Data-Driven Variational Multiscale Reduced Order Models and LES-ROMs

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ICAM
Virginia Tech

Algorithms for Dimension and Complexity Reduction

ICERM

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1. LES
2. LES-ROM
3. Data-Driven Variational Multiscale ROM
4. Numerical Analysis
5. Conclusions

Collaborators

- students, postdocs
  - Birgul Koc (student, Virginia Tech)
  - Changhong Mou (student, Virginia Tech)
  - Ludovica Saccaro (student, Politecnico di Milano / Virginia Tech)
  - Xuping Xie (postdoc, Courant, NYU)
  - Muhammad Mohebujjaman (postdoc, MIT)
  - Omer San (professor, Oklahoma State University)
  - David Wells (postdoc, UNC Chapel Hill)
  - Zhu Wang (professor, University of South Carolina)
- collaborators
  - Michael Schneier, Honghu Liu, Adrian Sandu, Samuele Rubino, Leo Rebholz, Eric Parish, Volker John, Simona Perotto, Max Gunzburger, Jeff Borggaard

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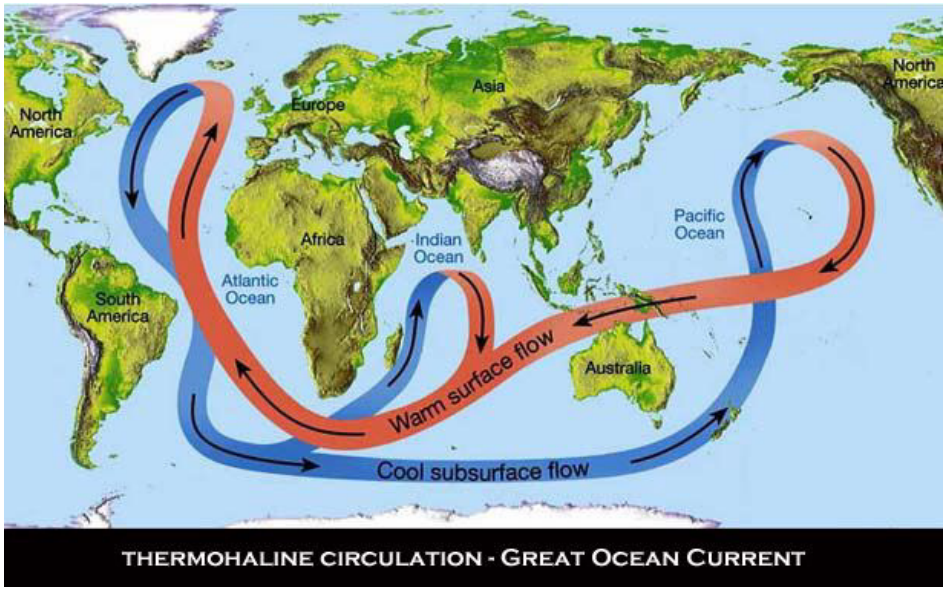
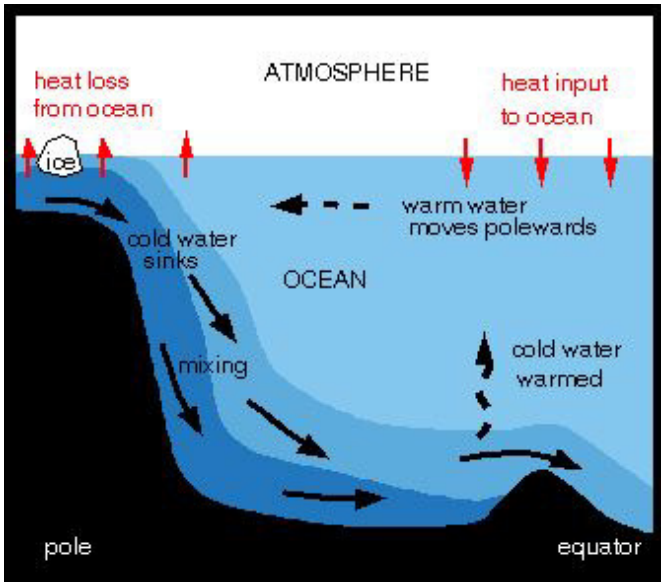
Collaborators

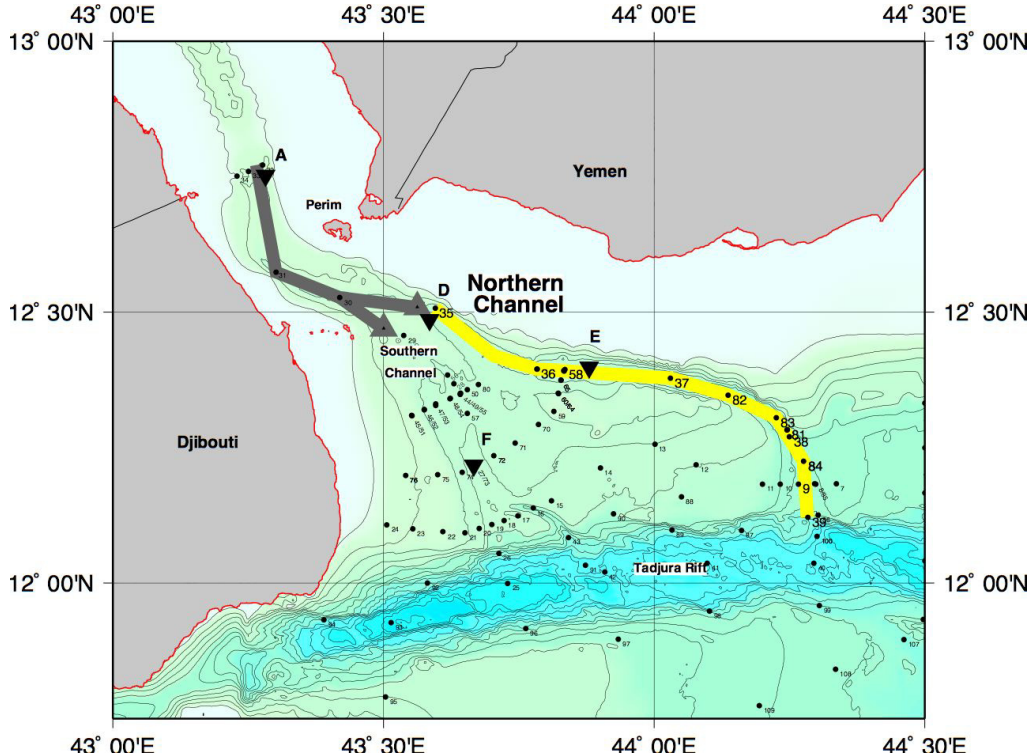
- Paul Fischer, Argonne National Laboratory
- Tamay Özgökmen, University of Miami
- Jinqiao Duan, Illinois Institute of Technology

Thermohaline Circulation





Red Sea Overflow



REDSOX winter cruise: topography and plume survey stations.

Direct Numerical Simulation (DNS)

- *all* scales
- $N \sim \mathcal{O}(Re^{9/4})$
- $U \sim 1\, m/s,\ L \sim 100\, m \Longrightarrow Re_{GC} \sim 10^8$
- $N_{GC} \sim 10^{18}$
- under-resolved

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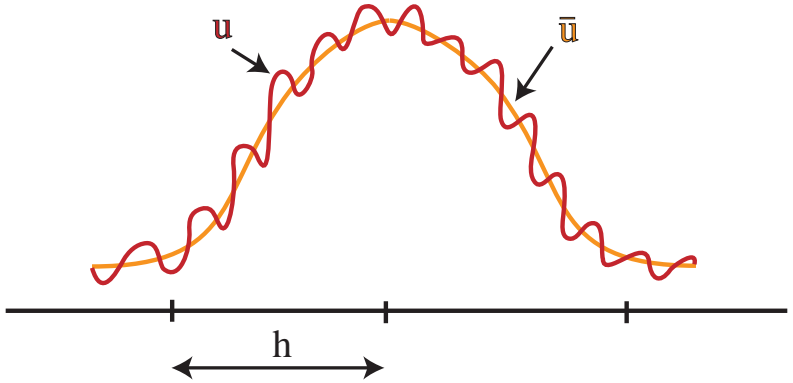

- spatial filter g_δ
- $\overline{\mathbf{u}} := g_\delta * \mathbf{u}$
- large scales
- $g_\delta *$ NSE

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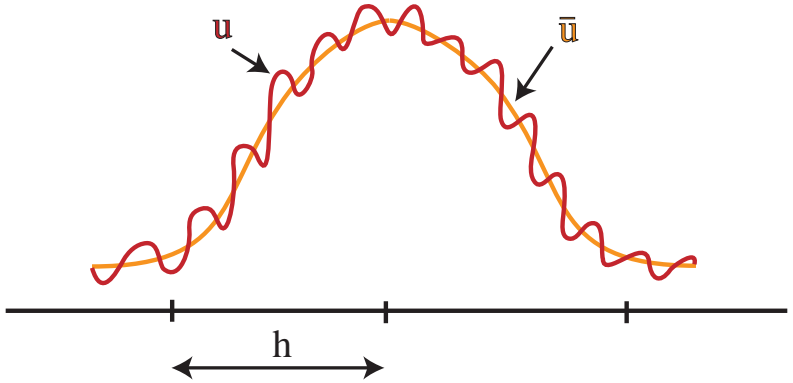

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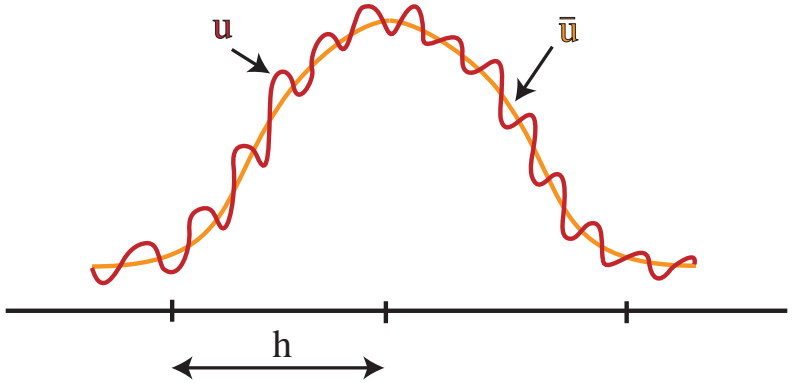

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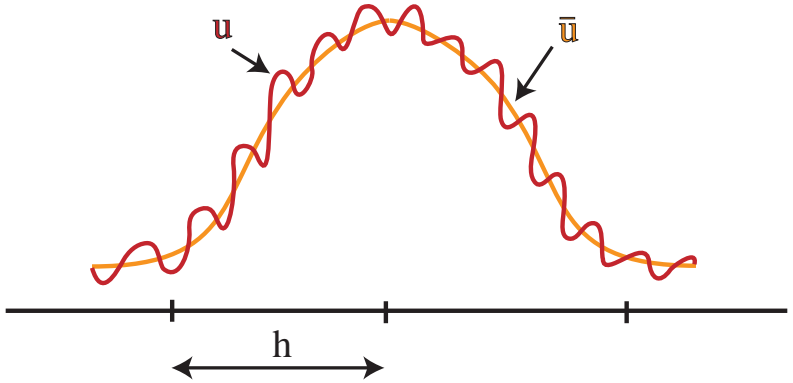

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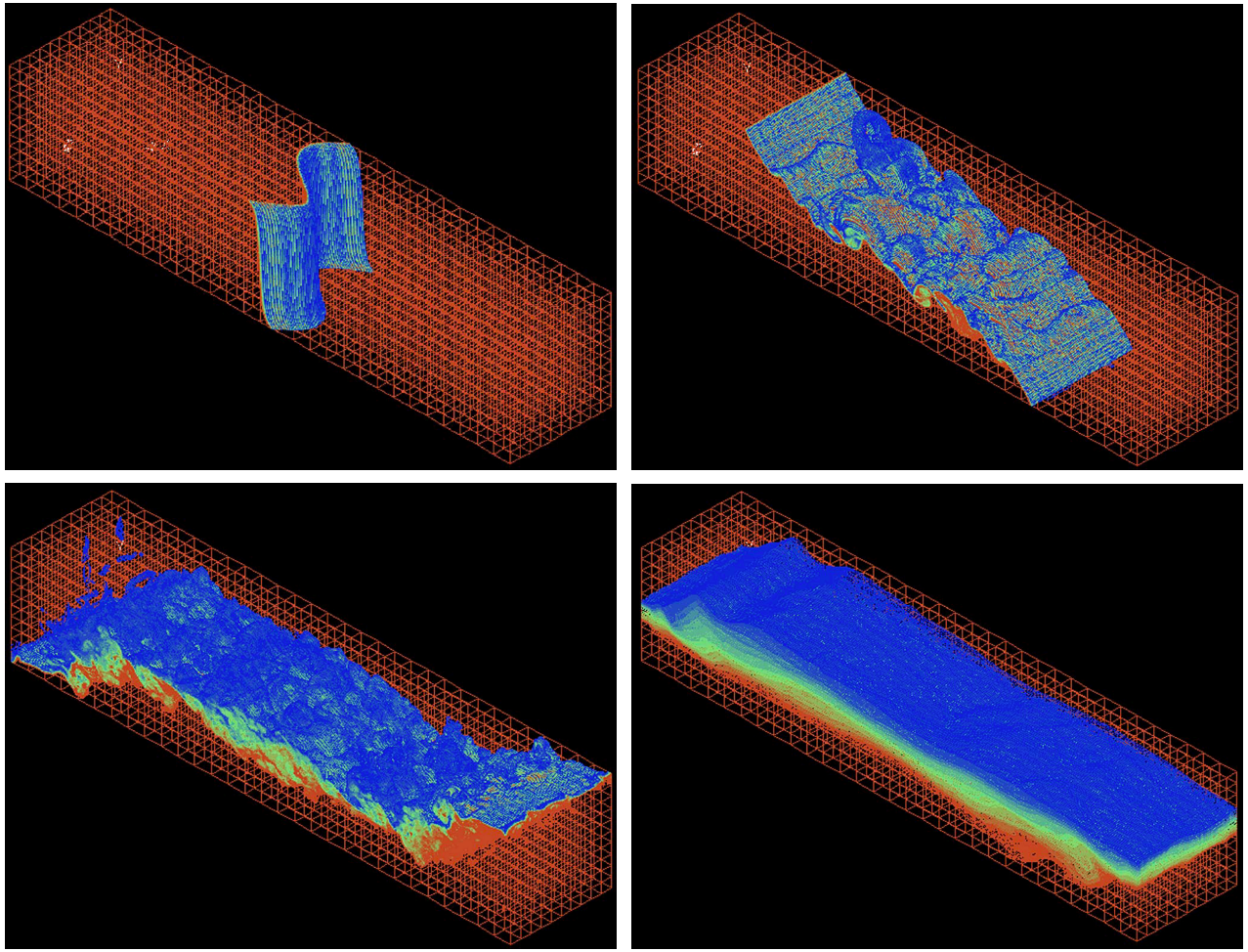
Large Eddy Simulation (LES)

