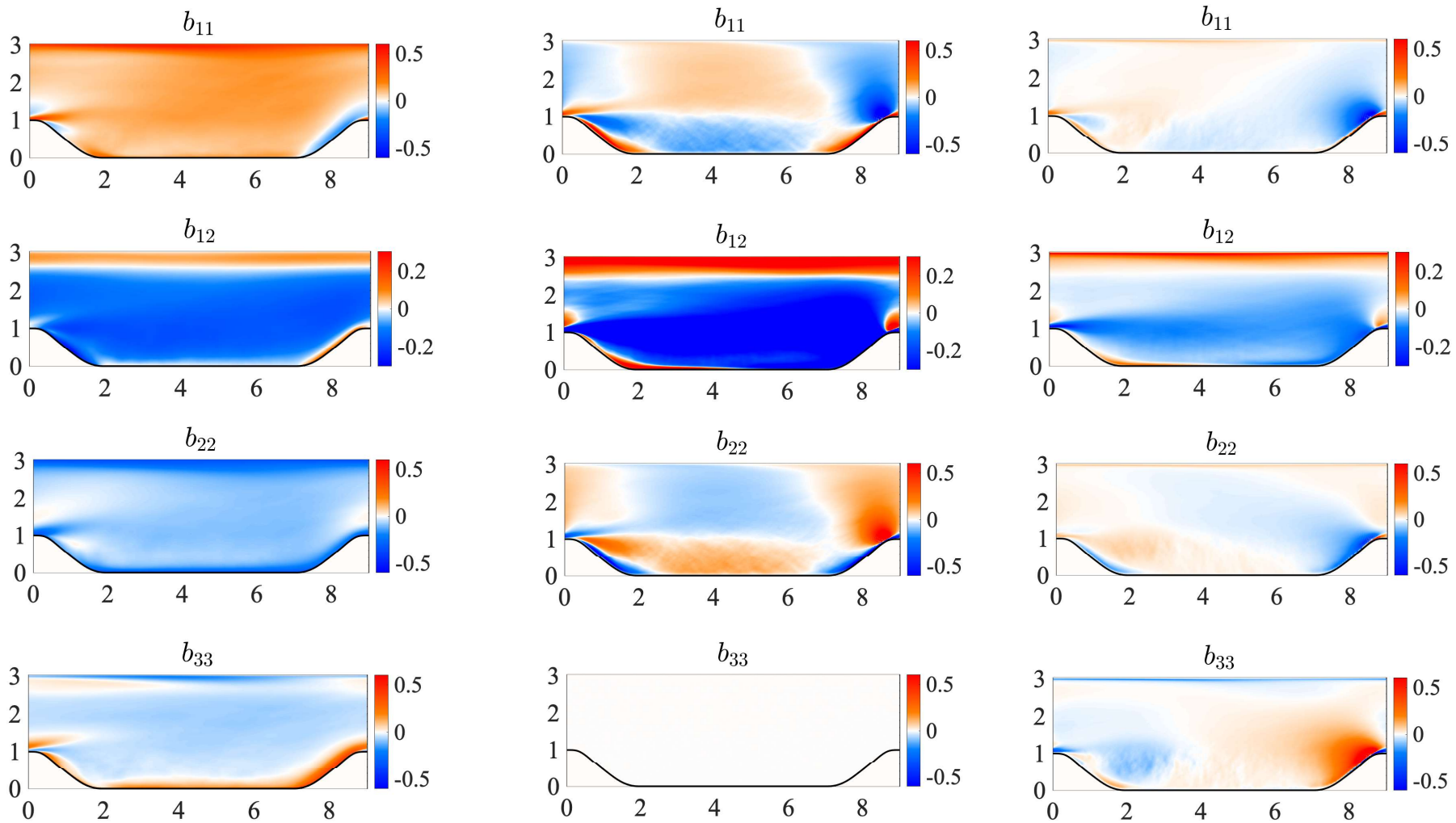
Fully resolved DNS:

- $(N_x, N_y, N_z) = (512, 380, 214)$
- $(L_x, L_y, L_z) = (9h, 3.036h, 4.5h)$
- Hill geometry corresponding to Breuer et. al (2009)

Steady data is averaged in z and over 44 flow-through times.

