Large Eddy Simulation Reduced Order Models (LES-ROMs) for Turbulent Flows

T. Iliescu

Department of Mathematics
Virginia Tech

Computational Learning for Model Reduction Workshop

ICERM, January 6-10, 2025

National Science Foundation DMS-2012253 2020-2025

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Collaborators

- students, postdocs
  - Ian Moore (student, Virginia Tech)
  - David Wells (research scientist, UNC Chapel Hill)
  - Zhu Wang (professor, University of South Carolina)
  - Xuping Xie (professor, Old Dominion University)
  - Changhong Mou (postdoc, Purdue)
  - Birgul Koc (postdoc, University of Seville)
  - Muhammad Mohebujjaman (professor, University of Alabama)
  - Omer San (professor, University of Tennessee)
  - Jorge Reyes (postdoc, Virginia Tech)
  - Ping-Hsuan Tsai (postdoc, Virginia Tech)
- collaborators
  - Maria Strazzullo, Claudio Canuto (Politecnico di Torino)
  - Francesco Ballarin, Anna Sanfilippo (Brescia), Alessandro Veneziani (Emory)
  - Honghu Liu (Virginia Tech), Michael Schneier (Bettis, Pitt), Max Gunzburger (Florida State)
  - Gianluigi Rozza, Michele Girfoglio, Anna Ivagnes (SISSA, Trieste)
  - Giovanni Stabile (Pisa), Tomas Chacon Rebollo, Samuele Rubino (Seville)
  - Paul Fischer (Illinois), Annalisa Quaini (Houston), Nan Chen (Wisconsin)

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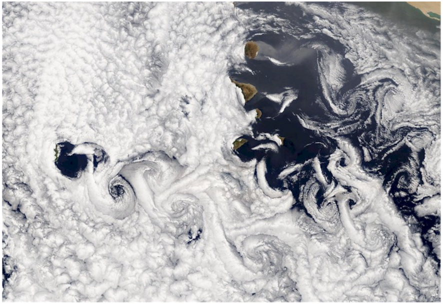
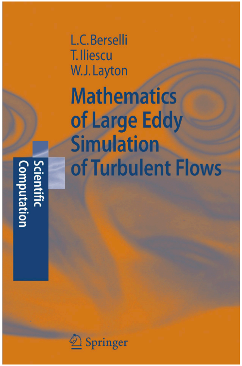
Commercial ROM Software for Real Turbulence



LES-ROMs

- bridge two distinct research fields (2010-2030)
  - large eddy simulation (LES)
  - reduced order model (ROM)
- sales pitch **LES-ROMs**
  - principles WHY? HOW?
  - *not* models
- case studies
  - Data-Driven LES-ROMs ☹
  - **Regularized ROMs (Reg-ROMs)** ☺

LES-ROMs



Physics of Fluids REVIEW scitation.org/journal/phf

On closures for reduced order models—A spectrum of first-principle to machine-learned avenues

Cite as: Phys. Fluids **33**, 091301 (2021); doi: 10.1063/5.0061577
Submitted: 28 June 2021 · Accepted: 1 September 2021 ·
Published Online: 22 September 2021

View Online Export Citation CrossMark

Shady E. Ahmed,[1] Suraj Pawar,[1] Omer San,[1,a)] Adil Rasheed,[2] Traian Iliescu,[3] and Bernd R. Noack[4,5]

AFFILIATIONS

[1]School of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, Oklahoma 74078, USA
[2]Department of Engineering Cybernetics, Norwegian University of Science and Technology, N-7465 Trondheim, Norway
[3]Department of Mathematics, Virginia Tech, Blacksburg, Virginia 24061, USA
[4]School of Mechanical Engineering and Automation, Harbin Institute of Technology, Shenzhen 518058, China
[5]Hermann-Föttinger-Institut für Strömungsmechanik, Technische Universität Berlin, D-10623 Berlin, Germany