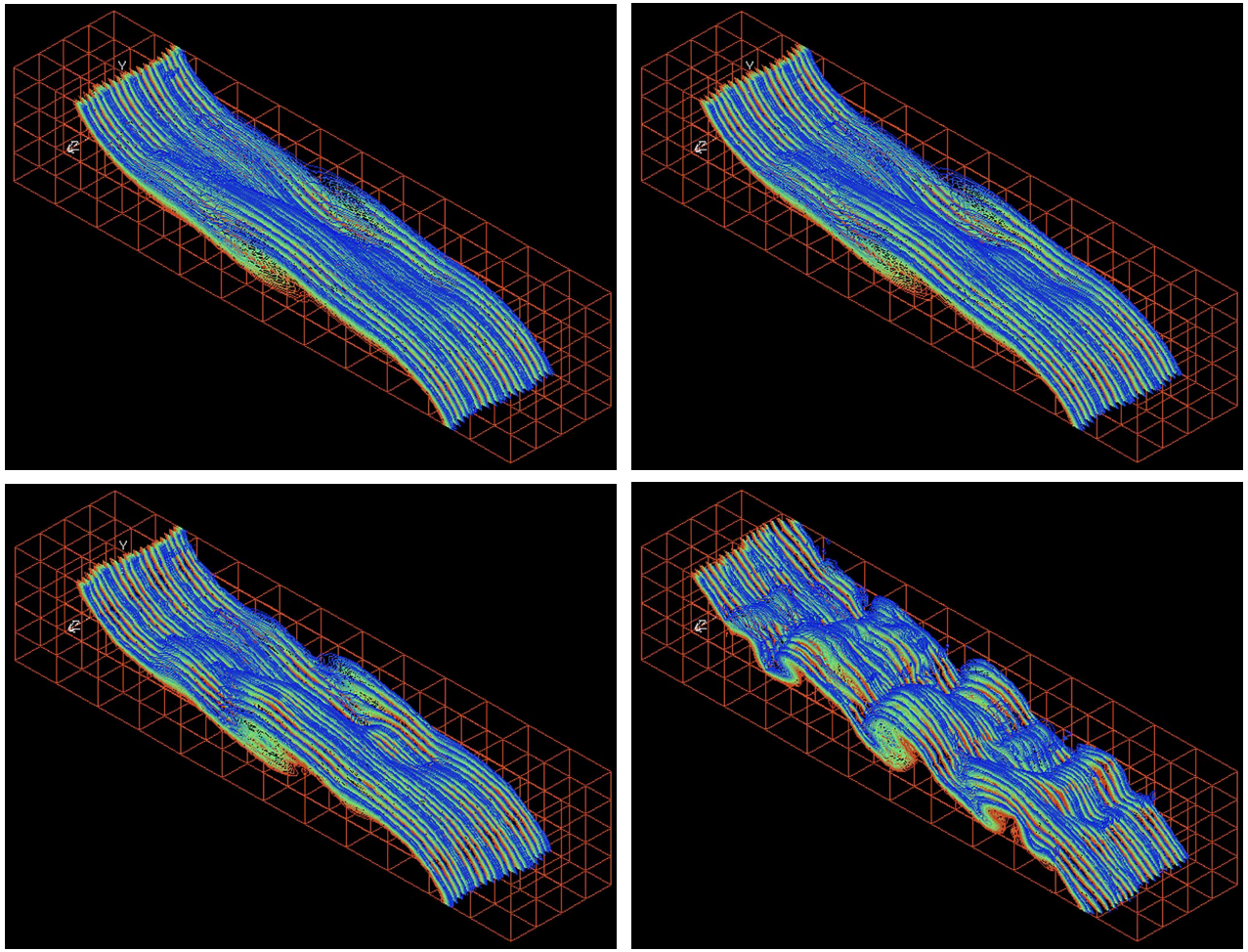
$$\begin{cases} \dfrac{D\overline{\mathbf{u}}}{Dt} - Re^{-1}\,\triangle\overline{\mathbf{u}} + \nabla\overline{p} + \nabla\cdot(\overline{\mathbf{u}\,\mathbf{u}} - \overline{\mathbf{u}}\,\overline{\mathbf{u}}) = 0 \\ \\ \nabla\cdot\overline{\mathbf{u}} = 0 \end{cases}$$

closure problem $\qquad \overline{\mathbf{u}\mathbf{u}} \neq \overline{\mathbf{u}}\,\overline{\mathbf{u}}$

DNS Density Perturbation



LES Density Perturbation



Computational Cost

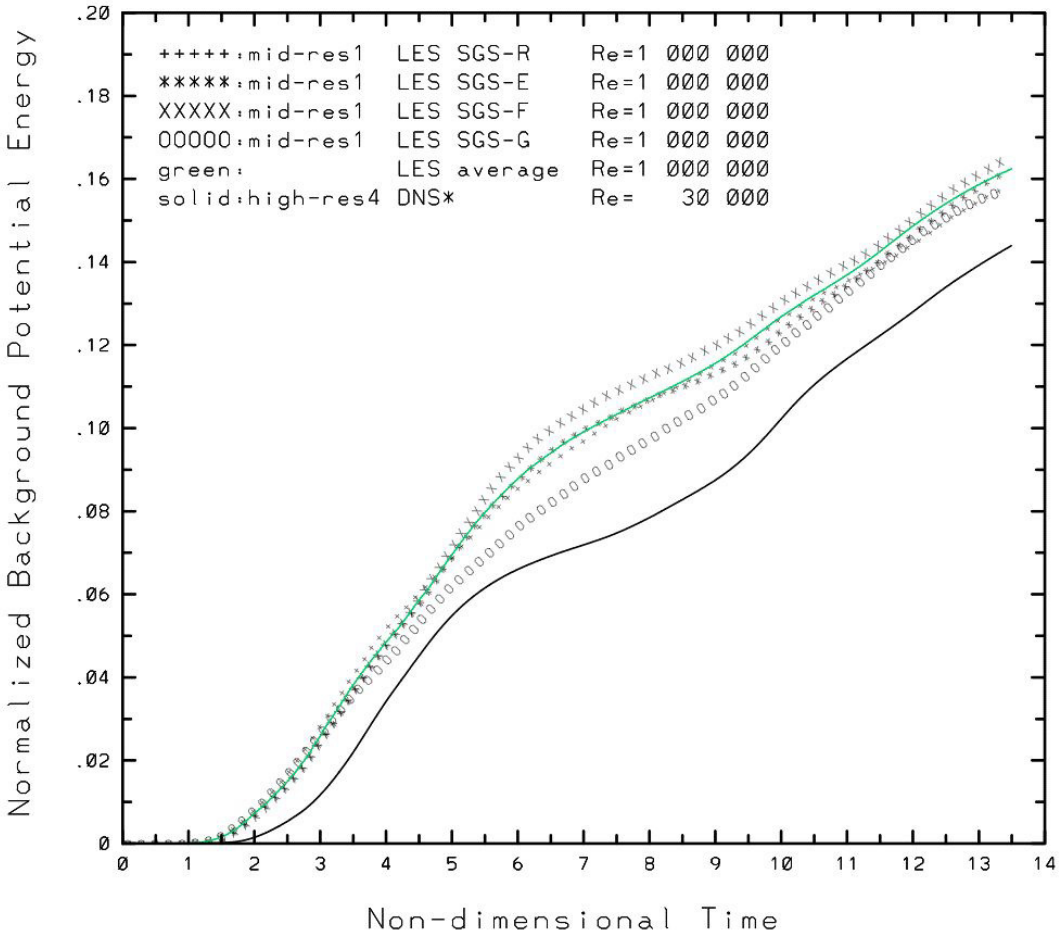
- *accuracy - fixed*
- $\boxed{CPU_{DNS} \approx 1000 * CPU_{LES}}$

Lock-Exchange Problem

Özgökmen, Iliescu, Fischer

Ocean Modelling, 2009

LES Model Comparison $Re = 1{,}000{,}000$



Take Home Message

$$\boxed{\text{realistic flows} \Longrightarrow \text{under-resolved} \Longrightarrow \text{LES}}$$

ROM Closure Modeling

(1) FUNCTIONAL

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  - mixing length: Lumley
  - Smagorinsky: Noack, Ullman & Lang, Wang, Rozza, Avila
  - variational multiscale: Iollo, Wang, Rubino, Codina, Rozza, Stabile, Duraisamy, Parish
  - *dynamic subgrid-scale*: Wang, San

(2) STRUCTURAL

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- LES
  - Wang, Rozza, Avila, Duraisamy, Parish, Carlberg, Iollo, Rubino, Codina, Stabile, San, Taddei, Patera, Maday, Kramer, Peherstorfer, ...

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(2) STRUCTURAL

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(2) STRUCTURAL

- non-LES
  - Xiao, Fu, Duraisamy, Parish, Tezaur, Wang, Carlberg, Kalashnikova, Peherstorfer, Rowley
- LES
  - Wang, Wan, Duraisamy, Parish, Xiao, Carlberg, Kalashnikova, Peherstorfer

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  - Xiao, Fu, Duraisamy, Parish, Tinoco, Wang, Ouil, Ouil, Ouil, Ouil, Ouil, Ouil, Ouil
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  - Wang, San, Iliescu, Duraisamy, Parish, Stabile, Rozza, Codina, Rubino, Iollo, Carlberg, Kalashnikova/Tezaur, Balajewicz, Noack, Ullman & Lang

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Galerkin ROM (G-ROM)

- $\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u})$
- $\mathbf{u}_r = \sum_{j=1}^{r} a_j \, \varphi_j$
- $\left(\dot{\mathbf{u}}_r \, , \varphi_i\right) = \left(\mathbf{f}(\mathbf{u}_r) \, , \varphi_i\right) \qquad i = 1, \ldots, r$
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$$\boxed{\dot{\boldsymbol{a}} = \mathbf{f}(\boldsymbol{a})}$$

[1] NSE $\quad \dot{\boldsymbol{a}} = A\,\boldsymbol{a} + \boldsymbol{a}^\top B\,\boldsymbol{a}$

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ROM Closure

- drastic ROM truncation $\{\varphi_1, \ldots, \varphi_{1000}\} \implies \{\varphi_1, \ldots, \varphi_{10}\}$
- under-resolved regime
- ROM closure

$$\dot{\boldsymbol{a}} = \mathbf{f}(\boldsymbol{a}) + \text{Closure}(\boldsymbol{a})$$

- closure term
  - effect of $\{\varphi_{11}, \ldots, \varphi_{1000}\}$ on $\{\varphi_1, \ldots, \varphi_{10}\}$
  - low-dimensional
- closure model
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- drastic ROM truncation $\{\varphi_1, \ldots, \varphi_{1000}\} \implies \{\varphi_1, \ldots, \varphi_{10}\}$
- under-resolved regime
- ROM closure

$$\dot{\boldsymbol{a}} = \mathbf{f}(\boldsymbol{a}) + \text{Closure}(\boldsymbol{a})$$