Improved model using minimal dataset

DNS	LEVM	Sparse Regression



$\epsilon = \|\|b_{ij}^{\mathrm{DNS}} - b_{ij}^{\mathrm{model}}\|\|_2 / \|\|b_{ij}^{\mathrm{DNS}}\|\|_2$	1.76	1.11

Algebraic form of improved model

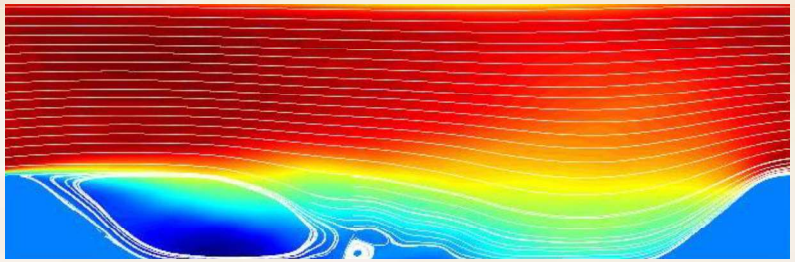
$\mathcal{T}^{(n)}$	LEVM	Sparse Regression
$\boldsymbol{S}$	-0.09	-0.0158
$\boldsymbol{SR} - \boldsymbol{RS}$	0	0
$\boldsymbol{S}^2 - \frac{1}{3}\mathrm{tr}(\boldsymbol{S}^2)\mathbf{I}$	0	-0.012
$\boldsymbol{R}^2 - \frac{1}{3}\mathrm{tr}(\boldsymbol{R}^2)\mathbf{I}$	0	-0.0125
$\boldsymbol{RS}^2 - \boldsymbol{S}^2\boldsymbol{R}$	0	0
$\boldsymbol{RR}^2\boldsymbol{S} - \boldsymbol{SRR}^2 - \frac{2}{3}\mathrm{tr}(\boldsymbol{SR}^2)\mathbf{I}$	0	0
$\boldsymbol{RSR}^2 - \boldsymbol{R}^2\boldsymbol{SR}$	0	0
$\boldsymbol{SRS}^2 - \boldsymbol{S}^2\boldsymbol{RS}$	0	0
$\boldsymbol{R}^2\boldsymbol{S}^2 + \boldsymbol{S}^2\boldsymbol{R}^2 - \frac{2}{3}\mathrm{tr}(\boldsymbol{S}^2\boldsymbol{R}^2)\mathbf{I}$	0	0
$\boldsymbol{RS}^2\boldsymbol{R}^2 - \boldsymbol{R}^2\boldsymbol{S}^2\boldsymbol{R}$	0	0
error	1.76	1.11

Modeling parameters:

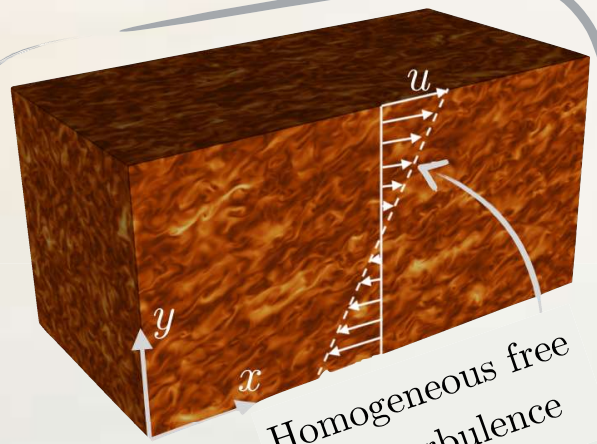
$\lambda = 0.1$

training set: 380 points at $x/h = 1.3$

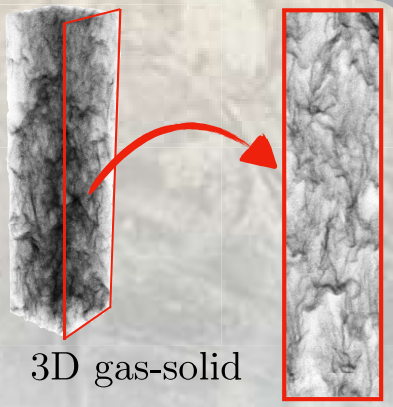
Turbulence over periodic hills



2D gas-solid sedimenting flow

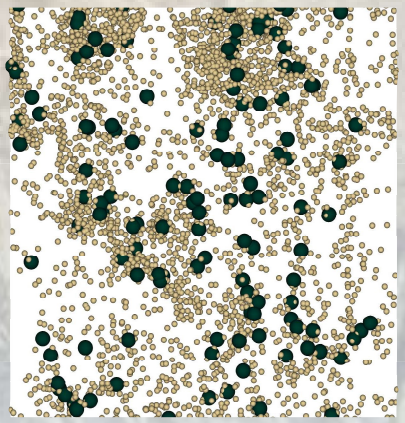


Homogeneous free shear turbulence



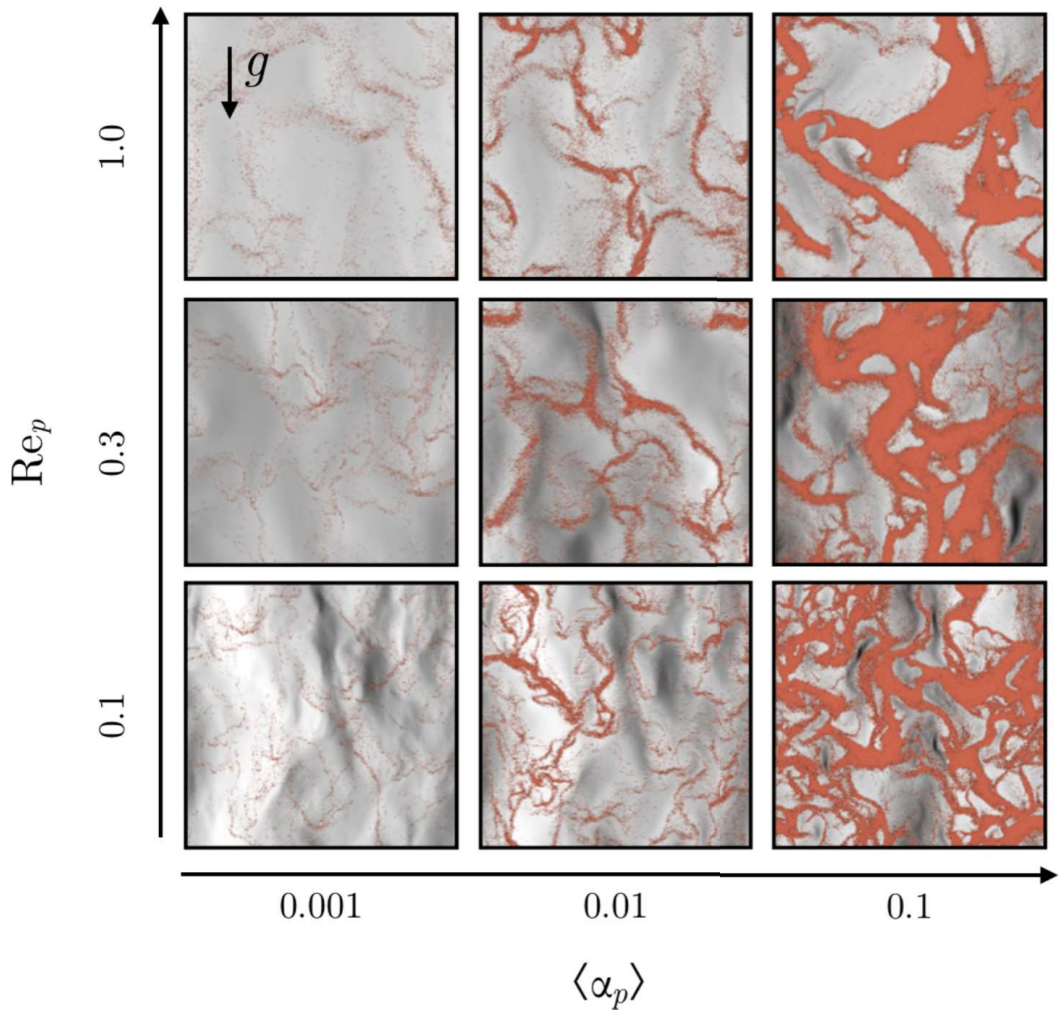
3D gas-solid sedimenting flow

GOAL: Develop accurate, tractable multiphase RANS models that capture relevant physics across scales



Increasing modeling difficulty

Multiphase behavior is complex



- Initially, particles are randomly distributed and gas is quiescent.
- Gravitational body force leads to spontaneous clustering.
- Two-way coupling between phases induces turbulence in gas phase.
- Multiphase dynamics are governed by high dimensional parameter space.