[a)]Author to whom correspondence should be addressed: osan@okstate.edu

ABSTRACT

For over a century, reduced order models (ROMs) have been a fundamental discipline of theoretical fluid mechanics. Early examples include Galerkin models inspired by the Orr–Sommerfeld stability equation and numerous vortex models, of which the von Kármán vortex street is one of the most prominent. Subsequent ROMs typically relied on first principles, like mathematical Galerkin models, weakly nonlinear stability theory, and two- and three-dimensional vortex models. Aubry *et al.* [J. Fluid Mech. **192**, 115–173 (1988)] pioneered the data-driven proper orthogonal decomposition (POD) modeling. In early POD modeling, available data were used to build an optimal basis, which was then utilized in a classical Galerkin procedure to construct the ROM, but data have made a profound impact on ROMs beyond the Galerkin expansion. In this paper, we take a modest step and illustrate the impact of data-driven modeling on one significant ROM area. Specifically, we focus on ROM closures, which are correction terms that are added to the classical ROMs in order to model the effect of the discarded ROM modes in under-resolved simulations. Through simple examples, we illustrate the main modeling principles used to construct the classical ROMs, motivate and introduce modern ROM closures, and show how data-driven modeling, artificial intelligence, and machine learning have changed the standard ROM methodology over the last two decades. Finally, we outline our vision on how the state-of-the-art data-driven modeling can continue to reshape the field of reduced order modeling.

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LES-ROMs

fluids

MDPI

Review

Bridging Large Eddy Simulation and Reduced-Order Modeling of Convection-Dominated Flows through Spatial Filtering: Review and Perspectives

Annalisa Quaini [1,†], Omer San [2,†], Alessandro Veneziani [3,†] and Traian Iliescu [4,*,†]

[1] Department of Mathematics, University of Houston, 3551 Cullen Blvd, Houston, TX 77204, USA; quaini@math.uh.edu
[2] Department of Mechanical, Aerospace and Biomedical Engineering, University of Tennessee, 1512 Middle Drive, Knoxville, TN 37996, USA; osan@utk.edu
[3] Department of Mathematics, Emory University, 400 Dowman Drive, Atlanta, GA 30322, USA; avenez2@emory.edu
[4] Department of Mathematics, Virginia Tech, 225 Stanger Street, Blacksburg, VA 24061, USA
* Correspondence: iliescu@vt.edu
† These authors contributed equally to this work.

Abstract: Reduced-order models (ROMs) have achieved a lot of success in reducing the computational cost of traditional numerical methods across many disciplines. In fluid dynamics, ROMs have been successful in providing efficient and relatively accurate solutions for the numerical simulation of laminar flows. For convection-dominated (e.g., turbulent) flows, however, standard ROMs generally yield inaccurate results, usually affected by spurious oscillations. Thus, ROMs are usually equipped with numerical stabilization or closure models in order to account for the effect of the discarded modes. The literature on ROM closures and stabilizations is large and growing fast. In this paper, instead of reviewing all the ROM closures and stabilizations, we took a more modest step and focused on one particular type of ROM closure and stabilization that is inspired by large eddy simulation (LES), a classical strategy in computational fluid dynamics (CFD). These ROMs, which we call LES-ROMs, are extremely easy to implement, very efficient, and accurate. Indeed, LES-ROMs are modular and generally require minimal modifications to standard ("legacy") ROM formulations. Furthermore, the computational overhead of these modifications is minimal. Finally, carefully tuned LES-ROMs can accurately capture the average physical quantities of interest in challenging convection-dominated flows in science and engineering applications. LES-ROMs are constructed by leveraging spatial filtering, which is the same principle used to build classical LES models. This ensures a modeling consistency between LES-ROMs and the approaches that generated the data used to train them. It also "bridges" two distinct research fields (LES and ROMs) that have been disconnected until now. This paper is a review of LES-ROMs, with a particular focus on the LES concepts and models that enable the construction of LES-inspired ROMs and the bridging of LES and reduced-order modeling. This paper starts with a description of a versatile LES strategy called evolve–filter–relax (EFR) that has been successfully used as a full-order method for both incompressible and compressible convection-dominated flows. We present evidence of this success. We then show how the EFR strategy, and spatial filtering in general, can be leveraged to construct LES-ROMs (e.g., EFR-ROM). Several applications of LES-ROMs to the numerical simulation of incompressible and compressible convection-dominated flows are presented. Finally, we draw conclusions and outline several research directions and open questions in LES-ROM development. While we do not claim this review to be comprehensive, we certainly hope it serves as a brief and friendly introduction to this exciting research area, which we believe has a lot of potential in the practical numerical simulation of convection-dominated flows in science, engineering, and medicine.

