Reduced Order Models on a Variational Multi-Scale Model of Navier–Stokes: focus on wall law functions for boundary layer treatment preliminary study

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CFC - Cannes - 26th April 2023

Motivation

Fluid Simulations

- Which **scale** can we approximate?
- Computational **costs** vs **accuracy**
- Large Eddy Simulations (LES)
- Variational Multi-Scale (**VMS**)
- Weak Boundary conditions and **Wall-Law** for boundary layers to improve accuracy
- Turbulence

Model order reduction

- **Parametric** context or time prediction
- Further reduce costs
- **Reduce** the computational cost for a new parameter/time
- Good approximation
- Challenges:
  - Representability (turbulence, moving discontinuities)
  - Stability

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- Wall Law model
- **POD-Galerkin**
- Flow past cylinder

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- No special techniques for advection dominated structures

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In the future

- VMS-Smagorinsky model
- Hyper-reduction
- NN for wall laws

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Navier–Stokes VMS[1]

Navier–Stokes equations (strong)

$$
\begin{cases}
\frac{\partial \underline{u}}{\partial t} + (\underline{u} \cdot \nabla)\underline{u} + \nabla p - 2\,\mathrm{div}(\nu \nabla^s \underline{u}) = 0 \\
\nabla \cdot \underline{u} = 0 \\
\text{B.C. and I.C.}
\end{cases}
$$

[1] Y. Bazilevs, T.J.R. Hughes / Computers & Fluids 36 (2007) 12–26

Navier–Stokes VMS[1]

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Weak formulation

$$\begin{cases} \left(\underline{v}, \frac{\partial \underline{u}}{\partial t}\right)_\Omega - (\nabla \underline{v}, \underline{u} \otimes \underline{u})_\Omega + (q, \nabla \cdot \underline{u})_\Omega - \\ (\nabla \cdot \underline{v}, p)_\Omega + (\nabla^s \underline{v}, 2\nu \nabla^s \underline{u})_\Omega = 0 \\ \text{Dirichlet B.C. for } \underline{u} \text{ and } p \text{ and I.C.} \end{cases}$$

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Variational Multi-Scale Resiudal based (FEM)

- $\underline{u} = \underline{u}_h + \underline{u}'$ (all variables)
- Residual based

$$\underline{u}'_h = -\tau_M \underline{r}_M(\underline{u}_h, p_h)$$

$$p'_h = -\tau_C r_C(\underline{u}_h)$$

$$\underline{r}_M(\underline{u}_h, p_h) = \frac{\partial \underline{u}_h}{\partial t} + \mathrm{div}(\underline{u}_h \otimes \underline{u}_h) + \nabla p_h - \mathrm{div}(2\nu\nabla^s \underline{u}_h)$$

$$\tau_M = \left(\frac{4}{\Delta t^2} + \underline{u}_h \cdot G\underline{u}_h + C_{inv}\nu^2 G : G\right)^{-\frac{1}{2}}$$

$$r_C(\underline{u}_h) = \mathrm{div}(\underline{u}_h), \qquad \tau_C = (\tau_M \underline{g}\cdot\underline{g})^{-1}$$

$$G = \left(\frac{d\xi}{dx}\right)^T \frac{d\xi}{dx}, \qquad \underline{g}_i = \sum_j \left(\frac{d\xi}{dx}\right)_{ji}$$

[1] Y. Bazilevs, T.J.R. Hughes / Computers & Fluids 36 (2007) 12–26

Navier–Stokes VMS[1]

Weak VMS formulation

$$
\begin{aligned}
&a^{VMS}(\underline{u}_h, p_h, \underline{v}_h, q_h) := \\
&\sum_e (\underline{v}_h, \partial_t \underline{u}_h)_{\Omega_e} - (\nabla \underline{v}_h, \underline{u}_h \otimes \underline{u}_h)_\Omega + (q_h, \nabla \cdot \underline{u}_h)_\Omega \\
&-\sum_e (\nabla \cdot \underline{v}_h, p_h)_{\Omega_e} + (\nabla^s \underline{v}_h, 2\nu \nabla^s \underline{u}_h)_\Omega \\
&+2\sum_e \left(\underline{u}_h \cdot \nabla^s \underline{v}_h, \underline{u}_h'\right)_{\Omega_e} - \sum_e \left(\nabla \underline{v}_h, \underline{u}_h' \otimes \underline{u}_h'\right)_{\Omega_e} \\
&+\sum_e \left(\nabla \cdot \underline{v}_h, p_h'\right)_{\Omega_e} = 0
\end{aligned}
$$

