Identification of compact closures for the multiphase RANS equations, with application to strongly-coupled gas-solid flows

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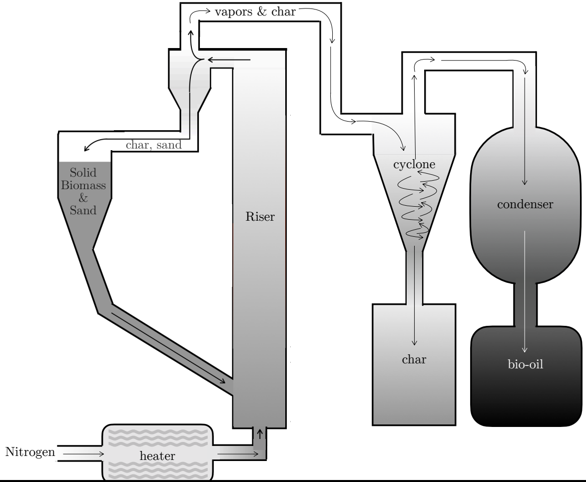
Fluidized bed reactors upgrade feedstock into usable fuel

While gas-solid flows are pervasive, we frame this work in the context of ***fluidized bed reactors.***



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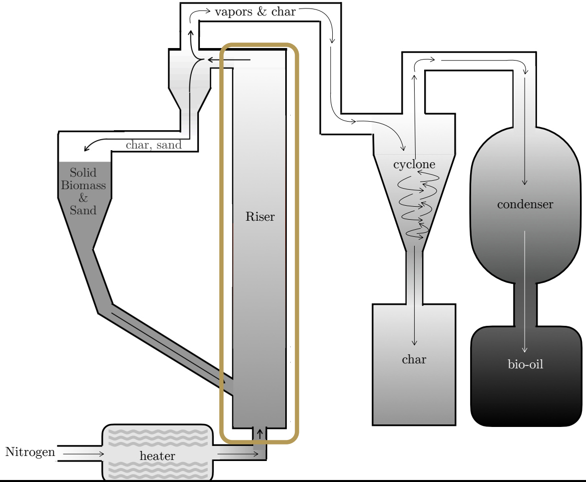


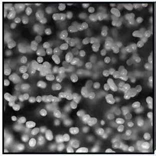
The multiscale challenge of a fluidized bed reactor

Microscale

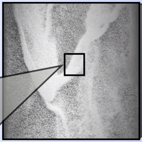
Particle diameter: $O(10^{-4})$ [m]

Physics:

Wakes past particles,
Collisions,
Surface reactions,
Phase change,
Heat transfer

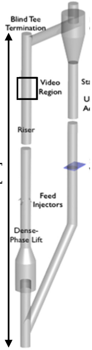


Experiments [4]



Mesoscale

Length scale: $O(10^{-2})$ to $O(10)$ m
Number of particles: $> O(10^4)$
Clustering and bubbling
Turbulence modulation



22 [m]

Macroscale

Reactor geometry: $O(10)$ [m]
Number of particles $O(10^{12})$

10^{-8} [m] — length scale — 10^{2} [m]

[4] Shaffer & Gopalan (2013)

The multiscale challenge of a fluidized bed reactor

Microscale physics impact ***macroscale*** quantities of interest!

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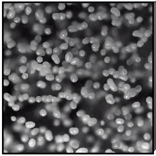

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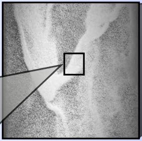

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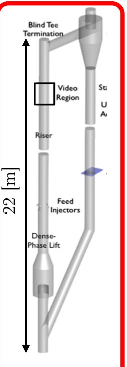

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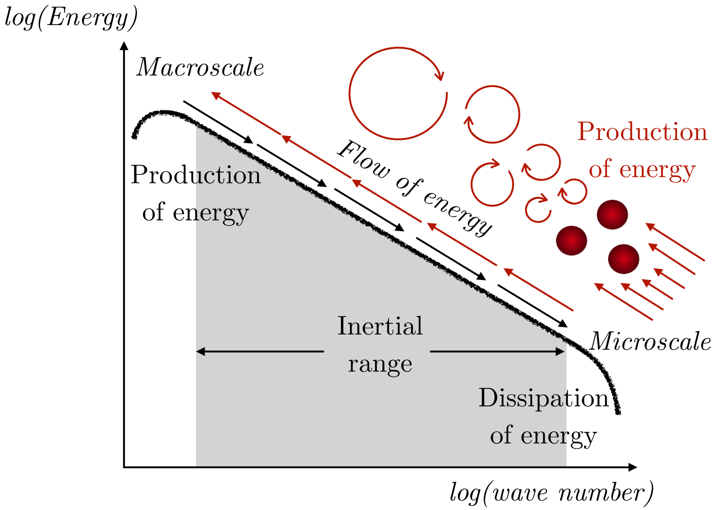