RANS equations for fully-developed CIT

Phase-averaging of the mesoscale equations yields RANS equations for two-way coupled turbulent flows.

$$\frac{1}{2}\frac{\partial \langle u_f'^2 \rangle_f}{\partial t} = \frac{1}{\rho_f}\left(\underbrace{\left\langle p_f \frac{\partial u_f'}{\partial x} \right\rangle_f}_{\text{Pres. Strain}} - \underbrace{\left\langle \sigma_{f,xi} \frac{\partial u_f'}{\partial x_i} \right\rangle_f}_{\text{Visc. Diff.}} \right)$$

$$+ \underbrace{\frac{\varphi}{\tau_p}\left(\langle u_f' u_p' \rangle_p - \langle u_f'^2 \rangle_p \right)}_{\text{Drag Exchange}}$$

$$+ \underbrace{\frac{\varphi}{\tau_p}\langle u_f' \rangle_p \langle u_p \rangle_p}_{\text{Drag Prod.}} + \frac{\varphi}{\tau_p}\left(\underbrace{\left\langle u_f' \frac{\partial p_f'}{\partial x} \right\rangle_p}_{\text{Press. Exch.}} - \underbrace{\left\langle u_f' \frac{\partial \sigma_{f,xi}'}{\partial x_i} \right\rangle_p}_{\text{Visc. Exch.}} \right)$$

τ_p: particle settling time

φ: mass loading

$(\cdot)'$: fluctuation of quantity $(\cdot)$

R.O. Fox (2014), *JFM*; Capecelatro *et al* (2015), *JFM*

RANS equations for fully-developed CIT

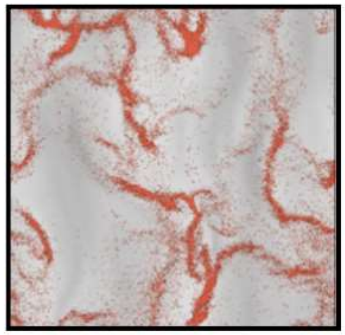
$$\frac{1}{2}\frac{\partial \langle u_f'^2 \rangle_f}{\partial t} = \underbrace{+\frac{\varphi}{\tau_p}\langle u_f' \rangle_p \langle u_p \rangle_p}_{\text{Drag Prod.}} + \frac{\varphi}{\tau_p}\left(\underbrace{\left\langle u_f' \frac{\partial p_f'}{\partial x} \right\rangle_p}_{\text{Press. Exch.}} - \underbrace{\left\langle u_f' \frac{\partial \sigma_{f,xi}'}{\partial x_i} \right\rangle_p}_{\text{Visc. Exch.}} \right)$$

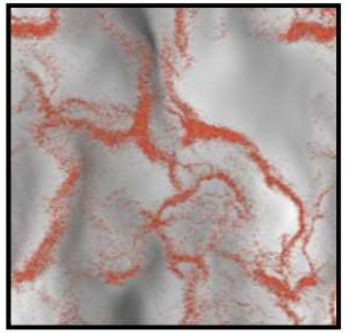
Drag Production

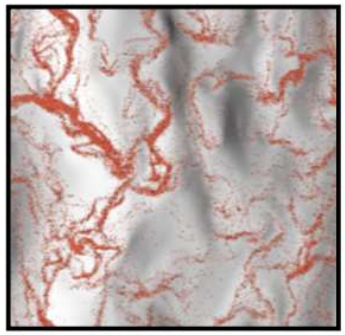
- Sole source of turbulent kinetic energy
- Only present in the gravity-aligned direction and in coupled flows.
- In the absence of clustering, particles are uncorrelated and $\langle u_f' \rangle_p$ is zero.
- The fluid velocity fluctuation *seen by the particle*: $\langle u_f' \rangle_p$