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  - effect of $\{\varphi_{11}, \ldots, \varphi_{1000}\}$ on $\{\varphi_1, \ldots, \varphi_{10}\}$
  - low-dimensional
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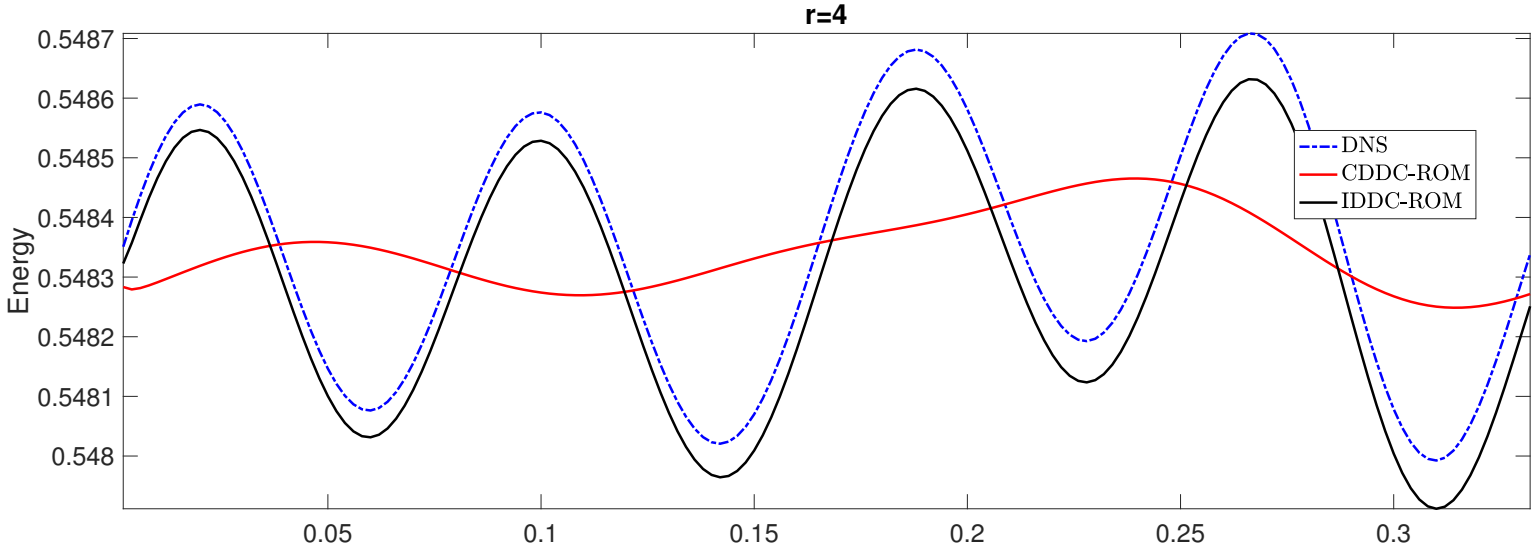
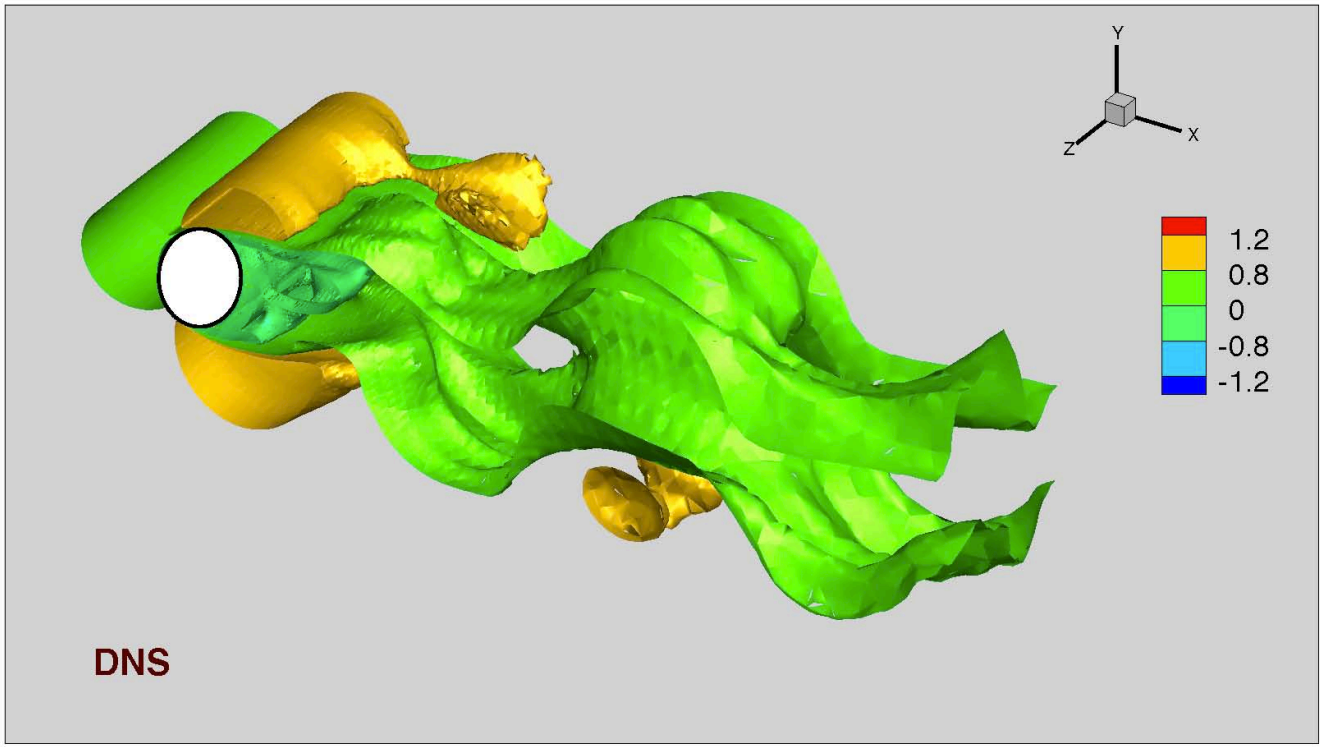
Ideal Closure



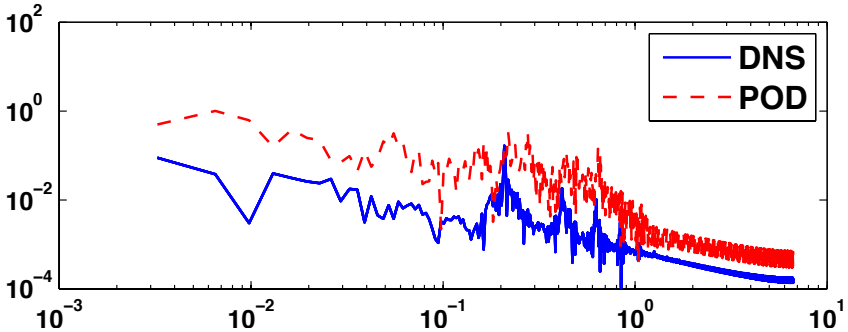
EV-ROMs

3D flow past a cylinder $\boxed{\mathrm{Re} = 1000}$

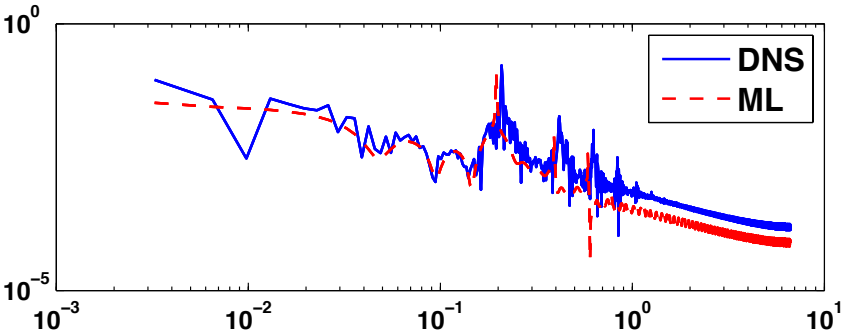


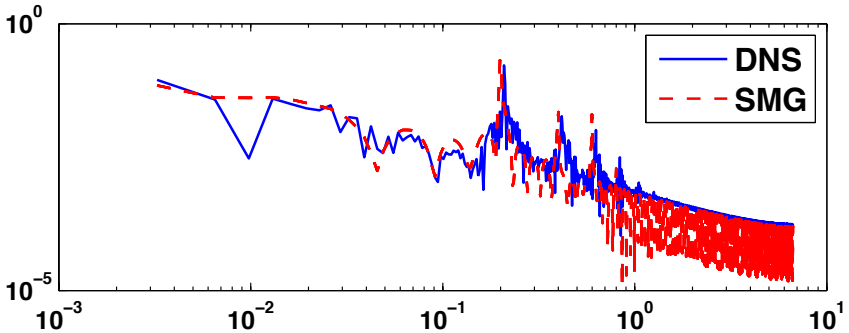
Wang, Akhtar, Borggaard, Iliescu, *Comput. Meth. Appl. Mech. Eng.*, 2012

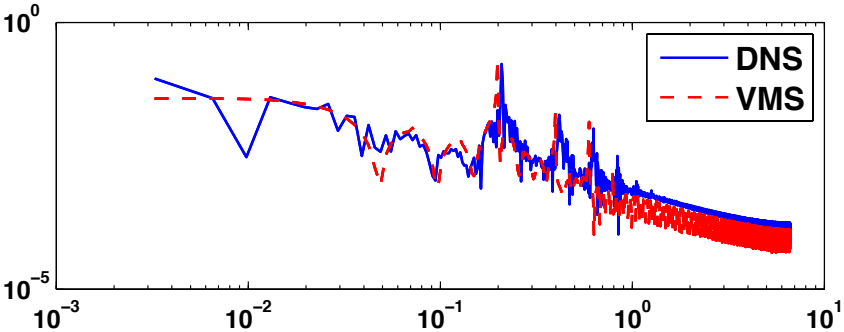
EV-ROMs Energy Spectrum

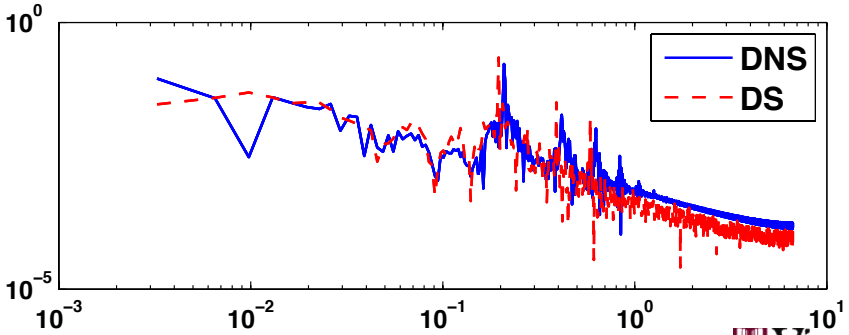


VMS-ROM; DS-ROM – accurate

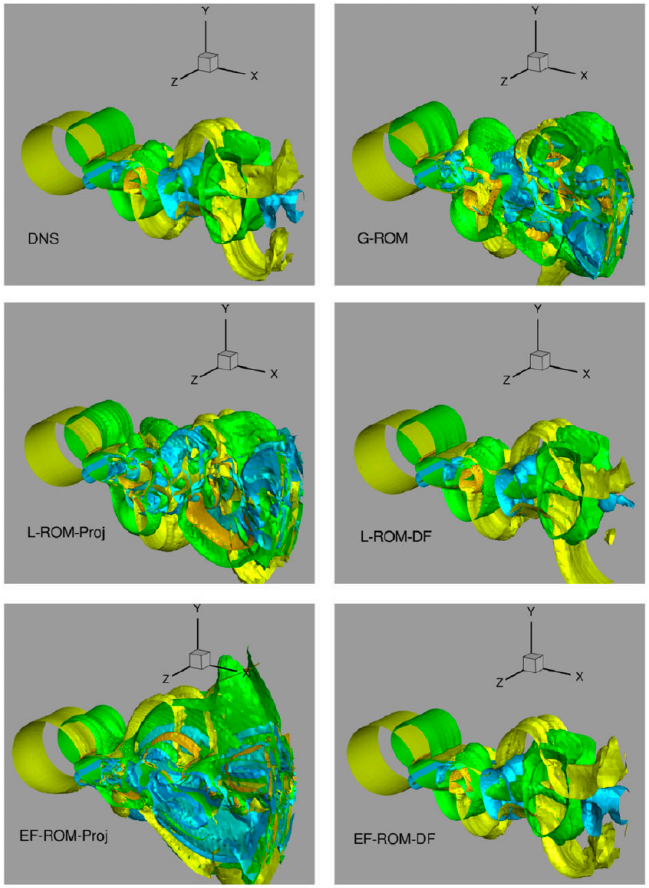








Regularized ROMs



Wells, Wang, Xie, Iliescu, *Int. J. Num. Meth. Fluids*, 2017

Gunzburger, Iliescu, Mohebujjaman, Schneier, *SIAM-ASA J. Uncertain.*, 2019

Gunzburger, Iliescu, Schneier, *IMA J. Numer. Anal.1*, 2019

Approximate Deconvolution ROM (AD-ROM)

- spatial filter $\boxed{\left(\left(I - \delta^2 \Delta \right) \overline{\mathbf{u}}^r, \varphi_j \right) = \left(\mathbf{u}^r, \varphi_j \right)}$