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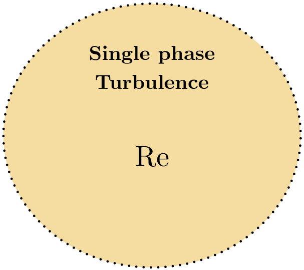

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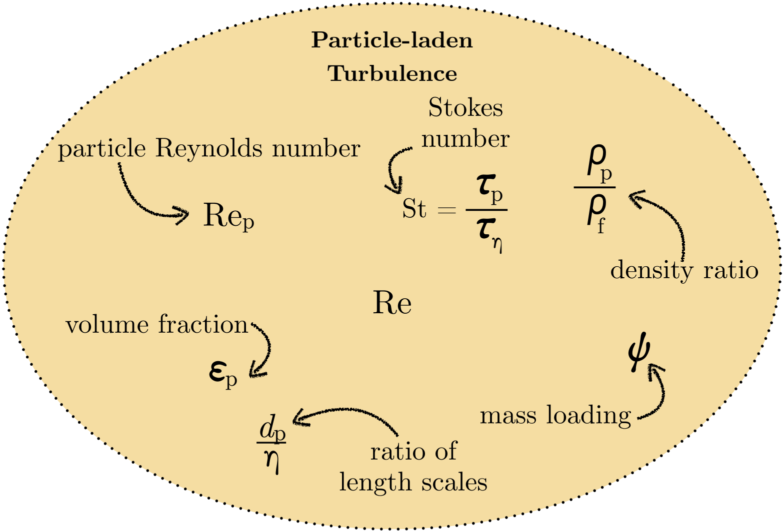
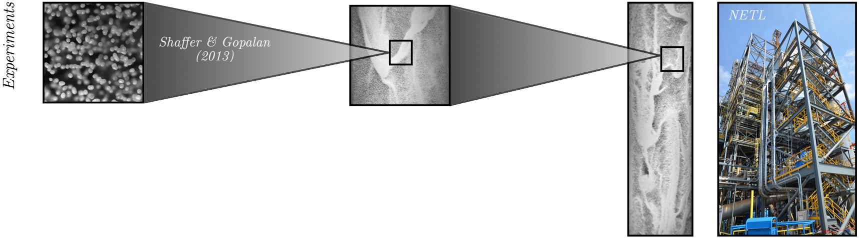


Computational strategies vary across scales of interest.

Modeling strategies at scales of interest

microscale → *mesoscale* → *macroscale*

10^{-6} [s] — timescale — 10^{4} [s]



Multiphase RANS

Treats both phases as continuous

Heavy reliance on models

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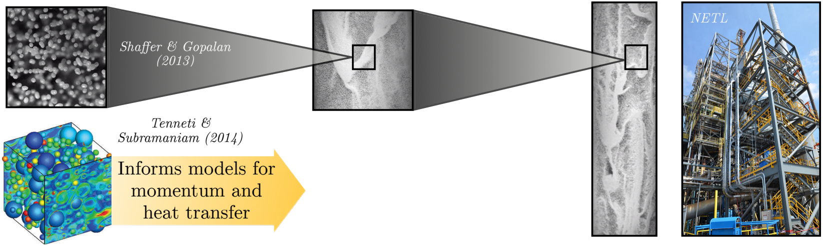