Sparse identification of fully-developed CIT

$$\mathcal{P}_{11}^{drag} = \frac{\varphi}{\tau_p}\langle u_f' \rangle_p \langle u_p \rangle_p$$







Nondimensionalize drag production with dissipation: $\mathcal{P}_{11}^{drag}/\varepsilon_f$

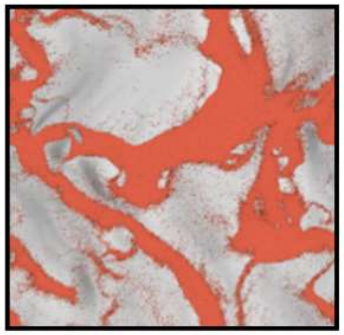
Form minimal tensor basis based upon the following tensors:

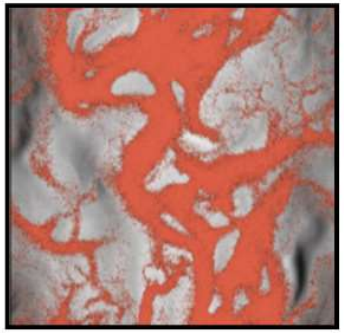
$$\boldsymbol{G}_f = \frac{k_f}{\varepsilon_f^2}\boldsymbol{g}^{\mathrm{T}}\boldsymbol{g}$$

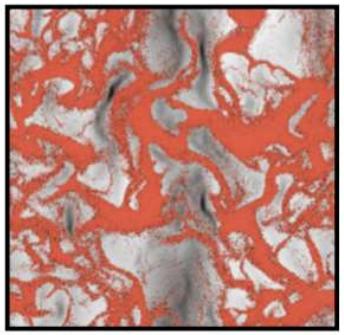
$$\boldsymbol{G}_p = \frac{k_p}{\varepsilon_p^2}\boldsymbol{g}^{\mathrm{T}}\boldsymbol{g}$$

$$\boldsymbol{b}_f = \frac{\langle \boldsymbol{u}_f'''^2 \rangle_f}{2k_f} - \frac{1}{2}\delta_{ij}$$

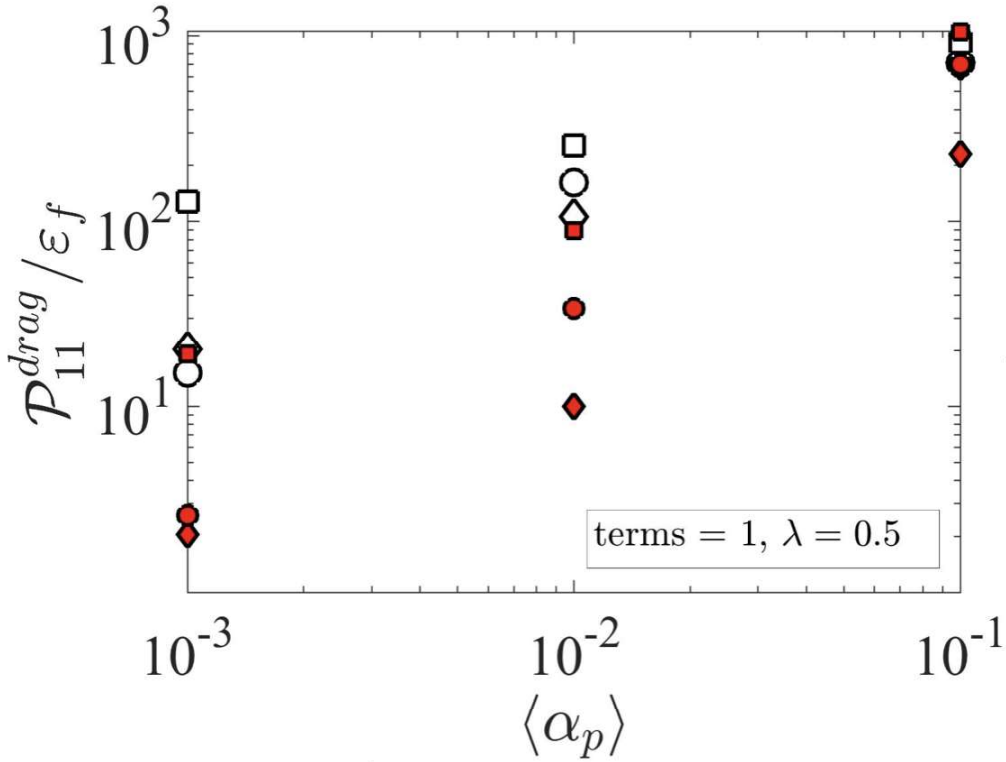
$$\boldsymbol{b}_p = \frac{\langle \boldsymbol{u}_p''^2 \rangle_p}{2k_p} - \frac{1}{2}\delta_{ij}$$