- approximate deconvolution ROM (AD-ROM)

$$\boxed{\left(\frac{\partial \mathbf{w}_r}{\partial t}, \varphi_k \right) + Re^{-1} \left(\nabla \mathbf{w}_r, \nabla \varphi_k \right) + \left(\left(\mathbf{w}_r^{AD} \cdot \nabla \right) \mathbf{w}_r^{AD}, \overline{\varphi_k} \right) = 0}$$

$$\mathbf{w}_r^{AD} = \left(G + \mu \, I \right)^{-1} \mathbf{w}_r$$

- *Xie, Wang, Wells, Iliescu, Comput. Meth. Appl. Mech. Eng., 2017*

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Variational Multiscale (VMS)

- Hughes 2000
- amazing success
  - SIMPLE
  - general Galerkin system
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  - hierarchical spaces
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    - Scale-similarity
    - Eddy-viscosity
  - VMS-ROM
    - VMS-ROM
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Two-Scale Data-Driven VMS-ROM

- resolved ROM scales $\mathbf{X}_1 := \text{span}\{\varphi_1, \ldots, \varphi_r\}$
- unresolved ROM scales $\mathbf{X}_2 := \text{span}\{\varphi_{r+1}, \ldots, \varphi_d\}$
- two-scale decomposition

$$\mathbf{u}_d = \sum_{j=1}^{d} a_j \, \varphi_j = \sum_{j=1}^{r} a_j \, \varphi_j + \sum_{j=r+1}^{d} a_j \, \varphi_j = \mathbf{u}_r + \mathbf{u}'$$

- $\mathbf{u}_r \in \mathbf{X}_1$ resolved ROM component of $\mathbf{u}$
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- VMS-ROM closure term

$$\left(\dot{\mathbf{u}}_r, \varphi_i\right) = \left(\mathbf{f}(\mathbf{u}_r), \varphi_i\right) + \underbrace{\boxed{\left[\left(\mathbf{f}(\mathbf{u}_d), \varphi_i\right) - \left(\mathbf{f}(\mathbf{u}_r), \varphi_i\right)\right]}}_{\text{VMS-ROM closure term}}, \quad \forall\, i = 1, \ldots, r$$

- VMS-ROM closure models
  - phenomenological eddy viscosity
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  - data-driven

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Two-Scale Data-Driven VMS-ROM

- ansatz

$$\left[\left(\mathbf{f}(\mathbf{u_d}), \varphi_\mathbf{i}\right) - \left(\mathbf{f}(\mathbf{u_r}), \varphi_\mathbf{i}\right)\right] \approx \left(\mathbf{g}(\mathbf{u_r}), \varphi_\mathbf{i}\right)$$

- low-dimensional least squares

$$\min_{\mathbf{g}\text{ parameters}} \sum_{j=1}^{M} \left\| \left[\left(\mathbf{f}(\mathbf{u}_d^{FOM}(t_j)), \varphi_i\right) - \left(\mathbf{f}(\mathbf{u}_r^{FOM}(t_j)), \varphi_i\right)\right] - \left(\mathbf{g}(\mathbf{u}_r^{FOM}(t_j)), \varphi_i\right) \right\|^2$$

- Two-Scale DD-VMS-ROM (2S-DD-VMS-ROM) [2]

$$\boxed{\left(\dot{\mathbf{u}}_r, \varphi_i\right) = \left(\mathbf{f}(\mathbf{u_r}), \varphi_\mathbf{i}\right) + \left(\mathbf{g}(\mathbf{u_r}), \varphi_\mathbf{i}\right)} \qquad i = 1, \ldots, r$$

[2] NSE $\quad \dot{\boldsymbol{a}} = \left(A + \widetilde{A}\right)\boldsymbol{a} + \boldsymbol{a}^\top \left(B + \widetilde{B}\right)\boldsymbol{a}$

Two-Scale Data-Driven VMS-ROM

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Two-Scale Data-Driven VMS-ROM

Algorithm 1 2S-DD-VMS-ROM

1: Use data (snapshots) to construct orthonormal basis $\{\varphi_1, \ldots, \varphi_d\}$, $\boxed{d = \mathcal{O}(10^3)}$.

2: In offline stage, solve least squares problem:

$$\min_{\mathbf{g}\text{ parameters}} \sum_{j=1}^{M} \left\| \left[\left(\mathbf{f}(\mathbf{u}_d(t_j)), \varphi_i \right) - \left(\mathbf{f}(\mathbf{u}_r(t_j)), \varphi_i \right) \right] - \left(\mathbf{g}(\mathbf{u}_r(t_j)), \varphi_i \right) \right\|^2 . \tag{1}$$

3: In offline stage, compute ROM operators of r-dimensional 2S-DD-VMS-ROM, $\boxed{r = \mathcal{O}(10)}$:

$$\left(\dot{\mathbf{u}}_r, \varphi_i \right) = \left(\mathbf{f}(\mathbf{u}_r), \varphi_i \right) + \left(\mathbf{g}(\mathbf{u}_r), \varphi_i \right), \qquad i = 1, \ldots, r. \tag{2}$$

4: In online stage, use 2S-DD-VMS-ROM (2) for different parameters and/or longer time.

Two-Scale Data-Driven VMS-ROM NSE

Algorithm 2 2S-DD-VMS-ROM for NSE

1: Use data (snapshots) to construct orthonormal basis $\{\varphi_1, \ldots, \varphi_d\}$, $\boxed{d = \mathcal{O}(10^3)}$.

2: In offline stage, construct r-dimensional operators A and B, $\boxed{r = \mathcal{O}(10)}$.

3: In offline stage, construct r-dimensional operators $\tilde{A}$ and $\widetilde{B}$, $\boxed{r = \mathcal{O}(10)}$, which solve least squares problem:

$$\min_{\tilde{A},\widetilde{B}} \sum_{j=1}^{M} \Bigg\| - \left[\Big(\left(\mathbf{u}_d(t_j) \cdot \nabla\right) \mathbf{u}_d(t_j) \,, \varphi_i \Big) - \Big(\left(\mathbf{u}_r(t_j) \cdot \nabla\right) \mathbf{u}_r(t_j) \,, \varphi_i \Big) \right] - \Big(\tilde{A}\, \boldsymbol{a}^{DNS}(t_j) + \boldsymbol{a}^{DNS}(t_j)^\top \tilde{B}\, \boldsymbol{a}^{DNS}(t_j) \Big) \Bigg\|^2 . \tag{3}$$

4: In online stage, for different parameters and/or longer time, repeatedly use 2S-DD-VMS-ROM

$$\dot{\boldsymbol{a}} = (A + \tilde{A})\boldsymbol{a} + \boldsymbol{a}^\top (B + \tilde{B})\boldsymbol{a} \,. \tag{4}$$

Three-Scale Data-Driven VMS-ROM

- large resolved ROM scales $\mathbf{X}_1 := \text{span}\{\varphi_1, \ldots, \varphi_{r_1}\}$
- snall resolved ROM scales $\mathbf{X}_2 := \text{span}\{\varphi_{r_1+1}, \ldots, \varphi_r\}$
- unresolved ROM scales $\mathbf{X}_3 := \text{span}\{\varphi_{r+1}, \ldots, \varphi_d\}$
- three-scale decomposition

$$\mathbf{u}_d = \sum_{j=1}^{d} a_j \varphi_j = \sum_{j=1}^{r_1} a_j \varphi_j + \sum_{j=r_1+1}^{r} a_j \varphi_j + \sum_{j=r+1}^{d} a_j \varphi_j = \mathbf{u}_L + \mathbf{u}_S + \mathbf{u}'$$

- $\mathbf{u}_L \in \mathbf{X}_1$ large resolved ROM component of $\mathbf{u}$
- $\mathbf{u}_S \in \mathbf{X}_2$ small resolved ROM component of $\mathbf{u}$
- $\mathbf{u}' \in \mathbf{X}_3$ unresolved ROM component of $\mathbf{u}$

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- $\mathbf{u}_L \in \mathbf{X}_1$: large resolved ROM component of $\mathbf{u}$
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$$\mathbf{u}_d = \sum_{j=1}^{d} a_j \varphi_j = \sum_{j=1}^{r_1} a_j \varphi_j + \sum_{j=r_1+1}^{r} a_j \varphi_j + \sum_{j=r+1}^{d} a_j \varphi_j = \mathbf{u}_L + \mathbf{u}_S + \mathbf{u}'$$

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- $\mathbf{u}_S \in \mathbf{X}_2$ small resolved ROM component of $\mathbf{u}$
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Three-Scale Data-Driven VMS-ROM

- large resolved ROM scales $\mathbf{X}_1 := \text{span}\{\varphi_1, \ldots, \varphi_{r_1}\}$
- snall resolved ROM scales $\mathbf{X}_2 := \text{span}\{\varphi_{r_1+1}, \ldots, \varphi_r\}$
- unresolved ROM scales $\mathbf{X}_3 := \text{span}\{\varphi_{r+1}, \ldots, \varphi_d\}$
- three-scale decomposition

$$\mathbf{u}_d = \sum_{j=1}^{d} a_j \varphi_j = \sum_{j=1}^{r_1} a_j \varphi_j + \sum_{j=r_1+1}^{r} a_j \varphi_j + \sum_{j=r+1}^{d} a_j \varphi_j = \mathbf{u}_L + \mathbf{u}_S + \mathbf{u}'$$

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Three-Scale Data-Driven VMS-ROM

- large-small VMS-ROM closure terms

$$\left(\dot{\mathbf{u}}_L, \varphi_i\right) = \left(\mathbf{f}(\mathbf{u_L} + \mathbf{u_S}), \varphi_\mathbf{i}\right) + \boxed{\left[\left(\mathbf{f}(\mathbf{u_d}), \varphi_\mathbf{i}\right) - \left(\mathbf{f}(\mathbf{u_L} + \mathbf{u_S}), \varphi_\mathbf{i}\right)\right]} \qquad \forall\, i = 1, \ldots, r_1$$

- small-unresolved VMS-ROM closure terms

$$\left(\dot{\mathbf{u}}_S, \varphi_i\right) = \left(\mathbf{f}(\mathbf{u_L} + \mathbf{u_S}), \varphi_\mathbf{i}\right) + \boxed{\left[\left(\mathbf{f}(\mathbf{u_d}), \varphi_\mathbf{i}\right) - \left(\mathbf{f}(\mathbf{u_L} + \mathbf{u_S}), \varphi_\mathbf{i}\right)\right]} \qquad \forall\, i = r_1 + 1, \ldots, r$$

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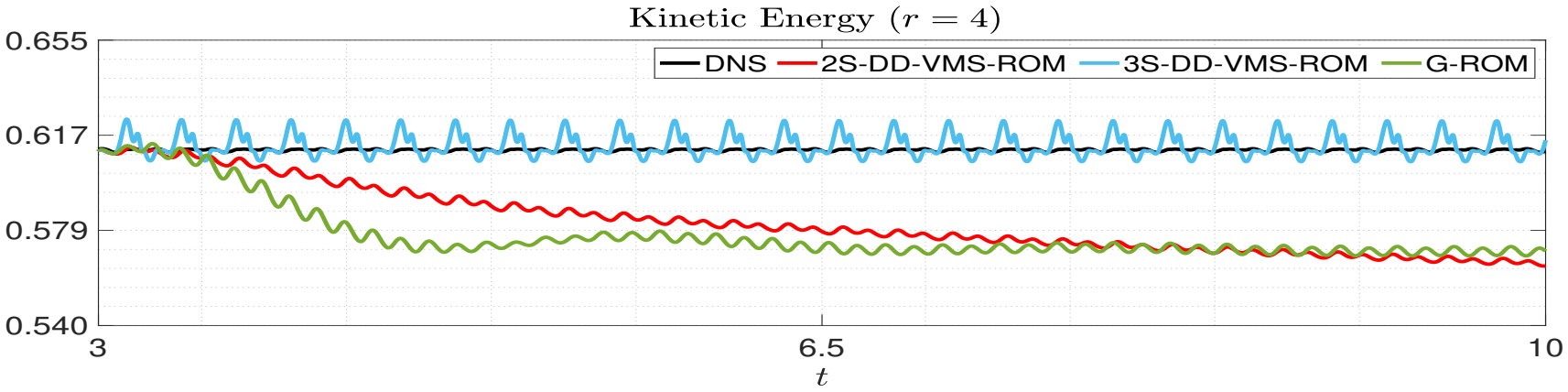
Three-Scale Data-Driven VMS-ROM

- Three-Scale DD-VMS-ROM (3S-DD-VMS-ROM)