Keywords: large eddy simulation; reduced-order modeling; spatial filtering; machine learning; incompressible fluids; compressible fluids; cardiovascular modeling; atmospheric modeling

check for updates

Citation: Quaini, A.; San, O.; Veneziani, A.; Iliescu, T. Bridging Large Eddy Simulation and Reduced-Order Modeling of Convection-Dominated Flows through Spatial Filtering: Review and Perspectives. *Fluids* **2024**, *9*, 178. https://doi.org/10.3390/fluids9080178

Academic Editors: D. Andrew S. Rees and Giuliano De Stefano

Received: 29 June 2024
Revised: 29 July 2024
Accepted: 31 July 2024
Published: 4 August 2024

Fluids **2024**, *9*, 178. https://doi.org/10.3390/fluids9080178 https://www.mdpi.com/journal/fluids

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ROM+ML4LES+

- "Reduced Order Modeling and Machine Learning for Large Eddy Simulation and Related Topics (ROM+ML4LES+)"
- organizers Veneziani, Quaini, San, Iliescu
- **October, 2025, Virginia Tech**

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Vision

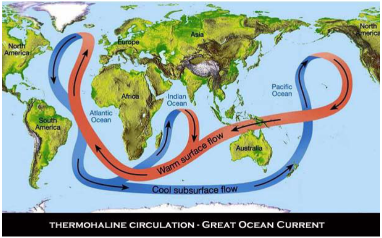
How will commercial software for ROMs for fluids look in 2030?

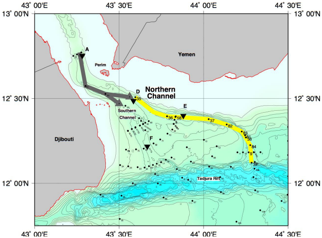
LES-ROMs

Turbulence

- chaotic
  - unpredictable
- multiscale
  - spectrum of scales
  - nonlinear interaction
- convection-dominated
  - incompressible flows *both* diffusion and convection
  - $\neq$ transport
- under-resolved regime
  - not enough DOFs

Thermohaline Circulation   Red Sea Overflow

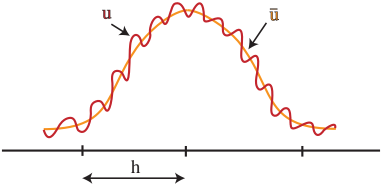




Direct Numerical Simulation (DNS)

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

Large Eddy Simulation (LES)



1. spatial filter g_δ
   - (i) physical space (Gaussian, differential)
   - (ii) Fourier space (sharp cutoff)
2. filtered variables $\boxed{\overline{\mathbf{u}} := g_\delta * \mathbf{u}}$ large scales
3. filtered equations $g_\delta *$ NSE
4. solve for filtered variables

Large Eddy Simulation (LES)

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

- closure problem $\boxed{\overline{\mathbf{u}\mathbf{u}} \neq \overline{\mathbf{u}}\, \overline{\mathbf{u}}}$
- closure model
  1. functional (physical)
  2. structural (mathematical)

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LES Testing

- LES testing $\boxed{\Longrightarrow}$ **under-resolved** turbulent channel flow
  - turbulent channel flow ✓ $\boxed{\Longrightarrow}$ LES model used ☺
  - turbulent channel flow ✗ $\boxed{\Longrightarrow}$ LES model **NOT** used ☹
- DNS benchmark database
  - Moser, Kim, Mansour, *Phys. Fluids*, 1999
  - Lee, Moser, *J. Fluid Mech.*, 2015

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LES Turbulent Channel Flow

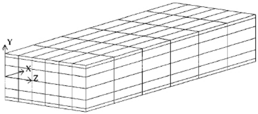


FIG. 3. Spectral element meshes: $Re_\tau=180$ (top), and $Re_\tau=395$ (bottom).