Particle Resolved DNS

$O(10^3)$ particles

Fully resolves hydrodynamics & heat transfer

Chemical kinetics modeled

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length scale

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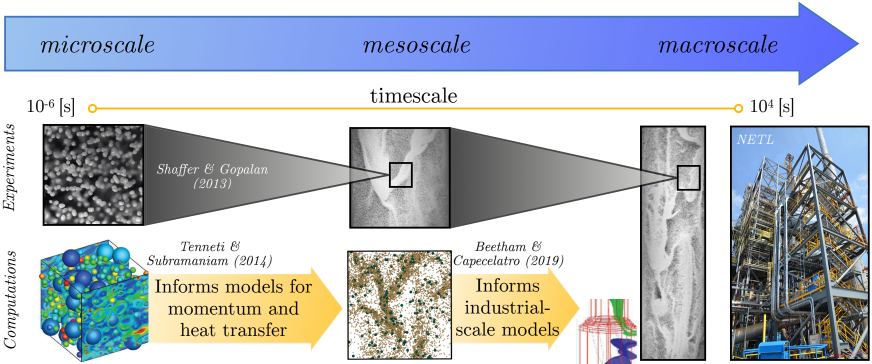


Particle Resolved DNS	Euler—Lagrange	Multiphase RANS
$O(10^3)$ particles	$O(10^8)$ particles	Treats both phases as continuous
Fully resolves hydrodynamics & heat transfer	Resolves inter-particle contact	Heavy reliance on models
Chemical kinetics modeled	Mass, momentum and heat transfer modeled	

Tenneti & Subramaniam (2014)

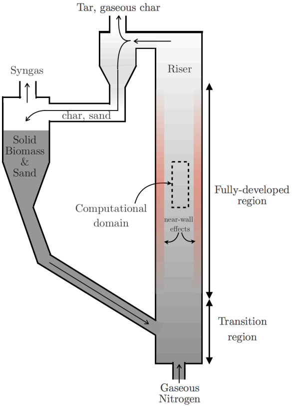
10^{-6} [m] — length scale — 10^{2} [m]

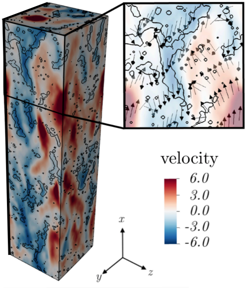
Simulating industrial-scale systems requires ***improved models.***

To date, multiphase RANS models
that are accurate across regimes, ***do not exist.***

Modeling a canonical two-phase flow

Configuration under study: Gravity-driven gas-solid flow





Chosen because:

- Simple configuration where two-way coupling drives the turbulence.
- Directly related to the fully-developed, interior region of a circulating fluidized bed.

Modeling goals:

- learn interpretable, accurate models across ***multiphase*** flow conditions
- learn models that are robust to sparse training data

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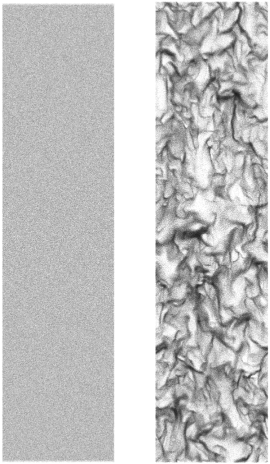
$t = 0$ fully developed



Configuration details:

- Particles are initially randomly distributed in a quiescent gas
- Particles fall under gravity and spontaneously form clusters

Density ratio:	$\rho_p/\rho_f = 1000$
Particle diameter:	$d_p = 90\mu$m
Gravity:	$g = (0.8, 2.4, 8.0)$m/s
Volume fractions:	$\langle\alpha_p\rangle = (0.1, 2.55, 5.0) \times 10^{-2}$
Mass loading:	$\varphi = (1.0, 26.2, 52.6)$
Characteristic cluster length:	$\mathcal{L} = \tau_p g$: $(5 \times 10^{-4}, 1.5 \times 10^{-3}, 5 \times 10^{-3})$
Particle Reynolds number	$\mathrm{Re}_p = \tau_p g d_p/\nu_f^2$: $(0.1, 0.3, 1)$

These parameters were chosen for consistency with fluidized bed conditions.