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- $\underline{u} = \underline{u}_h + \underline{u}'$ (all variables)
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\begin{aligned}
\underline{u}_h' &= -\tau_M \underline{r}_M(\underline{u}_h, p_h) \\
p_h' &= -\tau_C r_C(\underline{u}_h) \\
\underline{r}_M(\underline{u}_h, p_h) &= \frac{\partial \underline{u}_h}{\partial t} + \mathrm{div}(\underline{u}_h \otimes \underline{u}_h) + \nabla p_h \\
&\quad - \mathrm{div}(2\nu \nabla^s \underline{u}_h)
\end{aligned}
$$

$$
\tau_M = \left(\frac{4}{\Delta t^2} + \underline{u}_h \cdot G \underline{u}_h + C_{inv} \nu^2 G : G \right)^{-\frac{1}{2}}
$$

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r_C(\underline{u}_h) = \mathrm{div}(\underline{u}_h), \qquad \tau_C = (\tau_M \underline{g} \cdot \underline{g})^{-1}
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&a^{VMS}(\underline{u}_h, p_h, \underline{v}_h, q_h) := \\
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&- \sum_e (\nabla \cdot \underline{v}_h, p_h)_{\Omega_e} + (\nabla^s \underline{v}_h, 2\nu \nabla^s \underline{u}_h)_\Omega \\
&+2 \sum_e \left(\underline{u}_h \cdot \nabla^s \underline{v}_h, \underline{u}_h'\right)_{\Omega_e} - \sum_e \left(\nabla \underline{v}_h, \underline{u}_h' \otimes \underline{u}_h'\right)_{\Omega_e} \\
&+ \sum_e \left(\nabla \cdot \underline{v}_h, p_h'\right)_{\Omega_e} = 0
\end{aligned}
$$

Advantages

- Coarse scale $\Longrightarrow$ Discretized
- Fine scale $\Longrightarrow$ Modeled
- Extra accuracy by modeling higher order terms without solving them
- Stabilization effect: we can use $\mathbb{P}^p$ for both velocity and pressure (no need of $\mathbb{P}^1\mathbb{P}^2$ formulations)
- Duality: LES modeling and stabilization

[2] Y. Bazilevs, T.J.R. Hughes / Computers & Fluids 36 (2007) 12–26

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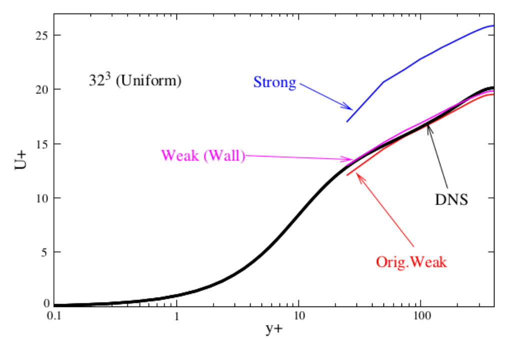
Boundary conditions

No slip Boundary conditions

- Can create boundary layers
- If strongly huge impact on the solution



(a) Mean stream-wise velocity

Weak Enforcement of no slip BC

$$
\begin{aligned}
a^{VMS}_{weakBC}(\underline{u}_h, p_h, \underline{v}_h, q_h) &:= a^{VMS}(\underline{u}_h, p_h, \underline{v}_h, q_h) \\
&-\sum_b (\underline{v}_h, 2\nu\nabla^s \underline{u}_h \cdot \underline{n})_{\partial\Omega\cap\Gamma_b} \\
&-\sum_b (2\nu\nabla^s \underline{v}_h \cdot \underline{n}, \underline{u}_h - \underline{0})_{\partial\Omega\cap\Gamma_b} \\
&+\sum_b \left(\underline{v}_h \frac{C_b^I \nu}{h_b}, \underline{u}_h - \underline{0}\right)_{\partial\Omega\cap\Gamma_b} = 0
\end{aligned}
$$

- Consistency term
- Adjoint consistency term
- Penalization of Dirichlet BC

Spalding Wall Law[3,4]