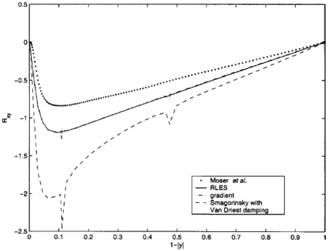
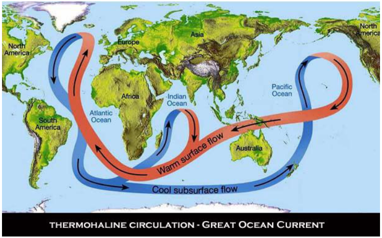
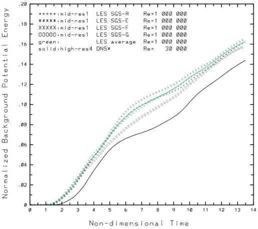


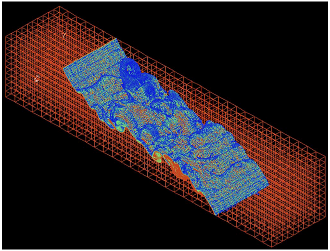
FIG. 12. The x, y component of the Reynolds stress, $Re_\tau=395$. We compared the RLES model (12), the gradient model (9), and the Smagorinsky model with Van Driest damping with the fine DNS of Moser, Kim, and Mansour (Ref. 42).

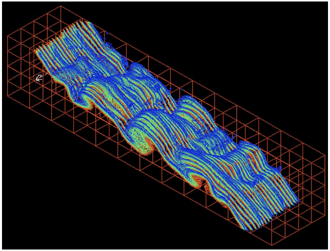
Iliescu, Fischer, *Phys. Fluids*, 2003

LES Thermohaline Circulation



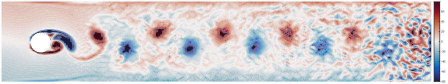


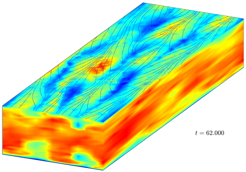


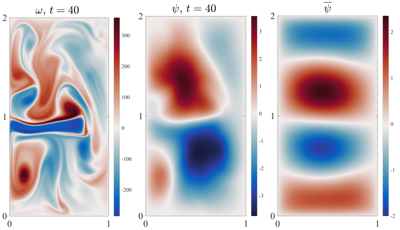


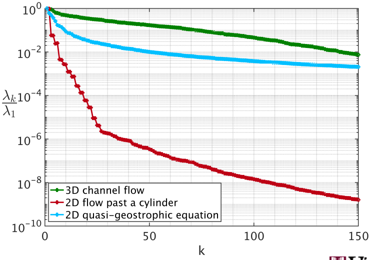
Özgökmen, Iliescu, Fischer, *Ocean Model.*, 2009

ROM (**Lack of**) Testing

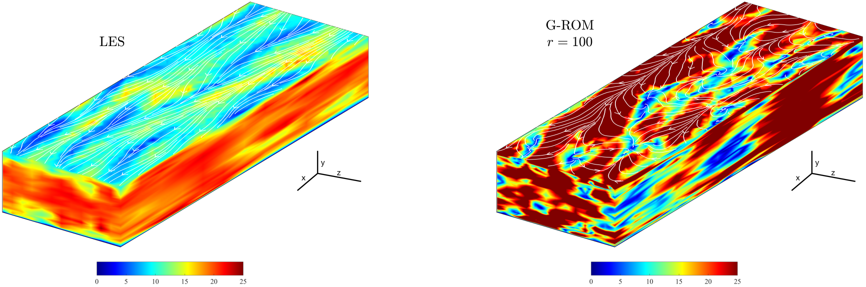






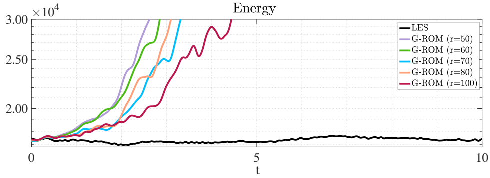


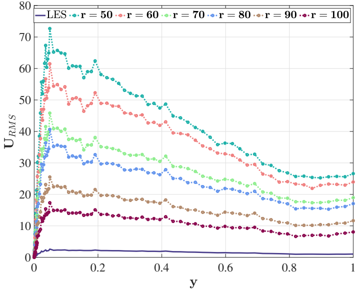
G-ROM



Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.,* 2023

G-ROM





Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.*, 2023

Data-Driven LES-ROMs

Algorithm 1 d2-VMS-ROM for NSE

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

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 a least squares problem:

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

4: In online stage, for different parameters and/or longer time, repeatedly use d2-VMS-ROM

$$\boxed{\overset{\bullet}{\boldsymbol{a}} = (A + \tilde{A})\boldsymbol{a} + \boldsymbol{a}^\top (B + \tilde{B})\boldsymbol{a} .} \qquad (2)$$

Xie, Mohebujjaman, Rebholz, Iliescu, *SIAM J. Sci. Comput.*, **2018**

Mou, Koc, San, Rebholz, Iliescu, *Comput. Meth. Appl. Mech. Eng.*, 2021

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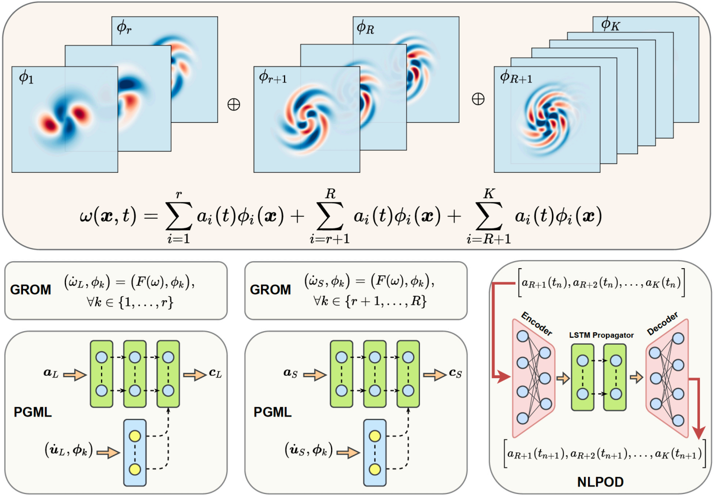
Physics Guided Machine Learning (PGML)



Ahmed, San, Rasheed, Iliescu, Veneziani *SIAM J. Sci. Comp.*, 2023

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Data-Driven LES-ROMs

- evolution

  Xie, Mohebujjaman, Rebholz, Iliescu, *SIAM J. Sci. Comput.*, 2018

  Mou, Koc, San, Rebholz, Iliescu, *Comput. Methods Appl. Mech. Engrg.*, 2021

- physical constraints

  Mohebujjaman, Rebholz, Iliescu, *Int. J. Num. Meth. Fluids*, 2019

- pressure

  Ivagnes, Stabile, Mola, Iliescu, Rozza *J. Comput. Phys.*, 2023

  Ivagnes, Stabile, Mola, Iliescu, Rozza, *Apl. Math. Comput.*, 2023

- machine learning

  Xie, Webster, Iliescu, *Fluids*, 2020

  Ahmed, San, Rasheed, Iliescu, Veneziani, *SIAM J. Sci. Comput.*, 2023

- stochastic modeling, data assimilation

  Mou, Chen, Iliescu *J. Comp. Phys.*, 2023

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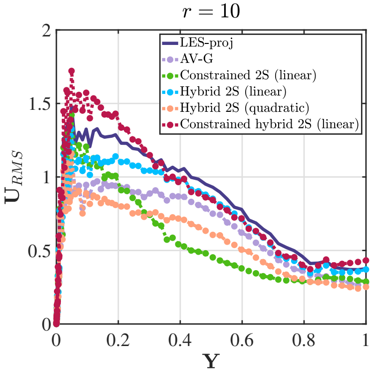
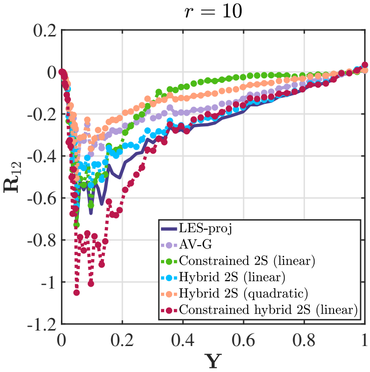
Data-Driven LES-ROMs