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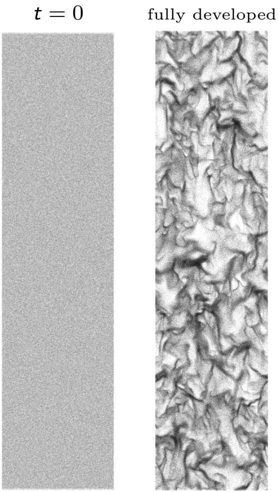

Computational details:

NGA (Desjardins et al. (2008))

1. Fully-conservative, finite volume DNS/LES code
2. Semi-implicit Crank-Nicolson for time advancement

Lagrangian Particle Tracking (Capecelatro et al. (2013))

1. Particle position and velocity calculated using Newton's second law
2. Soft-sphere collisional model ($e = 0.85$)
3. 2nd order Runge Kutta used for particle ODEs

Interphase exchange

1. Fluid and particles are coupled through drag and volume fraction
2. Tenneti (2011) drag law (Re_p and α_p dependent) for interphase momentum exchange

Simulation details

1. Boundary Conditions: periodic in all directions
2. Grid size: $(512 \times 128 \times 128)$
3. $L_x/\mathcal{L} = (316, 105, 32)$
4. Since fully periodic, mean mass flow rate is forced to 0

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Modeling a canonical two-phase flow

The multiphase RANS equations in the fluid-phase (Capecelatro et al. (2015)):

$$\frac{1}{2}\frac{\partial\langle u_f'''^2\rangle_f}{\partial t} = \underbrace{\frac{1}{\rho_f}\left\langle p_f \frac{\partial\langle u_f'''\rangle}{\partial x}\right\rangle}_{\text{pressure strain (PS)}} - \underbrace{\frac{1}{\rho_f}\left\langle \sigma_{f,1i}\frac{\partial\langle u_f'''\rangle}{\partial x}\right\rangle}_{\text{viscous dissipation (VD)}} + \underbrace{\frac{\varphi}{\tau_p^\star}\left(\langle u_f'''\rangle\langle u_p''\rangle_p - \langle u_f'''^2\rangle_p\right)}_{\text{drag exchange (DE)}} + \underbrace{\frac{\varphi}{\tau_p^\star}\langle u_f'''\rangle\langle u_p\rangle_p}_{\text{drag production (DP)}} + \underbrace{\frac{\varphi}{\rho_p}\left\langle u_f''' \frac{\partial p_f'}{\partial x}\right\rangle_p}_{\text{pressure exchange (PE)}} - \underbrace{\frac{\varphi}{\rho_p}\left\langle u_f''' \frac{\partial \sigma_{f,1i}'}{\partial x_i}\right\rangle_p}_{\text{viscous exchange (VE)}}$$

$$\frac{1}{2}\frac{\partial\langle v_f'''^2\rangle_f}{\partial t} = \underbrace{\frac{1}{\rho_f}\left\langle p_f \frac{\partial\langle v_f'''\rangle}{\partial y}\right\rangle}_{\text{pressure strain (PS)}} - \underbrace{\frac{1}{\rho_f}\left\langle \sigma_{f,2i}\frac{\partial\langle v_f'''\rangle}{\partial x}\right\rangle}_{\text{viscous dissipation (VD)}} + \underbrace{\frac{\varphi}{\tau_p^\star}\left(\langle v_f''' v_p''\rangle_p - \langle v_f'''^2\rangle_p\right)}_{\text{drag exchange (DE)}} + \underbrace{\frac{\varphi}{\rho_p}\left\langle v_f''' \frac{\partial p_f'}{\partial y}\right\rangle_p}_{\text{pressure exchange (PE)}} - \underbrace{\frac{\varphi}{\rho_p}\left\langle v_f''' \frac{\partial \sigma_{f,2i}'}{\partial x_i}\right\rangle_p}_{\text{viscous exchange (VE)}}$$

We cannot extend models from single phase or augment existing models. So, what is the best approach to modeling these systems?

Sparse regression with embedded form invariance

We employ a sparse regression approach that postulates that a model for $\mathcal{D}_{ij}$ takes the form,