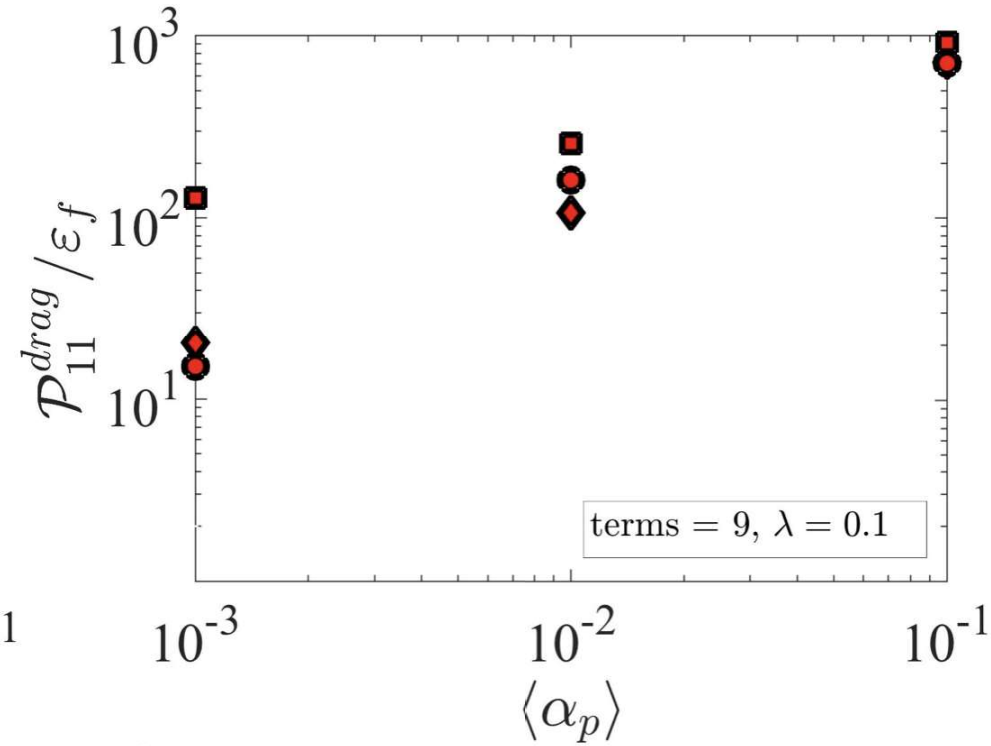






Sparse identification of fully-developed CIT





Re_p	
◇	0.1
○	0.3
□	1.0

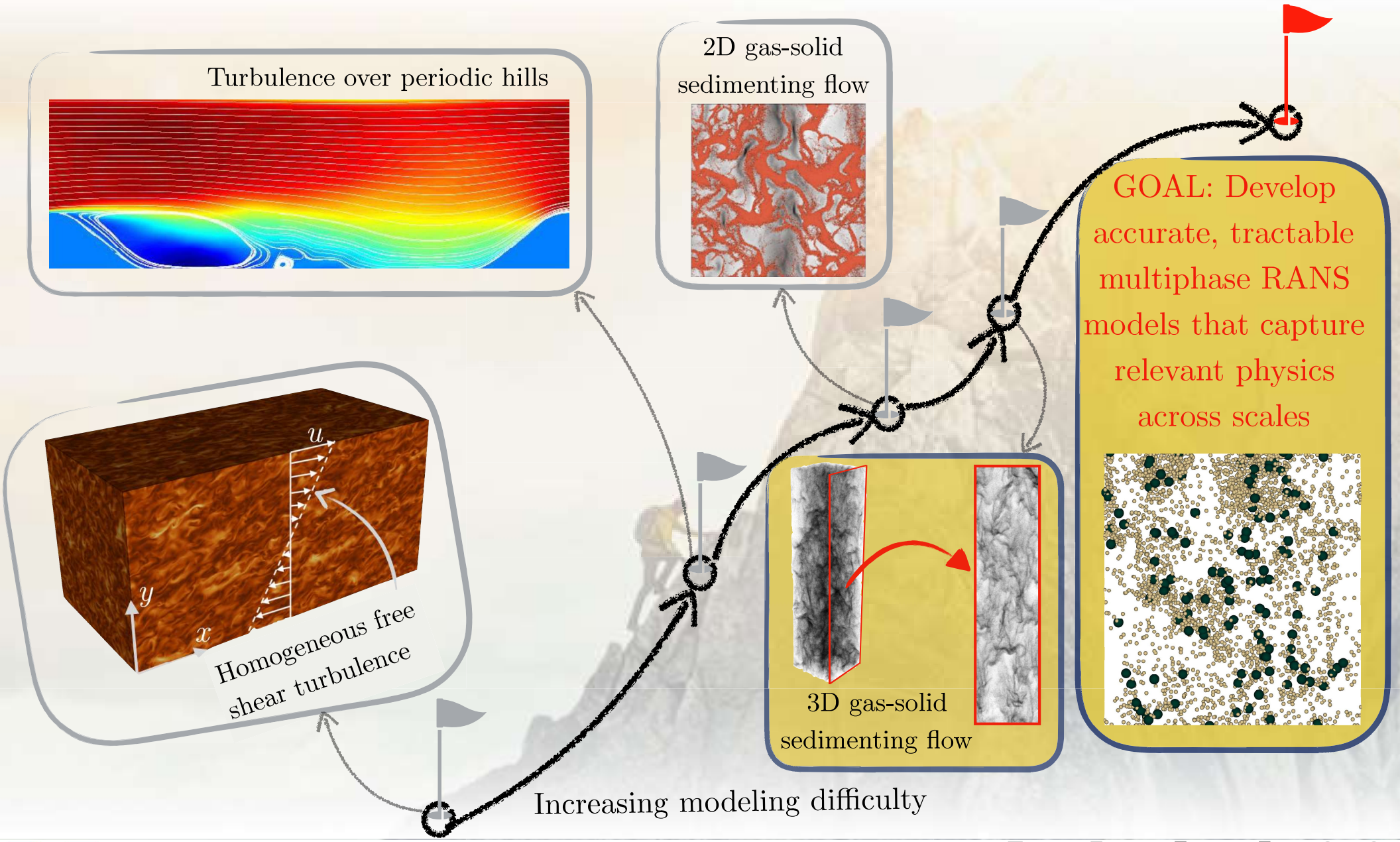
$$\frac{\mathcal{P}^{drag}}{\varepsilon_f} = 7.54\,\varphi\langle\alpha_p\rangle\boldsymbol{G}_f$$

$$\frac{\mathcal{P}^{drag}}{\varepsilon_f} = 6.31\varphi\left(7.54\,\langle\alpha_p\rangle + 0.30\mathrm{Re}_p + 0.32\mathrm{Re}_p^4\right)\boldsymbol{G}_f + 3.32\varphi\left[\left(3.4\mathrm{Re}_p^3 - 2.4\mathrm{Re}_p + 0.14\right)\langle\alpha_p\rangle - 0.84\mathrm{Re}_p^4 + 2.4\mathrm{Re}_p^2 + 0.05\mathrm{Re}_p\right]\boldsymbol{G}_p$$

Sparse identification only selects gravity-based terms.

Sparse identification uncovers complex dependencies on flow conditions that improve model accuracy.