- data ☹
- hybrid = data + physics ☺

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Data-Driven Variational Multiscale ROM Verifiability

Theorem (Koc, Mou, Liu, Wang, Rozza, Iliescu, *J. Sci. Comput.*, 2022)

Accurate ROM closure $\Longrightarrow$ accurate ROM approximation:

$$\|\boldsymbol{e}^n\|^2 + \Delta t \sum_{j=0}^{n} Re^{-1} \left\|\nabla \boldsymbol{e}^j\right\|^2 \leq \exp\left(\Delta t \sum_{j=0}^{n} \frac{d_j}{1 - \Delta t\, d_j}\right)$$
$$\left(\Delta t \sum_{j=0}^{n} Re^{-1} \left\| P_r \left(\boldsymbol{\tau}^{FOM}(\boldsymbol{u}_R^j) - \boldsymbol{\tau}^{ROM}\left(P_r(\mathbf{u}_R^j)\right)\right)\right\|^2\right).$$

Proof.

1. Galerkin + filtering $\Longrightarrow$ mathematical framework
2. data-driven closure $\Longrightarrow$ accurate closure
3. Galerkin + data $\Longrightarrow$ accurate ROM

□

LES-ROM Criteria

- accuracy ✓
- efficiency ✓
- mathematics ✓
- commercial ROM software ✗
- **WHY?**

LES-ROM Criteria

NOT easy to implement ☹

ROM Filters   Projection

- given $\mathbf{u}_R \in \mathbf{X}^R = \text{span}\left\{\varphi_1, \ldots, \varphi_r, \varphi_{r+1}, \ldots\ldots\ldots\ldots, \varphi_R\right\}$
- find $\overline{\mathbf{u}}_R \in \mathbf{X}^r = \{\varphi_1, \ldots, \varphi_r\}$
- $\boxed{\left(\overline{\mathbf{u}}_R, \varphi_j\right) = \left(\mathbf{u}_R, \varphi_j\right)} \qquad \forall j = 1, \ldots r$

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

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

Kaneko, Tsai, Fischer, *Nucl. Eng. Des.*, 2020

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ROM Filters   Differential

- given $\mathbf{u}_r \in \mathbf{X}^r$
- find $\overline{\mathbf{u}}_r \in \mathbf{X}^r$
- $$\boxed{\left(\left(\mathbb{I} - \delta^2 \Delta \right) \overline{\mathbf{u}}^r, \varphi_j \right) = \left(\mathbf{u}^r, \varphi_j \right)} \qquad \forall j = 1, \ldots r$$
- $$\boxed{\left(\mathbb{I} + \delta^2 S_r \right) \overline{\boldsymbol{a}}_r = \boldsymbol{a}_r}$$
- low-dimensional linear system

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

ROM Lengthscale

- input
  1. FOM
     - mesh size h
     - solution $\mathbf{u}^{FOM}$
     - computational domain lengthscale L
  2. ROM
     - dimension r
     - total number of ROM basis functions R
     - eigenvalues λ_i
     - basis functions $\boldsymbol{\varphi}_i$
- output
  - $\boxed{\delta = ?}$

Dimensional Lengthscale δ_1

- definition

$$\delta_1 := \left(\frac{\int_0^{L_1} \int_0^{L_2} \int_0^{L_3} \sum_{i=1}^3 u_i^{\prime\, FOM} u_i^{\prime\, FOM} \, dx_1 \, dx_2 \, dx_3}{\int_0^{L_1} \int_0^{L_2} \int_0^{L_3} \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial u_i^{\prime\, FOM}}{\partial x_j} \frac{\partial u_i^{\prime\, FOM}}{\partial x_j} \, dx_1 \, dx_2 \, dx_3} \right)^{1/2}$$

- check

$$[\delta_1] = \left(\frac{\frac{m}{s} \frac{m}{s} m^3}{\frac{1}{s} \frac{1}{s} m^3} \right)^{1/2} = m \qquad \checkmark$$