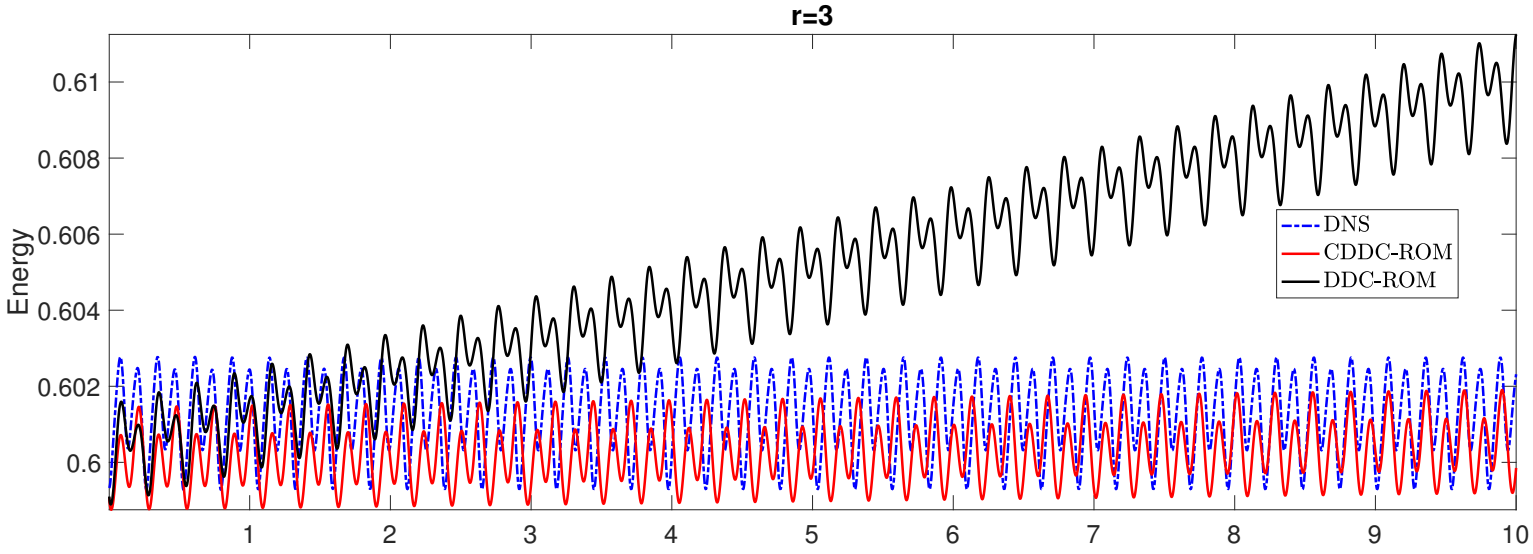
$$\begin{bmatrix} \dot{\boldsymbol{a}}_L \\ \\ \dot{\boldsymbol{a}}_S \end{bmatrix} = A\,\boldsymbol{a} + \boldsymbol{a}^\top B\,\boldsymbol{a} + \begin{bmatrix} \tilde{A}_L\,\boldsymbol{a} + \boldsymbol{a}^\top \widetilde{B}_L\,\boldsymbol{a} \\ \\ \tilde{A}_S\,\boldsymbol{a} + \boldsymbol{a}^\top \widetilde{B}_S\,\boldsymbol{a} \end{bmatrix}$$

DD-VMS-ROM $Re = 1000$ Predictive

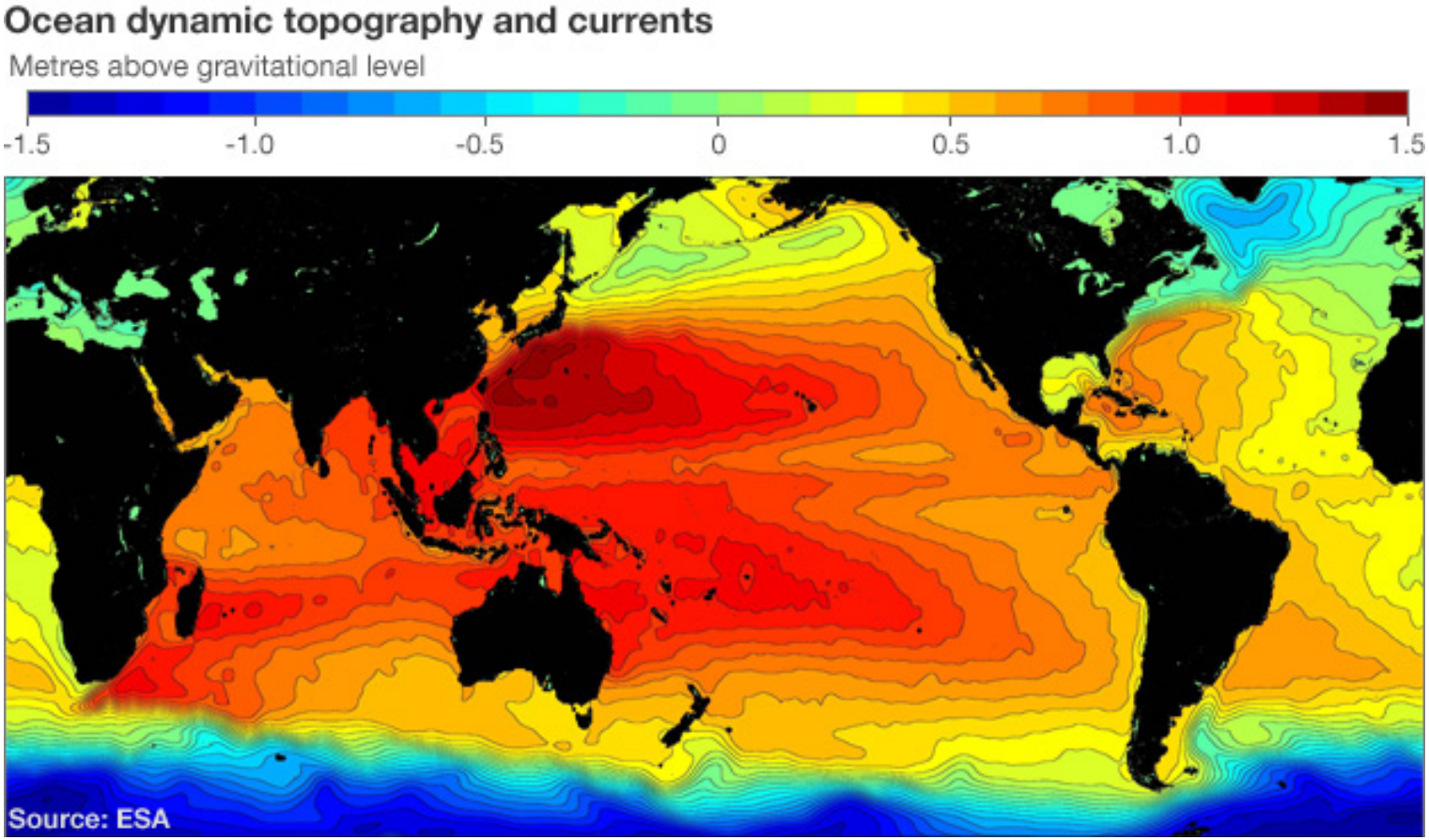


DD-VMS-ROM + Constraints Predictive

- $Re = 1000$
- 50% data



Quasi-Geostrophic Flow



Quasi-Geostrophic Equations (QGE)

$$\begin{aligned} \frac{\partial q}{\partial t} + J(\psi, q) &= Re^{-1}\,\Delta q + F \\ q &= Ro\,\Delta\psi + y \end{aligned}$$

- $J(\cdot,\cdot)$ Jacobian operator $J(\psi, q) := \frac{\partial \psi}{\partial x}\frac{\partial q}{\partial y} - \frac{\partial \psi}{\partial y}\frac{\partial q}{\partial x}$
- velocity $\mathbf{u} := \nabla^{\perp}\psi = \left(-\frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial x}\right)$
- Rossby number $Ro := \frac{U}{\beta\, L^2}$
- Reynolds number $Re := \frac{U\,L}{A}$

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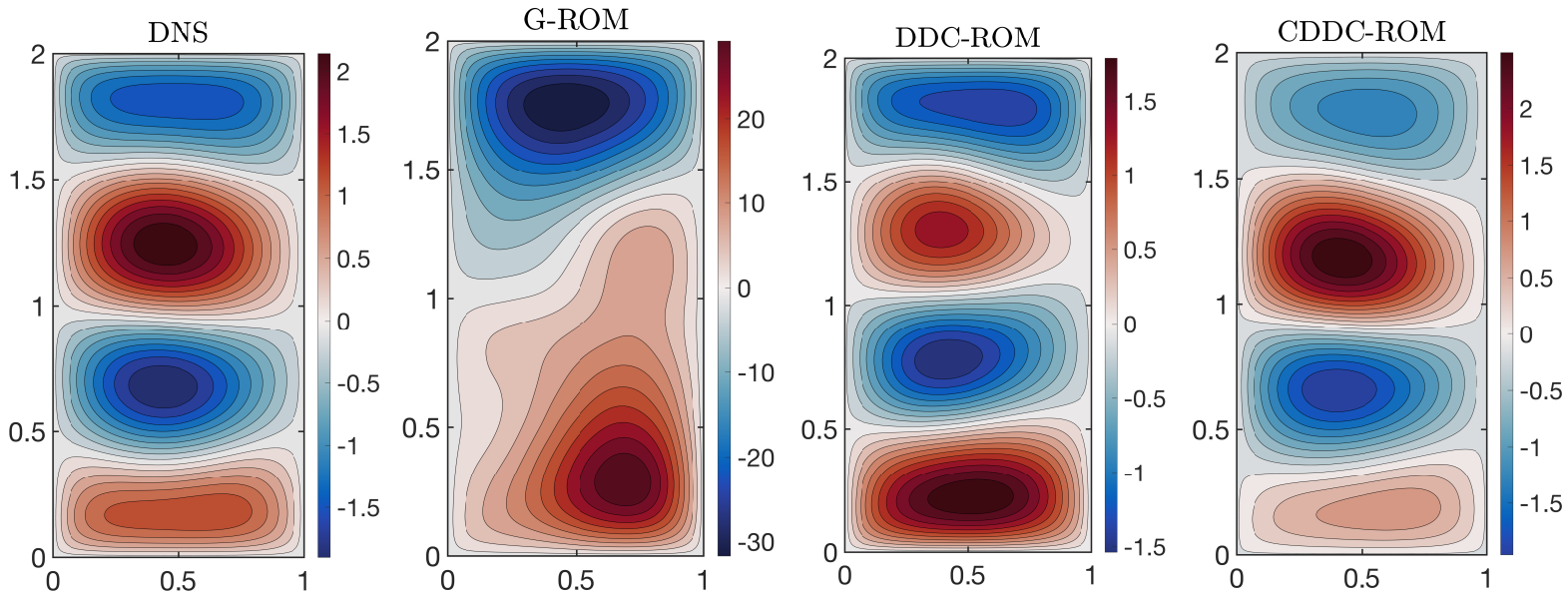
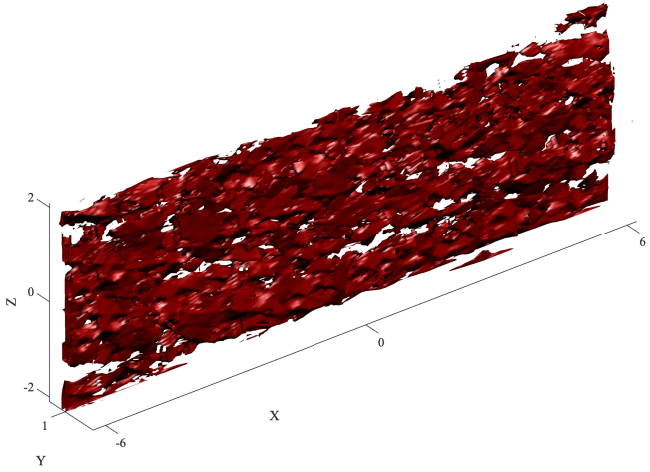
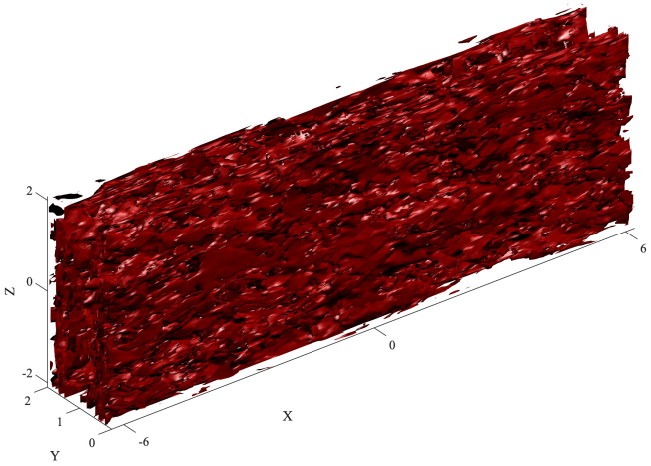
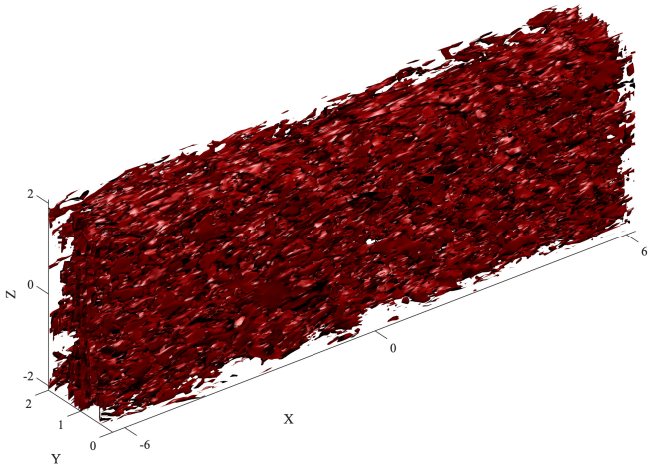
QGE: Time-Average