Weak penalty for no slip condition

$$\sum_b \left(\underline{v}_h \frac{C_b^I \nu}{h_b}, \underline{u}_h - \underline{0} \right)_{\partial\Omega\cap\Gamma_b}$$

- $C_b^I = 4$ user set coefficient
- $h_b = 2\left(\underline{n}^T G \underline{n}\right)^{-1/2}$ wall-normal element mesh size

Spalding Wall law

- More **physical intuition**
- Exploiting notion of fully developed turbulence
- No-slip Dirichlet BC replaced by **traction Neumann boundary**

$$\sum_b \left(\underline{v}_h, {u^*}^2 \frac{\underline{u}_h}{\|\underline{u}_h\|} \right)_{\partial\Omega\cap\Gamma_b}$$

- ${u^*}^2$ magnitude of the **wall shear stress**
- Consistent with the "law of the wall"

[3]D.B. Spalding, A single formula for the law of the wall, J. Appl. Mech. 28 (1961) 444–458
[4]Y. Bazilevs et al. / Comput. Methods Appl. Mech. Engrg. 196 (2007) 4853–4862

Spalding Wall Law

Spalding Law

$$\sum_b \left(\underline{v}_h, u^{*2} \frac{\underline{u}_h}{\|\underline{u}_h\|} \right)_{\partial\Omega \cap \Gamma_b}$$

- Empirical relation between the mean fluid speed and the normal distance to the wall
- Spalding Law

$$y^+ \overset{!}{=} f(u^+) = u^+ + e^{-\chi B} \left(e^{\chi u^+} - 1 - \chi u^+ - \frac{(\chi u^+)^2}{2} - \frac{(\chi u^+)^3}{6} \right),$$

$$y^+ := \frac{y u^*}{\nu} \text{ distance from the wall in nondimensional wall units,}$$

$$u^+ := \frac{\|\underline{u}_h\|}{u^*} \text{ mean fluid speed in nondimensional wall units,}$$

$$\chi = 0.4, \ B = 5.5.$$

Spalding Wall Law

Spalding Law

$$\sum_b \left(\underline{v}_h, u^{*2} \frac{\underline{u}_h}{\|\underline{u}_h\|} \right)_{\partial\Omega\cap\Gamma_b} = \sum_b \left(\underline{v}_h \frac{u^{*2}}{\|\underline{u}_h\|}, \underline{u}_h - \underline{0} \right)_{\partial\Omega\cap\Gamma_b} = \sum_b \left(\underline{v}_h \tau_B, \underline{u}_h - \underline{0} \right)_{\partial\Omega\cap\Gamma_b}, \quad \tau_B := \frac{u^{*2}}{\|\underline{u}_h\|}$$

- τ_B makes the connection with the weak formulation where $\tau_B = \frac{C_b^I \nu}{h_b}$
- One extra scalar nonlinear equation to be solved $y^+ \overset{!}{=} f(u^+)$ for each boundary cell (not too expensive)
- Rewrite the equation in terms of τ_B
- $r(\tau_B) = 0$ with $r'(\tau) > 0$ and $r''(\tau) < 0$ for $\tau > 0$
- Newton's method converges if τ^0 small enough (worst case bisection not too expensive)
- Initial guess $\tau^0 = \frac{C_b^I \nu}{h_b}$ (from weak formulation)

Full Order Model

FOM

- $\mathbb{P}^2 - \mathbb{P}^2$ **continuous Galerkin FEM** formulation
- Residual based Variational MultiScale discrete model
- Boundary consistency terms
- Weak penalty for no-slip BC
- **Spalding Wall Law** (very fast 1% cost)

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Test: Flow Past Cylinder

$\mathcal{R} = [0, 2.2] \times [-0.41, 0.41], \mathcal{C} = \mathcal{B}([0.2, 0], 0.05),$
$D = \mathcal{R} \backslash \mathcal{C}, \qquad T_{end} = 3, \qquad N_h = 3 \cdot 122145,$
$u_{in} = (\mu_1, 0), \quad \nu = \mu_2,$
$Re \in [2.5 \cdot 10^3, 2.5 \cdot 10^5],$
$\mu_1 \in [0.5, 5.0], \quad \mu_2 \in [2 \cdot 10^{-6}, 2 \cdot 10^{-5}],$
No slip BC on top, bottom and circle,

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Reduced Order Model[5]

Solution Manifold Compression

- Proper Orthogonal Decomposition (**POD**)
- Collection of **snapshots** $\{[u_h, p_h, \tau_{B,h}](t^{i_0}, \mu_1^{i_1}, \mu_2^{i_2})\}_{i\in\mathcal{T}} \in V_h$
- Generation of V_{RB} component by component
- No need of supremizer[5]

[5]Stabile, Giovanni, et al. "A reduced order variational multiscale approach for turbulent flows." Advances in Computational Mathematics 45 (2019): 2349-2368.