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

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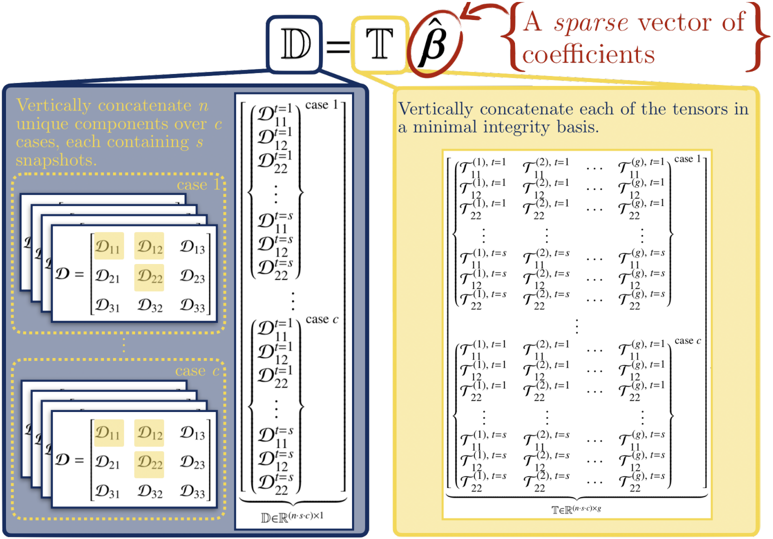
The notion of using an invariant tensor basis for turbulence modeling was established in the 1970s (see, e.g., Pope (1975).)

Sparse regression with embedded form invariance



Sparse regression with embedded form invariance

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

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.

We use the same optimization procedure as described in [6] Brunton et al. (2016)

Sparse regression with embedded form invariance

We can ensure form invariance due to

1. Linearity in the basis functions. This guarantees invariance[7] upon Galilean rotation, **Q**

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

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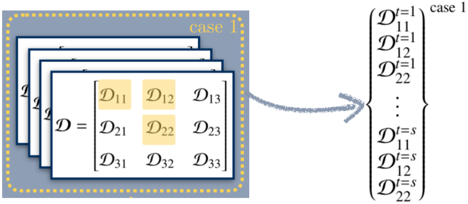
2. Formulating the problem as tall and skinny vectors. This ensures that β does not vary based on orientation.

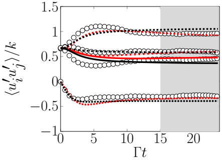


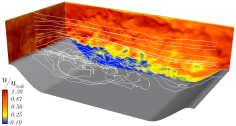
[7] Speziale et al. (1990)

Sparse regression learns accurate single phase models.

Our previous work has shown that sparse regression can formulate single-phase models that are:

- Accurate, even for flows with massive separation





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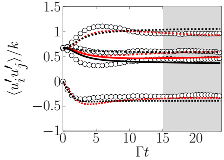
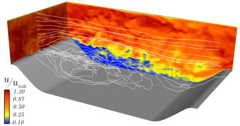
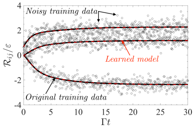
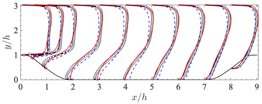




- Robust to noisy and sparse training data





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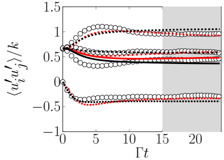

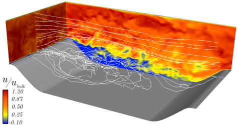

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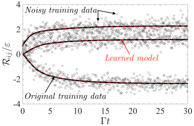
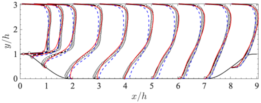
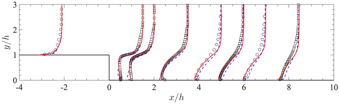




- Accurate outside the scope of their training



For more details see Beetham & Capecelatro (2020).

We now extend this approach to gravity-driven gas-solid flows.

Modeling a canonical two-phase flow

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Pressure strain − Viscous diffusion +
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Key challenges:

- Invariant basis has not yet been derived for this class of flows.
- Large parameter space and wide range of length and time scales.
- As configuration becomes more complex, the number of unclosed terms increases.

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

Modeling a canonical two-phase flow: Developing the basis

Challenge: An invariant basis, to date, has not been developed for this class of flows.

The following tensors are relevant for capturing flow physics:

(1) Particle-phase anisotropic stress tensor $\hat{\mathbb{R}}_p = \frac{\langle \boldsymbol{u}_p''' \boldsymbol{u}_p''' \rangle}{2k_p} - \frac{1}{3}\mathbb{I}$

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Modeling a canonical two-phase flow: Developing the basis

Challenge: An invariant basis, to date, has not been developed for this class of flows.