Channel Flow $Re_\tau = 395$ $(Re = 13{,}750)$







SUPG-ROM

- convection-dominated convection-diffusion-reaction

$$\frac{\partial u}{\partial t} - \varepsilon\,\Delta u + \mathbf{b}\cdot\nabla u + c\,u = f$$

- SUPG-ROM

$$\begin{aligned}\left(u_r^n - u_r^{n-1}, v_r\right) + \Delta t\, a_{\mathrm{SUPG},r}\left(u_r^n, v_r\right) &= \Delta t\,(f^n, v_r) + \Delta t\,\delta_r\,(f^n, \mathbf{b}^n\cdot\nabla v_r) \\ &- \delta_r\left(u_r^n - u_r^{n-1}, \mathbf{b}^n\cdot\nabla v_r\right)\end{aligned}$$

$$\begin{aligned}a_{\mathrm{SUPG},r}(u_r, v_r) &= (\varepsilon\nabla u_r, \nabla v_r) + (\mathbf{b}\cdot\nabla u_r, v_r) + (c\,u_r, v_r) \\ &+ \delta_r \sum_{K\in\mathcal{T}_h} (-\varepsilon\,\Delta u_r + \mathbf{b}\cdot\nabla u_r + c\,u_r, \mathbf{b}\cdot\nabla v_r)_K\end{aligned}$$

- fundamental question $\boxed{\delta_r = ?}$

Inverse Estimates

- FE inverse estimate

$$\|v_h\|_{m,K} \leq \mu_{\text{inv}}\, h_K{}^{l-m}\, \|v_h\|_{l,K} \qquad \forall\, v_h \in X_h$$

- ROM inverse estimate

$$\|\nabla v_r\| \leq \sqrt{\|S_r\|_2\, \|M_r^{-1}\|_2}\;\; \|v_r\| \qquad \forall\, v_r \in X_r$$

- $\boxed{X_r \subset X_h}$

FE Scaling

- minimize

$$\delta_r = \frac{h^{m+1/2} + \Lambda_0}{h^{m-1}(h^{3/2} + h + \varepsilon + \varepsilon^{1/2} h^{1/2}) + \Lambda_0(1 + h^{-1} + \varepsilon h^{-2})}$$

$$\Lambda_0 = \left(\sum_{j=r+1}^{R} \lambda_j \right)^{1/2}$$

- simplify $\boxed{\delta_r^{\mathrm{FE}} = h}$

ROM Scaling

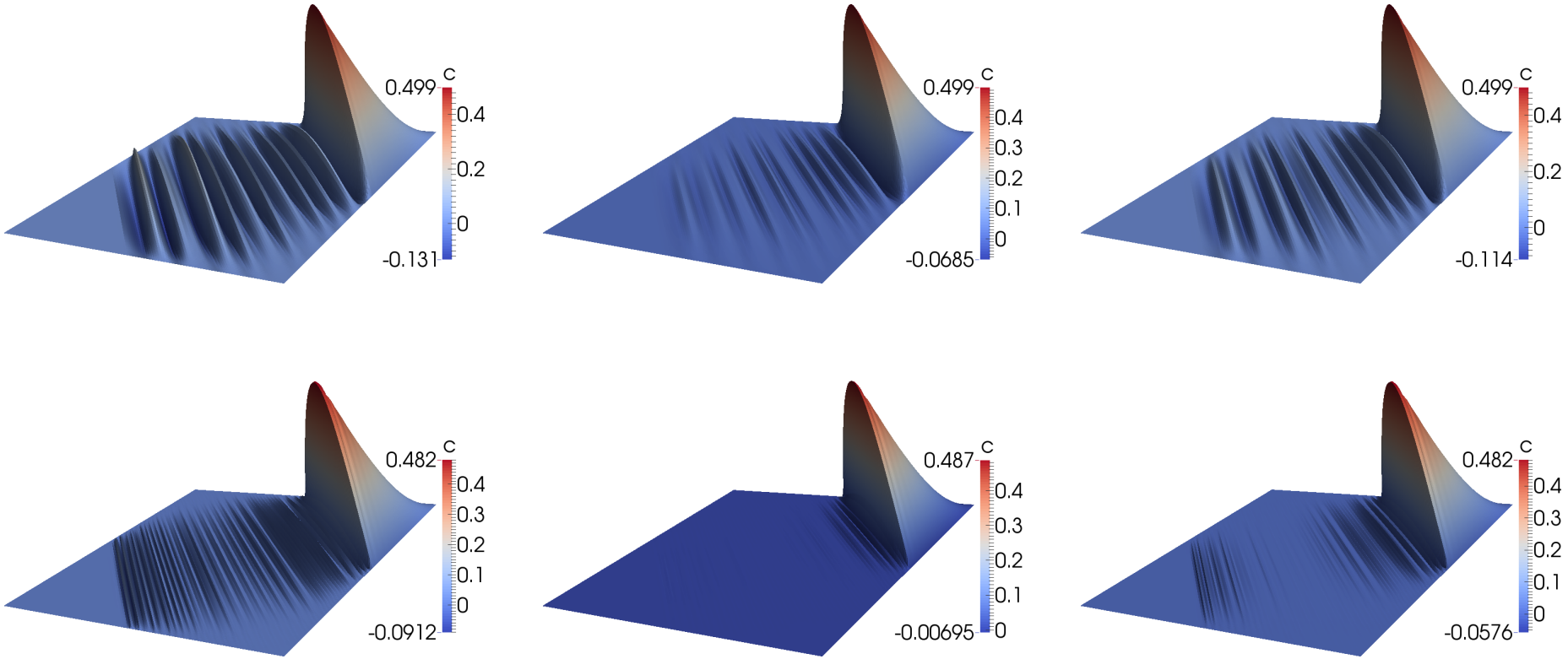
- minimize

$$\left(1+\delta_r^{-1/2}+\delta_r^{1/2}\right) C_\Lambda \Lambda_0 + \left(\varepsilon^{1/2}+\delta_r^{1/2}\right) C_\Lambda \Lambda_1 + \delta_r^{1/2}\varepsilon C_\Lambda \Lambda_2$$

$$\Lambda_0 = \left(\sum_{j=r+1}^{R} \lambda_j\right)^{1/2} \qquad \Lambda_1 = \left(\sum_{j=r+1}^{R} \lambda_j |\varphi_j|_1^2\right)^{1/2} \qquad \Lambda_2 = \left(\sum_{j=r+1}^{R} \lambda_j |\varphi_j|_2^2\right)^{1/2}$$

- simplify $\boxed{\delta_r^{\mathrm{POD}} = \dfrac{\Lambda_0}{\Lambda_1}}$

Numerical Test



G-ROM, FE-SUPG-ROM, POD-SUPG-ROM, $t = 1.0$, $r = 30,\ 130$.

- Giere, Iliescu, John, Wells, *Comput. Meth. Appl. Mech. Eng.*, 2015

Conclusions

- under-resolved ROMs
- closure
  - LES, spatial filter
  - variational multiscale + data
- simple
- physical constraints
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(1) EV-ROM

- NSF, AFOSR (2005-2015)
- Wang, Akhtar, Borggaard, Iliescu, *J. Comput. Phys.*, 2011
- Wang, Akhtar, Borggaard, Iliescu, *Comput. Meth. Appl. Mech. Eng.*, 2012
- Iliescu, Wang, *Math. Comput.*, 2013
- Iliescu, Wang, *SIAM J. Sci. Comput.*, 2014
- Wells, Xie, Wang, Iliescu, *Int. J. Num. Meth. Fluids*, 2017

(2) AD-ROM

- NSF (2015-2018)
- Xie, Wang, Wells, Iliescu, *Comput. Meth. Appl. Mech. Eng.*, 2017
- Gunzburger, Iliescu, Mohebujjaman, Schneier, *SIAM J. Uncertain. Quant.*, 2019

(3) DD-VMS-ROM

- NSF (2018-2021)
- Xie, Mohebujjaman, Rebholz, Iliescu, *SIAM J. Sci. Comput.*, 2018
- Mohebujjaman, Rebholz, Iliescu, *Int. J. Num. Meth. Fluids*, 2019
- Iliescu, Liu, Mou, *Int. J. Comput. Fluid Dyn.*, 2020
- Mou, Koc, San, Iliescu, 2020

VirginiaTech Invent the Future

Thank You!

Take Home Message

Galerkin + Data = ROM

Problem

- PDE $\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u})$ given
- FEM, FDM, FVM, ... given
- ROM
  - $r = \mathcal{O}(10)$ given
  - $\{\varphi_1, \ldots, \varphi_r\}$ given
  - model ???

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Variational Multiscale (VMS)

- Hughes 2000
- general PDE $\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u})$
- *hierarchical* spaces $\mathbf{X}_1, \quad \mathbf{X}_1 \oplus \mathbf{X}_2, \quad \mathbf{X}_1 \oplus \mathbf{X}_2 \oplus \mathbf{X}_3, \ldots$
- Galerkin projection

$$(\dot{\mathbf{u}}, \mathbf{v}_1) = (\mathbf{f}(\mathbf{u}), \mathbf{v}_1) \qquad \forall\, \mathbf{v}_1 \in \mathbf{X}_1$$

- not closed

$$(\mathbf{f}(\mathbf{u}), \mathbf{v}_1) = (\mathbf{f}(\mathbf{u}_1 + \mathbf{u}_2 + \mathbf{u}_3 + \ldots), \mathbf{v}_1) \qquad \forall\, \mathbf{v}_1 \in \mathbf{X}_1$$

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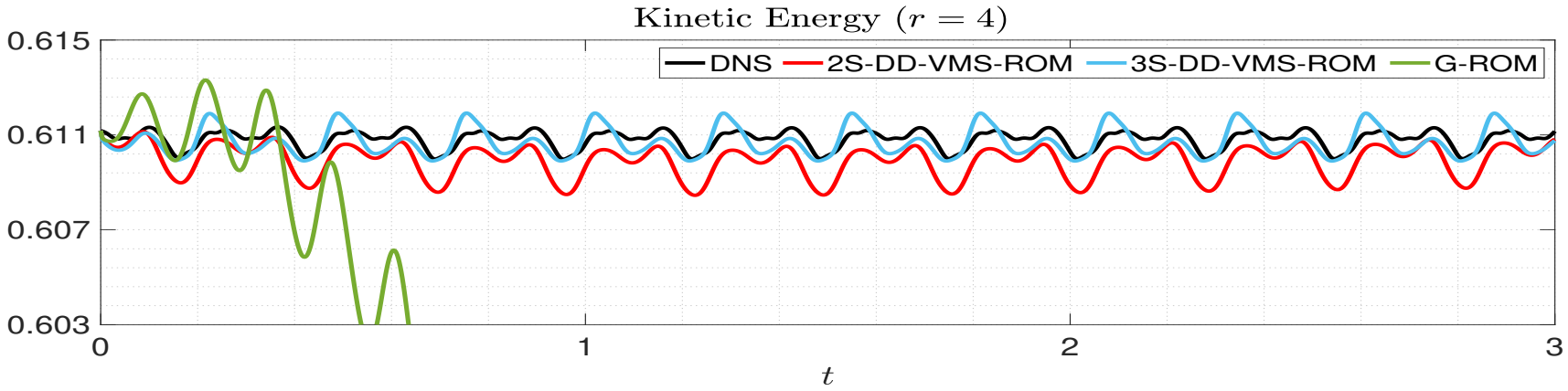
Paradigm Shift

Variational Multiscale in the Age of Data

DD-VMS-ROM $Re = 1000$ Reconstructive



Constrained DD-VMS-ROM

- G-ROM
  - $-\|\nabla \boldsymbol{u}_r\|^2 = \boldsymbol{a}^\top A\, \boldsymbol{a} \leq 0$
  - $\Big((\mathbf{u}_r \cdot \nabla)\, \mathbf{u}_r, \mathbf{u}_r \Big) = 0 \quad \Longleftrightarrow \quad \boldsymbol{a}^\top \left[\boldsymbol{a}^\top B\, \boldsymbol{a} \right] = 0$
- Constrained DD-VMS-ROM
  - $\boldsymbol{a}^\top [\tilde{A}\, \boldsymbol{a} + \boldsymbol{a}^\top \widetilde{B}\, \boldsymbol{a}] \leq 0$ [3]
  - $\boxed{\boldsymbol{a}^\top \tilde{A}\, \boldsymbol{a} \leq 0 \quad \text{and} \quad \boldsymbol{a}^\top \left[\boldsymbol{a}^\top \widetilde{B}\, \boldsymbol{a} \right] = 0}$

[3] Couplet, Sagaut, Basdevant, *J. Fluid Mech.*, 2003

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Constrained DD-VMS-ROM

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  - $\Big((\mathbf{u}_r \cdot \nabla)\, \mathbf{u}_r, \mathbf{u}_r \Big) = 0 \quad \Longleftrightarrow \quad \boldsymbol{a}^\top \left[\boldsymbol{a}^\top B\, \boldsymbol{a} \right] = 0$
- Constrained DD-VMS-ROM
  - $\boldsymbol{a}^\top [\tilde{A}\, \boldsymbol{a} + \boldsymbol{a}^\top \widetilde{B}\, \boldsymbol{a}] \leq 0$ [3]
  - $\boxed{\boldsymbol{a}^\top \tilde{A}\, \boldsymbol{a} \leq 0 \quad \text{and} \quad \boldsymbol{a}^\top \left[\boldsymbol{a}^\top \widetilde{B}\, \boldsymbol{a} \right] = 0}$

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Constrained DD-VMS-ROM NSE

Algorithm 3 Constrained DD-VMS-ROM for NSE

1: Use data (snapshots) to construct orthonormal basis $\{\varphi_1, \ldots, \varphi_d\}$, $\boxed{d = \mathcal{O}(10^3)}$.