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Reconstruction

- **POD-Galerkin**
  - $F(u_h) = 0 \Longrightarrow V_{RB}^T F(V_{RB} u_{RB}) = 0$
  - Less equations
  - **Hyper-reduction** needed to decrease costs (not today)
  - **Physics** based
  - Less nonlinear iterations
  - For the moment no computational advantage
- **POD-NN**

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- Generation of V_{RB} component by component
- No need of supremizer[5]

Spalding coefficient reconstruction

- For $\tau_{B,h}$ POD-Galerkin and then Newton
- Problem: **Newton does not converge** for reduced $\tau_{B,RB}$ equation
- Multi-layer perceptron NN $u_{RB} \to \tau_{B,RB}$?

Reconstruction

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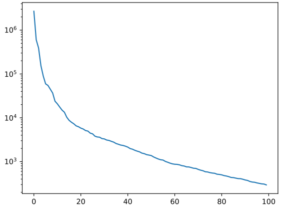
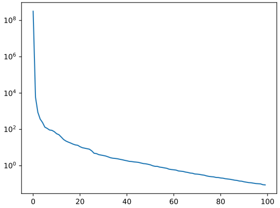
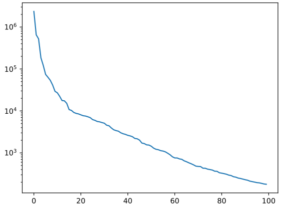
POD results: 20 parameters, 150 timesteps

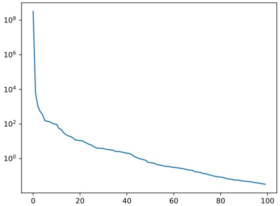
u | p | τ

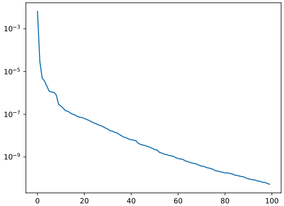




$\Leftarrow$ Weak BC, Spalding BC $\Downarrow$



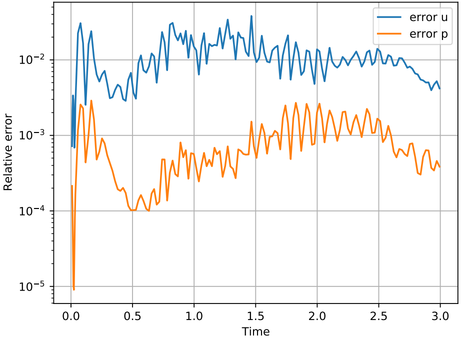




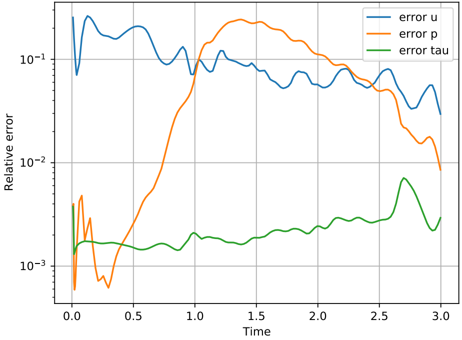
POD projection error: $(u_{in}, \nu) = (1, 2 \cdot 10^{-6})$