Next steps


Turbulence over periodic hills
2D gas-solid sedimenting flow
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u
y
x
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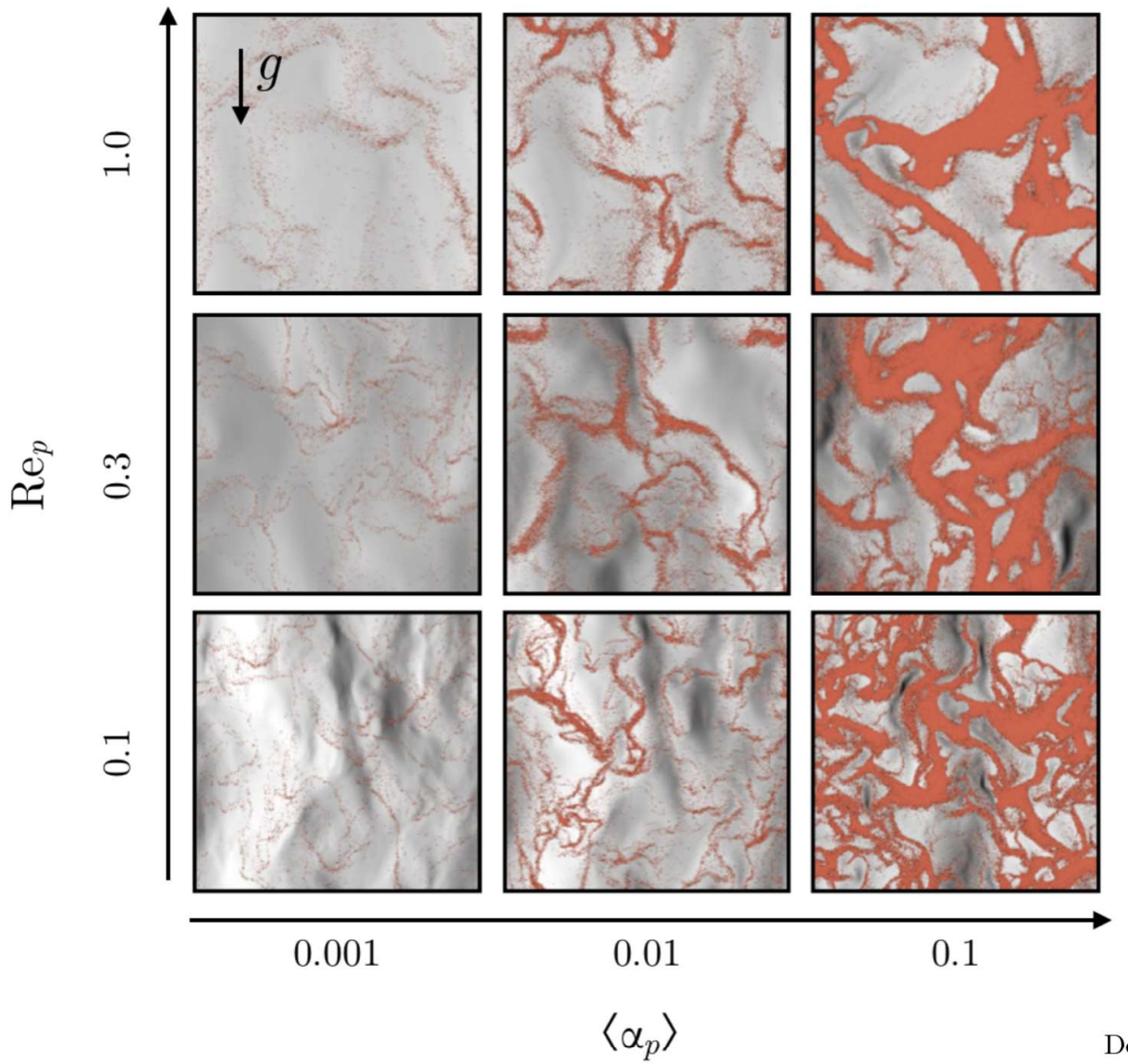
Questions?

This work is supported by the
NSF Graduate Research Fellowship Program

Multiphase dynamics governed by high dimensional parame



- Mesh: 512×512 ($896\,d_p \times 896\,d_p$)
- N_p = (12,359 57,362 266,278)
- Enforce mass flow rate = 0
- Density ratio = 1000

Computations carried out using NGA:

- Finite volume DNS/LES code
- Conservation of mass, momentum and kinetic energy
- Lagrangian particle tracking
- 2nd order RK for particle ODEs
- Soft-sphere collisional model
- Interphase exchange fully conservative.

Desjardins et al. (2008), Capecelatro et al. (2013)