2: In offline stage, construct r-dimensional operators A and B, $\boxed{r = \mathcal{O}(10)}$.

3: In offline stage, construct r-dimensional operators $\tilde{A}$ and $\widetilde{B}$, $\boxed{r = \mathcal{O}(10)}$, which solve least squares problem:

$$\min_{\substack{\tilde{A},\widetilde{B} \\ \boldsymbol{a}^\top \tilde{A}\, \boldsymbol{a} \leq 0 \\ \boldsymbol{a}^\top \left[\boldsymbol{a}^\top \widetilde{B}\, \boldsymbol{a}\right] = 0}} \sum_{j=1}^{M} \Bigg\| - \left[\Big(\left(\mathbf{u}_d(t_j)\cdot\nabla\right)\mathbf{u}_d(t_j), \varphi_i\Big) - \Big(\left(\mathbf{u}_r(t_j)\cdot\nabla\right)\mathbf{u}_r(t_j), \varphi_i\Big)\right] - \left(\tilde{A}\,\boldsymbol{a}^{DNS}(t_j) + \boldsymbol{a}^{DNS}(t_j)^\top \tilde{B}\,\boldsymbol{a}^{DNS}(t_j)\right)\Bigg\|^2 . \tag{5}$$

4: In online stage, for different parameters and/or longer time, repeatedly use DD-VMS-ROM

$$\dot{\boldsymbol{a}} = (A + \tilde{A})\boldsymbol{a} + \boldsymbol{a}^\top (B + \tilde{B})\boldsymbol{a} . \tag{6}$$

Quasi-Geostrophic Equations (QGE)

$$\begin{aligned} \frac{\partial q}{\partial t} + J(\psi, q) &= Re^{-1}\,\Delta q + F \\ q &= Ro\,\Delta\psi + y \end{aligned}$$

- $J(\cdot,\cdot)$ Jacobian operator $J(\psi, q) := \frac{\partial \psi}{\partial x}\frac{\partial q}{\partial y} - \frac{\partial \psi}{\partial y}\frac{\partial q}{\partial x}$
- velocity $\mathbf{u} := \nabla^{\perp}\psi = \left(-\frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial x}\right)$
- Rossby number $Ro := \frac{U}{\beta\, L^2}$
- Reynolds number $Re := \frac{U\,L}{A}$

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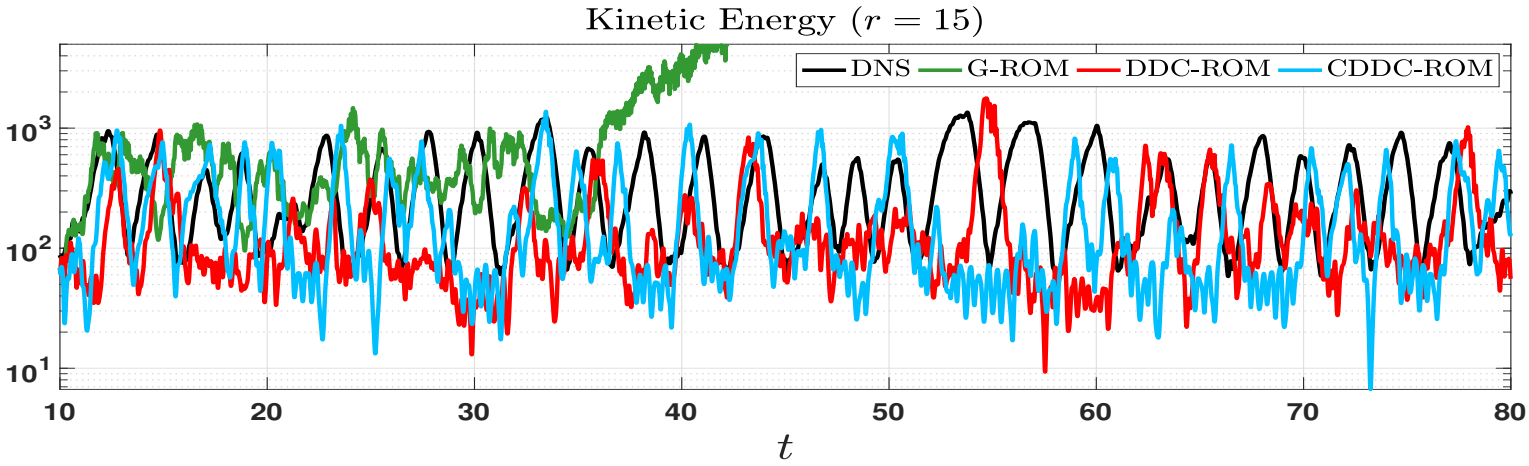
QGE: Time-Average



Related Work

- no ROM
  - 20th century Adrian, Moser
  - 21st century Iaccarino, Duraisamy, Ling, Xiao
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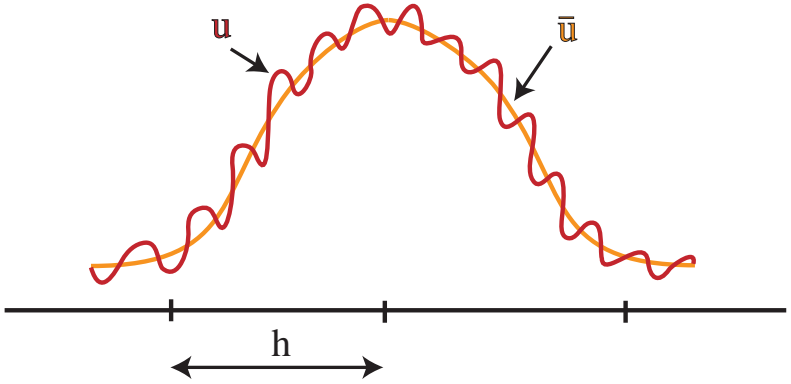
Connections

- Large Eddy Simulation



- Nonlinear Galerkin
- Bubble Functions

LES-ROM Framework

- standard LES derivation
  - filtered NSE

$$\left(\frac{\partial \overline{\mathbf{u}}}{\partial t}, \phi\right) + Re^{-1}\left(\nabla \overline{\mathbf{u}}, \nabla \phi\right) + \left(\overline{\mathbf{u} \cdot \nabla \mathbf{u}}, \phi\right) = \mathbf{0}$$

  - $\boxed{\text{“Correction”} = -\left(\overline{\mathbf{u} \cdot \nabla \mathbf{u}} + \overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}}, \phi\right)}$
  - closure model

$$\boxed{\overline{\mathbf{u} \cdot \nabla \mathbf{u}} = \text{function}(\overline{\mathbf{u}})}$$

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$$\left(\frac{\partial \mathbf{W}_r}{\partial t}, \varphi_i\right) + Re^{-1}\left(\nabla \mathbf{W}_r, \nabla \varphi_i\right) + \left(\text{function}(\mathbf{W}_r), \varphi_i\right) = \mathbf{0}$$

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VirginiaTech Invent the Future

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Approximate Deconvolution

- image processing, inverse problems
- deconvolution
  - given $\overline{\mathbf{u}}_r := G\,\mathbf{u}_r$
  - find $\mathbf{u}_r$
- exact deconvolution $\mathbf{u}_r{}^{ED} = G^{-1}\,\overline{\mathbf{u}}_r$
  - very bad idea
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- approximate deconvolution $\mathbf{u}_r{}^{AD} \approx \mathbf{u}_r{}^{ED} = G^{-1}\,\overline{\mathbf{u}}_r$
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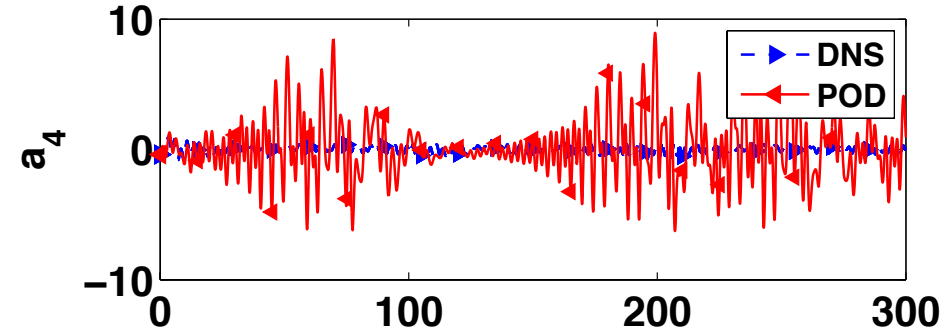
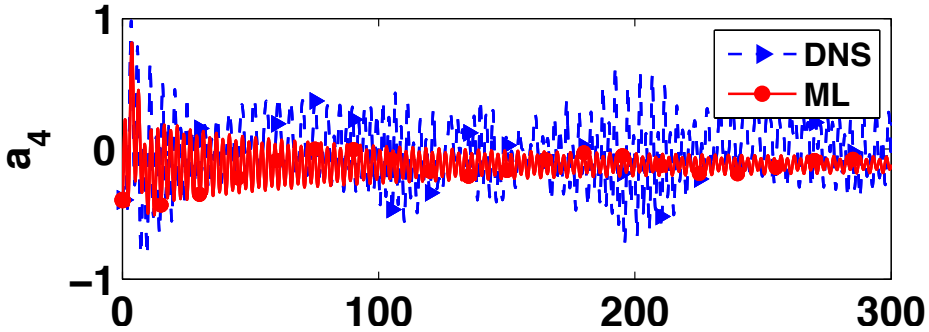
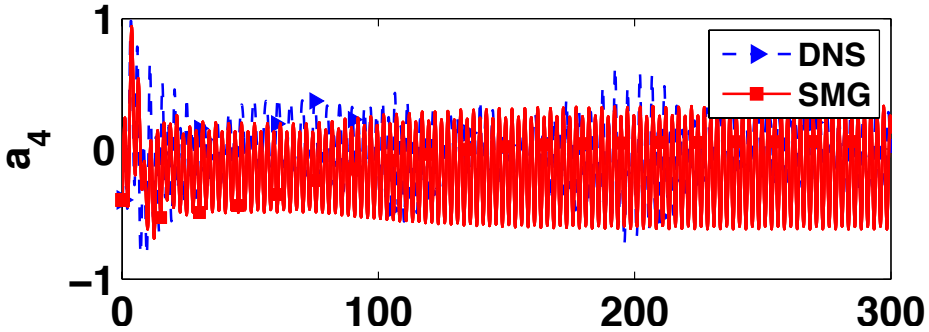
SOMETIMES
I QUESTION
MY SANITY.
BUT MY
UNICORN
SAID
I'M FINE.

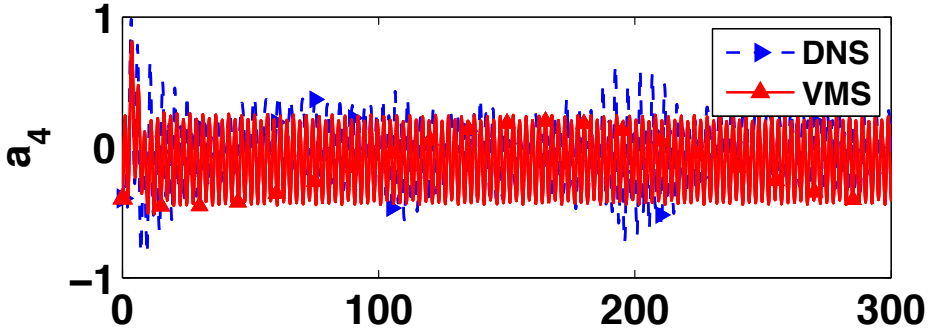
ROM Coefficients

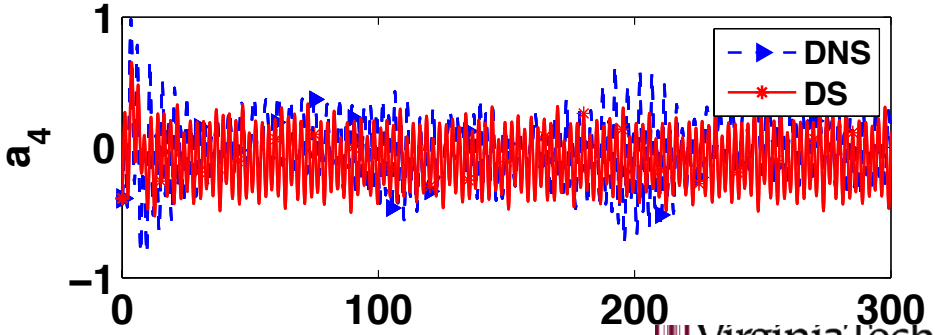


VMS-ROM; DS-ROM – accurate









DDF-ROM vs State-Of-The-Art ROMs: CPU Time

	L-ROM	EF-ROM	AD-ROM	DDF-ROM
$r = 6$	4.12	4.25	4.44	2.27
$r = 10$	6.72	6.91	7.26	4.42
$r = 15$	9.97	10.14	10.32	6.67

DDF-ROM: Computational Efficiency

Method	Proj	$\|u_{DNS} - u_{ROM}\|$			CPU time (seconds)		
		r=6	r=10	r=15	r=6	r=10	r=15
G-ROM		0.2208	0.1589	0.0848	2.06	3.28	4.79
DDF-ROM	X^r	0.2208	0.1589	0.0848	2.06	3.28	4.79
DDF-ROM	X^{r+1}	0.1214	0.0854	0.0654	2.16	3.43	4.95
DDF-ROM	X^{2r}	0.0928	0.0627	0.0446	2.75	4.42	6.67
DDF-ROM	X^{3r}	0.0923	0.0632	0.0452	3.44	5.61	8.57
DDF-ROM	X^d	0.0931	0.0638	0.0454	14.21	15.06	16.06