The following tensors are relevant for capturing flow physics:

(1) Particle-phase anisotropic stress tensor $\hat{\mathbb{R}}_p = \frac{\langle \boldsymbol{u}_p''' \boldsymbol{u}_p''' \rangle}{2k_p} - \frac{1}{3}\mathbb{I}$

(2) Fluid-phase anisotropic stress tensor $\hat{\mathbb{R}}_f = \frac{\langle \boldsymbol{u}_f''' \boldsymbol{u}_f''' \rangle_f}{2k_f} - \frac{1}{3}\mathbb{I}$

(3) Slip velocity tensor $\hat{\mathbb{U}}_r = \frac{\boldsymbol{U}_r}{\mathrm{tr}(\boldsymbol{U}_r)} - \frac{1}{3}\mathbb{I},$

Here, $\boldsymbol{U}_r = \boldsymbol{u}_r \otimes \boldsymbol{u}_r$, where $\boldsymbol{u}_r = \langle \boldsymbol{u}_p \rangle_p - \langle \boldsymbol{u}_f \rangle_f$ is the slip velocity vector.

Finally, since all the terms we seek to model are symmetric, the basis that we form also must contain only symmetric tensors.

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Following the procedure in [22] for developing invariant basis sets, we derive:

$\mathcal{T}^{(1)} = \mathbb{I}$	$\mathcal{T}^{(2)} = \hat{\mathbb{U}}_r$	$\mathcal{T}^{(3)} = \hat{\mathbb{U}}_r^2$
$\mathcal{T}^{(4)} = \left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f\right)^\dagger$	$\mathcal{T}^{(5)} = \left(\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_f\right)^\dagger$	$\mathcal{T}^{(6)} = \left(\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_f^2\right)^\dagger$
$\mathcal{T}^{(7)} = \left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p\right)^\dagger$	$\mathcal{T}^{(8)} = \left(\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p\right)^\dagger$	$\mathcal{T}^{(9)} = \left(\hat{\mathbb{R}}_f\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_p\right)^\dagger$
$\mathcal{T}^{(10)} = \left(\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_f^2\hat{\mathbb{R}}_p\right)^\dagger$	$\mathcal{T}^{(11)} = \left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_p\right)^\dagger$	$\mathcal{T}^{(12)} = \left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p\hat{\mathbb{U}}_r^2\right)^\dagger$
$\mathcal{T}^{(13)} = \hat{\mathbb{R}}_f$	$\mathcal{T}^{(14)} = \hat{\mathbb{R}}_f^2$	$\mathcal{T}^{(15)} = \hat{\mathbb{R}}_p$
$\mathcal{T}^{(16)} = \hat{\mathbb{R}}_p^2$	$\mathcal{T}^{(17)} = \left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_p\right)^\dagger$	$\mathcal{T}^{(18)} = \left(\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_p\right)^\dagger$
$\mathcal{T}^{(19)} = \left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_p^2\right)^\dagger$	$\mathcal{T}^{(20)} = \left(\hat{\mathbb{U}}_r^2\hat{\mathbb{R}}_p^2\right)^\dagger$	$\mathcal{T}^{(21)} = \left(\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p\right)^\dagger$
$\mathcal{T}^{(22)} = \left(\hat{\mathbb{R}}_f^2\hat{\mathbb{R}}_p\right)^\dagger$	$\mathcal{T}^{(23)} = \left(\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p^2\right)^\dagger$	$\mathcal{T}^{(24)} = \left(\hat{\mathbb{R}}_f^2\hat{\mathbb{R}}_p^2\right)^\dagger$
$\mathcal{S}^{(1)} = \mathrm{tr}\left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f^2\hat{\mathbb{R}}_p^2\right)$	$\mathcal{S}^{(2)} = \mathrm{tr}\left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p^2\right)$	$\mathcal{S}^{(3)} = \mathrm{tr}\left(\hat{\mathbb{U}}_r\hat{\mathbb{R}}_f\hat{\mathbb{R}}_p\right)$
$\mathcal{S}^{(4)} = Ar$	$\mathcal{S}^{(5)} = \varphi$	$\mathcal{S}^{(6)} = \langle\alpha_p\rangle$

where $(\cdot)^\dagger = (\cdot) + (\cdot)^{\mathrm{T}}$.