- Aubry, Holmes, Lumley, Stone, *J. Fluid Mech.*, 1988

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Energy Lengthscale δ_2

- principle

$$\Lambda \overset{\text{notation}}{=} \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{R} \lambda_i} = \frac{KE(\delta_2)}{KE(h)}$$

- tools
  - $KE(k) = \int_{k_0}^{k} E(k')\, dk'$
  - $E(k) \sim C\, \varepsilon^{2/3}\, k^{-5/3}$

- Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.*, 2023

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Energy Lengthscale δ_2

- formula

$$\delta_2 = \left[\Lambda \, h^{2/3} + (1 - \Lambda) \, L^{2/3} \right]^{3/2}$$

- dimensions ✓

- asymptotics ✓
  - $r \longrightarrow R \quad \Longrightarrow \quad \delta_2 \longrightarrow h$
  - $r \longrightarrow 1 \quad \Longrightarrow \quad \delta_2 \longrightarrow L$

- Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.*, 2023

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Numerical Results   Magnitude and Asymptotics

r	4	8	16	32	40	50
δ_1	4.64e-02	4.65e-02	4.68e-02	4.68e-02	4.66e-02	4.62e-02
δ_2	1.63e00	1.41e+00	1.08e+00	6.84e-01	5.56e-01	4.32e-01

Table: ROM lengthscales for different r values.

Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.*, 2023

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Evolve-Filter-Relax ROM (EFR-ROM)

- Evolve-Filter-Relax ROM (EFR-ROM)

(I) Evolve:
$$\left(\frac{\mathbf{w}_r^{n+1} - \mathbf{u}_r^n}{\Delta t}, \varphi_k \right) + Re^{-1} \left(\nabla \mathbf{u}_r^n, \nabla \varphi_k \right) + \left((\mathbf{u}_r^n \cdot \nabla) \mathbf{u}_r^n, \varphi_k \right) = 0$$

(II) Filter:
$$\mathbf{w}_r^{n+1} \longmapsto \overline{\mathbf{w}_r^{n+1}}$$

(III) Relax:
$$\mathbf{u}_r^{n+1} = (1 - \chi)\, \mathbf{w}_r^{n+1} + \chi\, \overline{\mathbf{w}_r^{n+1}}$$

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

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

Girfoglio, Quaini, Rozza, *J. Comp. Phys.*, 2021

Strazzullo, Girfoglio, Ballarin, Iliescu, Rozza, *Int. J. Num. Meth. Eng.*, 2022

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LES-ROM Criteria

Embarrassingly Easy to implement ☺

Almost Nonintrusive ☺

Leray ROM (L-ROM)

- Leray ROM (L-ROM)

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

$$\dot{\boldsymbol{a}} = A\,\boldsymbol{a} + \boldsymbol{a}^\top \, \overline{B}\,\boldsymbol{a}$$

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

Kaneko, Tsai, Fischer, *Nucl. Eng. Des.*, 2020

Time-Relaxation ROM (TR-ROM)

- Time-Relaxation ROM (TR-ROM)