LES, ROM Similarities: Basis

- homogeneous flow

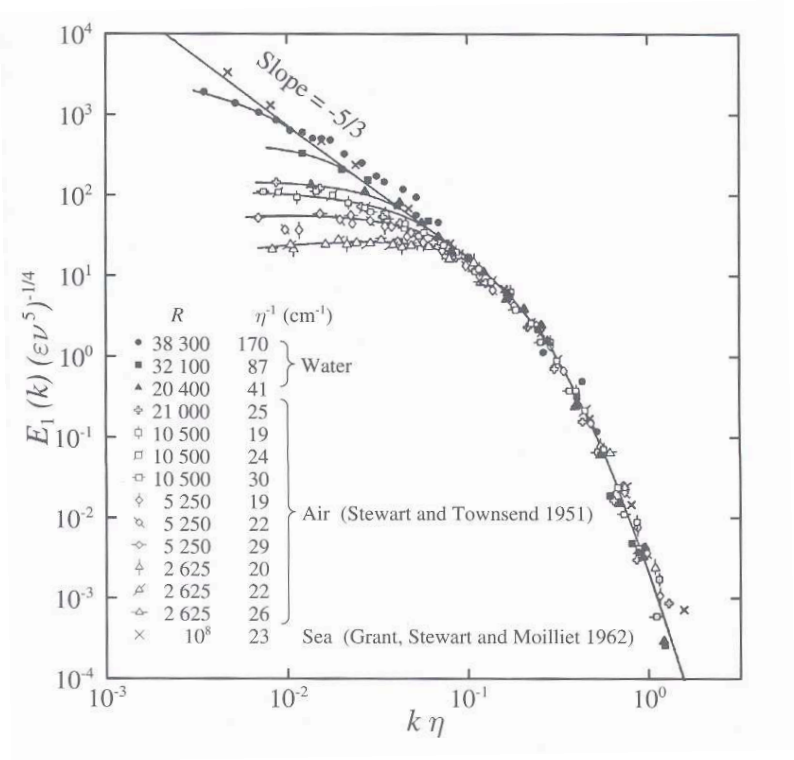
$$R(\mathbf{x}, \mathbf{x}') = R(\mathbf{x} - \mathbf{x}')$$

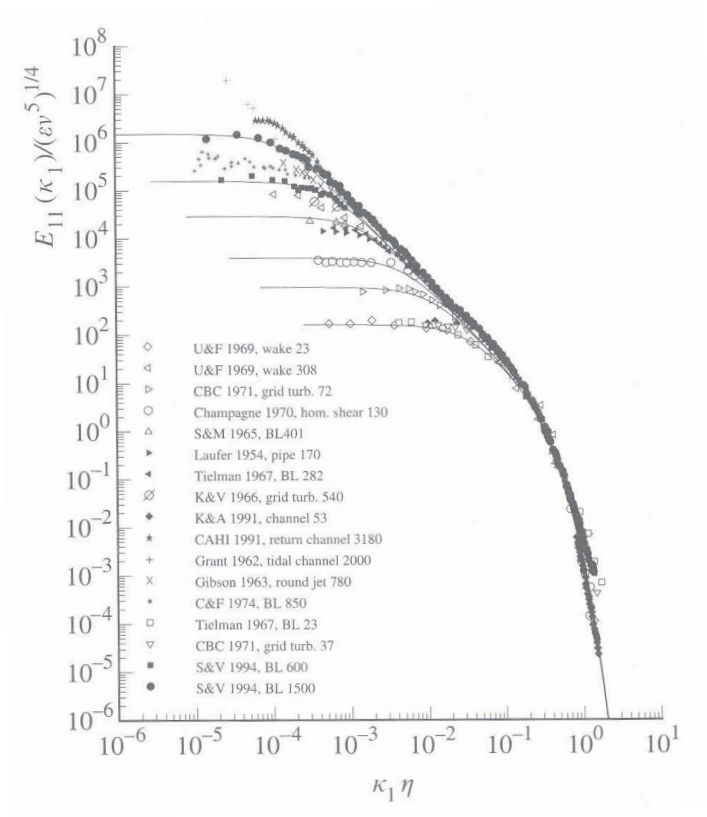
- translation invariant

Theorem (Holmes, Lumley, Berkooz, 1996)

If $R(\mathbf{x}, \mathbf{x}') = R(\mathbf{x} - \mathbf{x}')$ is homogeneous, then the eigenfunctions of the operator $\mathcal{R} = \int_\Omega R(\mathbf{x}, \mathbf{x}') \cdot d\mathbf{x}'$ (i.e., the POD modes) are Fourier modes.

Energy Cascade

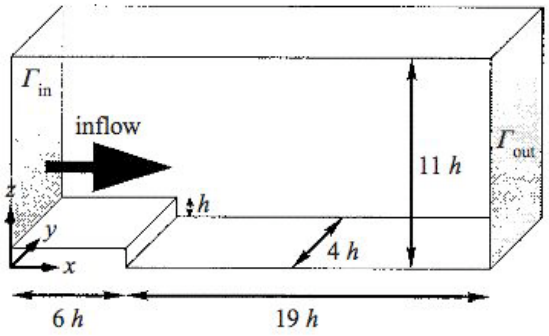




Energy cascade for different *Re*.

Energy Cascade – ROM

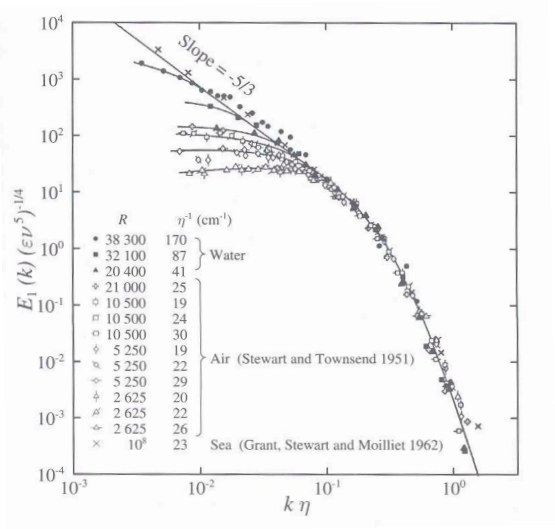
- forward energy transfer
  - Fourier ✓
  - POD ?
  - non-homogeneous



Couplet, Sagaut, Basdevant, *J. Fluid Mech.*, 2003.

Galerkin ROM Stable, Not Accurate

- stable [5] $$\|\mathbf{u}_r^n\|^2 + \nu\,\Delta t \sum_{n=1}^{M} \|\nabla \mathbf{u}_r^n\|^2 \leq \text{data}$$
- not accurate



- $\boxed{\text{Galerkin ROM} \neq \text{model large scales}}$

[5] Noel Walkington, Pitt seminar, 2013

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Data-Driven ROMs

- data DNS, experiment
- ansatz $\dot{\boldsymbol{a}} = A\,\boldsymbol{a} + \boldsymbol{a}^\top B\,\boldsymbol{a}$
- inverse problem $\Longrightarrow$ $\tilde{A}$, $\widetilde{B}$
- DD-ROM $\boxed{\dot{\boldsymbol{a}} = \tilde{A}\,\boldsymbol{a} + \boldsymbol{a}^\top \widetilde{B}\,\boldsymbol{a}}$
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ROM Spatial Filtering: Projection

- POD basis $\mathbf{X}^r = \{\varphi_1, \ldots, \varphi_{r_1}, \varphi_{r_1+1}, \ldots\ldots\ldots\ldots, \varphi_r\}$
- POD projection basis $\mathbf{X}^{r_1} = \{\varphi_1, \ldots, \varphi_{r_1}\}$
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DDF-ROM Step I: Filtered-ROM (F-ROM)

- LES-ROM + ROM projection

$$\left(\frac{\partial \overline{\mathbf{u}_d}^r}{\partial t}, \varphi_i\right) + Re^{-1}\left(\nabla \overline{\mathbf{u}_d}^r, \nabla \varphi_i\right) + \left(\left(\overline{\mathbf{u}_d}^r \cdot \nabla\right) \overline{\mathbf{u}_d}^r, \varphi_i\right) + \left(\tau_r^{SFS}, \varphi_i\right) = \mathbf{0}$$

- "Correction" = ROM subfilter-scale stress tensor

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- Burgers

$$
\begin{aligned}
(\tau_r^{SFS})_i &:= -\left(\overline{u_d \frac{\partial u_d}{\partial x}}^r - u_r \frac{\partial u_r}{\partial x}, \varphi_i \right) \\
&= -\Bigg(\overline{\Bigg[\left(\sum_{k_1=1}^{d} a_{k_1}^{snap}(t_j)\varphi_{k_1} \right) \left(\sum_{k_2=1}^{d} a_{k_2}^{snap}(t_j) \frac{\partial \varphi_{k_2}}{\partial x} \right)}^r \\
&\quad + \left(\sum_{k_3=1}^{r} a_{k_3}^{snap}(t_j)\varphi_{k_3} \right) \left(\sum_{k_4=1}^{r} a_{k_4}^{snap}(t_j) \frac{\partial \varphi_{k_4}}{\partial x} \right) \Bigg], \varphi_i \Bigg)
\end{aligned}
$$

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- closure problem ☹
- consistency ☺
  - "Correction"

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DDF-ROM Step II: Data-Driven Modeling

- ansatz $\tau(DNS) \approx \tilde{A}\,\boldsymbol{a} + \boldsymbol{a}^\top\,\widetilde{B}\,\boldsymbol{a}$
- inverse problem $\min_{\tilde{A},\widetilde{B}} \|\tau(DNS) - (\tilde{A}\,\boldsymbol{a} + \boldsymbol{a}^\top\,\widetilde{B}\,\boldsymbol{a})\|^2$
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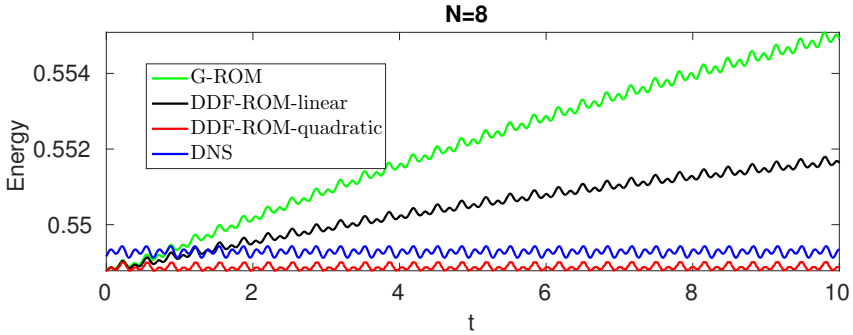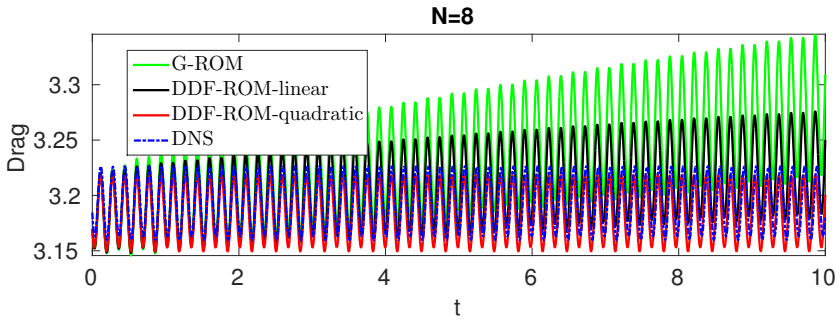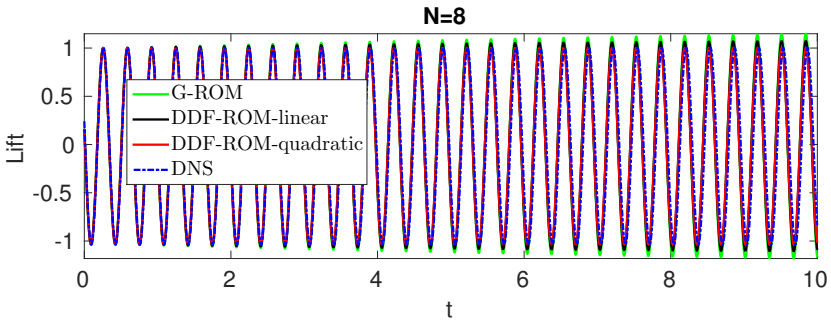
DDF-ROM: 2D Navier-Stokes