$$N^u_{POD} = N^p_{POD} = 100, \; N^\tau_{POD} = 30$$

Weak BC



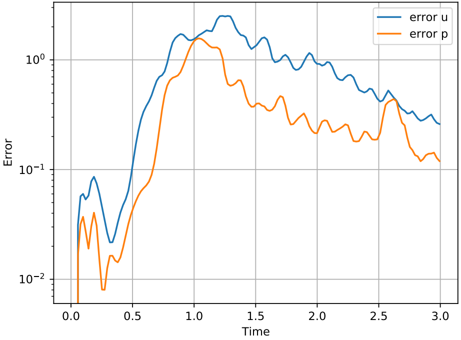
Spalding



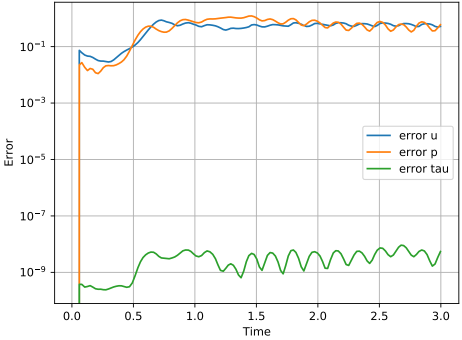
POD-Galerkin error: $(u_{in}, \nu) = (1, 2 \cdot 10^{-6})$

$$N^u_{POD} = N^p_{POD} = 100, \; \tau \text{ exact}$$

Weak BC



Spalding



Weak BC: POD-Galerkin (top) vs FOM (bottom)

Spalding BC: POD-Galerkin (top) vs FOM (bottom)

Comments on POD-Galerkin

Vortex shedding start

- The **vortex shedding** in FOM is dictated purely by the (triangular) mesh
- No reasons why also in ROM it should start at the same time and in the same direction
- Starting the ROM simulation after vortex shedding (at time $t = 1$)

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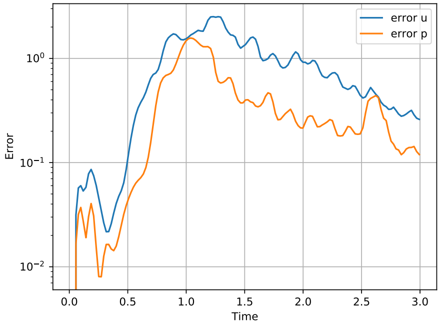
Weak BC ROM from $t = 0$



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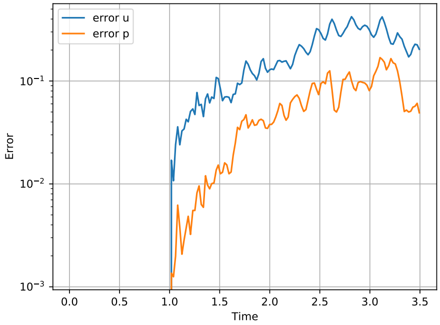

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Weak BC vs Spalding

- Spalding has larger error in representation
- Spalding has little worse behavior in POD-Galerkin
- In past simulations, τ_B computed as FOM (≈ 250 DOFs)

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Summary and perspectives[6]

Summary

- LES-VMS model for Navier-Stokes in FEM
- Weak Boundary Conditions
- Spalding Law
- POD-Galerkin

Perspectives

- Hyper-reduction (EIM or overcollocation)
- Extend to other models with Local Projection Stabilization (LPS) onto sub-filter scale[6]
- 3D turbulent simulations
- Improve the architecture for POD-NN to have a comparison with POD-Galerkin

[6] N. Ahmed, T. C. Rebollo, V. John and S. Rubino. Analysis of a Full Space–Time Discretization of the Navier–Stokes Equations by a Local Projection Stabilization Method. IMA Journal of Numerical Analysis, Vol. 37, pp. 1437–1467, 2017.

Literature

- Y. Bazilevs, T.J.R. Hughes. "Weak imposition of Dirichlet boundary conditions in fluid mechanics." Computers & Fluids 36 (2007) 12–26.
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THANK YOU!

POD-NN

- Training set as POD: 20 params, 150 timesteps (3000 snapshots)
- Goal: learn map $(t, \mu_0, \mu_1) \to u_{RB}$
- NN setting
  - multi-layer perceptron
  - 4 hidden nodes
  - 100 neurons each
  - Various activation functions
- For u and p the loss struggle at decaying
- For τ already better results, but dangerous to be used alone (time consistency)

Prediction of τ

It might be safer to predict $\tau_B(u)$

- Learn $u_{RB} \to \tau_{B,RB}$
- NN as before
- Errors $\approx 6\%$ on a test set
- Not really helpful in reducing the computational costs (solving for τ_B already cheap (1% of all costs)
- Still not physics based