[22] Spencer et al. (1958)

Modeling a canonical two-phase flow: Drag production

Drag production, $\mathcal{R}^{\mathrm{DP}}$, is the sole source of fluid-phase turbulent kinetic energy in the absence of mean shear.

$$\mathcal{R}^{\mathrm{DP}} = \frac{\varphi}{\tau_p^\star} \langle u_f''' \rangle_p \langle u_p \rangle_p$$

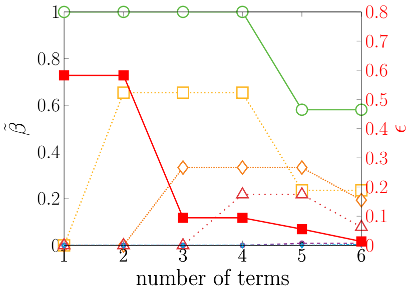
Phase averaging (PA) is defined as:

$$\langle (\cdot) \rangle_p = \frac{\langle \alpha_p (\cdot) \rangle}{\langle \alpha_p \rangle}$$

Where α_p is the particle volume fraction. Fluctuations about the PA velocity are denoted $\boldsymbol{u}_f''' = \boldsymbol{u}_p(\boldsymbol{x}, t) - \langle \boldsymbol{u}_f \rangle_f$.

- φ is the mass loading
- $\tau_p^\star$ is the drag time
- $\langle u_f''' \rangle_p$ is the fluid phase velocity *seen by the particles*
- $\langle u_p \rangle_p$ is the phase averaged particle velocity

Modeling a canonical two-phase flow: Drag production



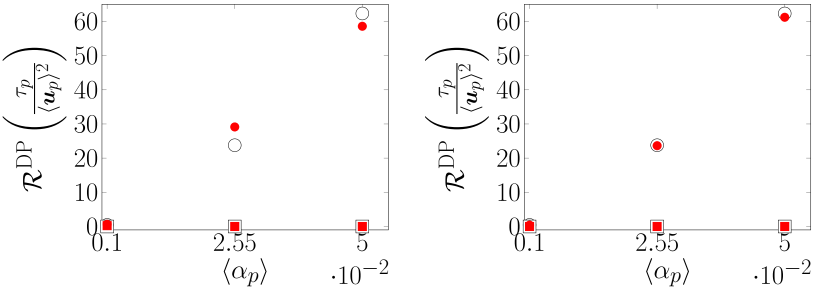
- ☛ Error is drastically reduced with a three terms and even further with six.
- ☛ Our method learns ***interpretable*** models. ✓

$$\mathcal{R}^{\mathrm{DP}} = \frac{\langle u_p \rangle_p^2}{\tau_p} \Big[\underbrace{1.11\varphi \hat{\mathbb{U}}_r}_{\text{term 1}} - \underbrace{0.73\varphi^{-2}\hat{\mathbb{U}}_r}_{\text{term 2}} + \underbrace{0.37\varphi\mathbb{I}}_{\text{term 3}} \Big]$$

$$\mathcal{R}^{\mathrm{DP}} = \frac{\langle u_p \rangle_p^2}{\tau_p} \Big[\underbrace{0.65\varphi \hat{\mathbb{U}}_r}_{\text{term 1}} - \underbrace{0.26\varphi^{-2}\hat{\mathbb{U}}_r}_{\text{term 2}} + \underbrace{0.22\varphi\mathbb{I}}_{\text{term 3}} - \underbrace{0.09\varphi^{-2}\mathbb{I}}_{\text{term 4}} + \underbrace{0.01\varphi^{2}\hat{\mathbb{U}}_r}_{\text{term 5}} + \underbrace{0.003\varphi^{2}\mathbb{I}}_{\text{term 6}} \Big]$$

Modeling a canonical two-phase flow: Drag production

Our method learned models that are
accurate across flow conditions. ✓



Three-term model

Six-term model

Cases shown correspond to $\boldsymbol{g} = 0.8$ m/s
EL data: ○ (stream-wise), □ (cross stream)

Learned model: ● (stream-wise) ■ (cross stream)

Application to transient flow

To assess model performance on temporally evolving flow, gravity is reversed.

$$\boldsymbol{g} = \begin{cases} (-g, 0, 0), & \text{if } \boldsymbol{t} < 0 \\ (g, 0, 0), & \text{if } \boldsymbol{t} \geq 0 \end{cases}.$$