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

Tsai, Fischer, Iliescu, *J. Comput. Phys.*, 2024

Reg-ROMs Developments

- model consistency

  Strazzullo, Girfoglio, Ballarin, Iliescu, Rozza, *Int. J. Num. Meth. Eng.*, 2022

- control

  Strazzullo, Ballarin, Iliescu, Canuto, *arXiv*, 2023

- approximate deconvolution

  Sanfilippo, Moore, Ballarin, Iliescu, *Finite Elem. Anal. Des.*, 2023

- parameter optimization

  Ivagnes, Strazzullo, Girfoglio, Iliescu, Rozza, *arXiv*, 2024

- variational multiscale

  Strazzullo, Ballarin, Iliescu, Chacon Rebollo, *arXiv*, 2024

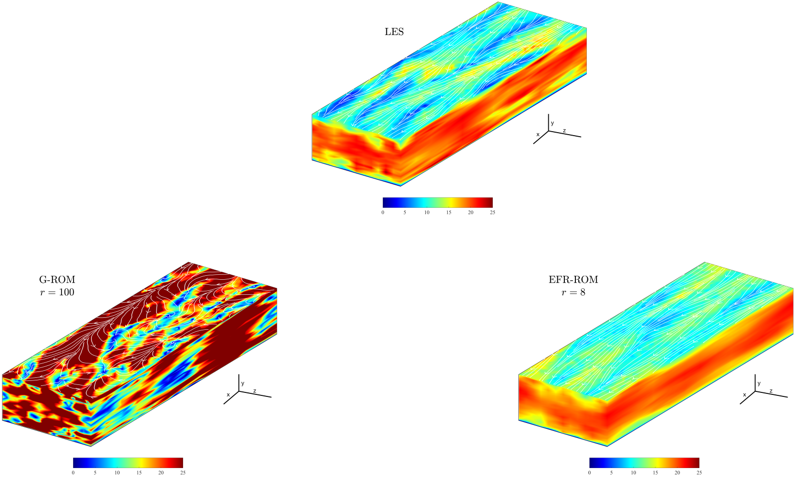
- numerical analysis

  Moore, Sanfilippo, Ballarin, Iliescu, *arXiv*, 2024

  Reyes, Tsai, Novo, Iliescu, *arXiv*, 2024

  Ballarin, Iliescu, *arXiv*, 2024

Turbulent Channel Flow $Re_\tau = 395$



Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.,* 2023

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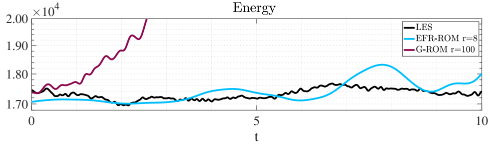
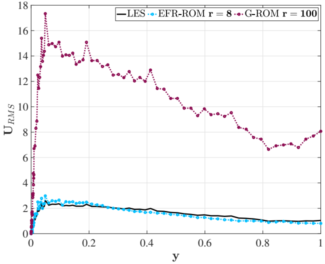
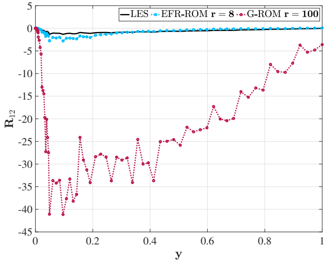
Turbulent Channel Flow $Re_\tau = 395$

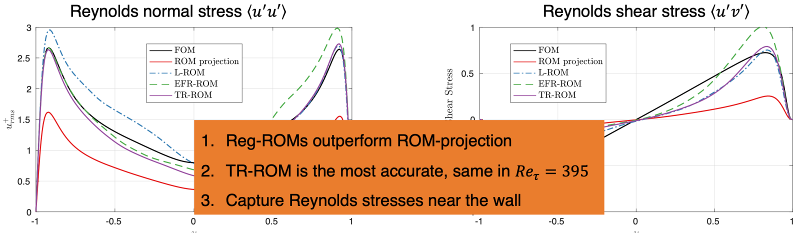




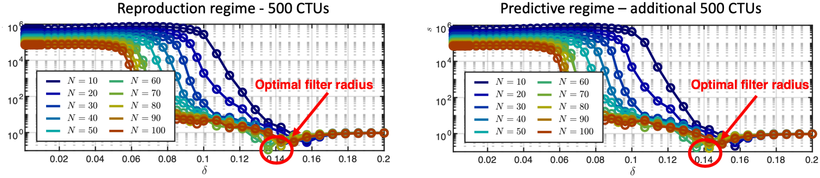


Mou, Merzari, San, Iliescu, *Nucl. Eng. Des.*, 2023

Turbulent Channel Flow $Re_\tau = 395$



1. Reg-ROMs outperform ROM-projection
2. TR-ROM is the most accurate, same in $Re_\tau = 395$
3. Capture Reynolds stresses near the wall



Reg-ROMs can be used for long-time prediction!

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Tsai, Fischer, Iliescu, *J. Comput. Phys.*, 2024

Conclusions

- LES-ROMs
  - ROM filters
  - ROM lengthscale
- Reg-ROMs
- turbulent channel flow

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Vision

How will commercial software for ROMs for fluids look in 2040?

LES-ROMs