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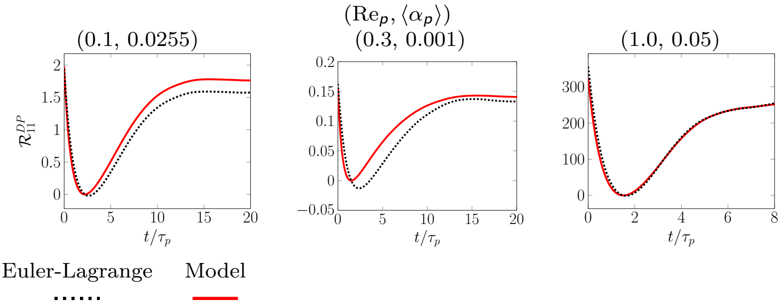

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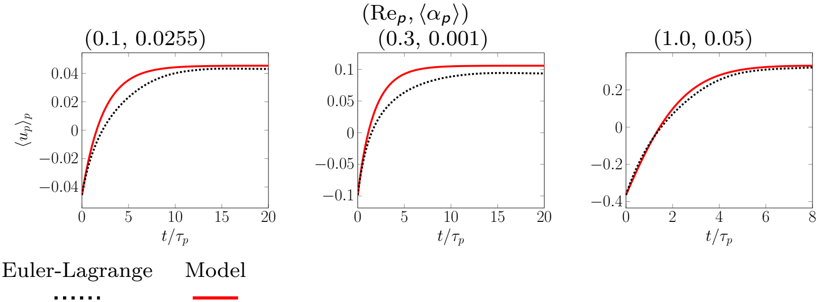
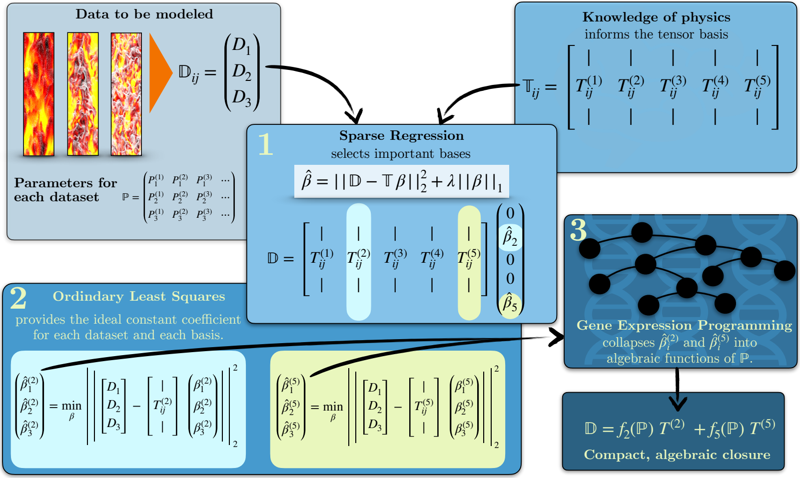


Sparse regression alone is tedious for determining non-constant coefficients.

Is there a better way?

GEP can be used to symbolically determine non-constant coefficients



Beetham & Capeclatro (2023)

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GEP enabled Sparse regression:

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	Sparse Regression		**Sparse Regression + GEP**	
Term	ϵ	*Number of terms*	ϵ	*Number of terms*
PS	0.15	3	0.06	3
DP	0.01	2	0.01	2
VD	0.07	4	0.09	2
DE	0.15	4	0.08	2

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Recall the closure for Drag Production:

Sparse Regression alone:

$$\mathcal{R}^{\mathrm{DP}} = \frac{\langle u_p \rangle_p^2}{\tau_p} \left(0.22\varphi - 0.09\varphi^{-2} + 0.003\varphi^3\right) \mathbb{I} + \left(0.65\varphi - 0.26\varphi^{-2} + 0.01\varphi^2\right) \hat{\mathbb{U}}_r$$

Sparse Regression + GEP:

$$\mathcal{R}^{\mathrm{DP}} = \frac{\langle u_p \rangle_p^2}{\tau_p} \left(0.258\varphi + (0.03\varphi)^3 + 1.9\frac{\langle \varepsilon_p \rangle}{\mathcal{S}^{(2)}}\right) \mathbb{I} + \left(1.9\varphi - 5.8\varphi^{1/2}\right) \hat{\mathbb{U}}_r$$

Questions?

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