

Reliable and efficient model reduction of parametrized aerodynamics problems - error estimation and adaptivity

Masayuki Yano

University of Toronto
Institute for Aerospace Studies

Joint work with Eugene Du & Michael Sleeman

Algorithms for Dimension and Complexity Reduction
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Students:



Eugene Du



Michael Sleeman

Acknowledgment: Anthony Patera

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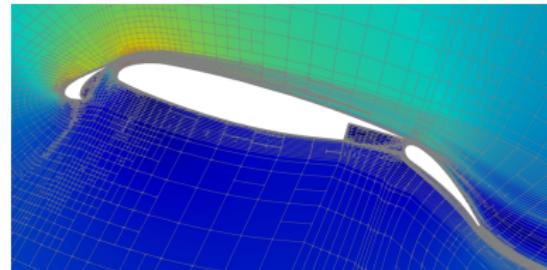
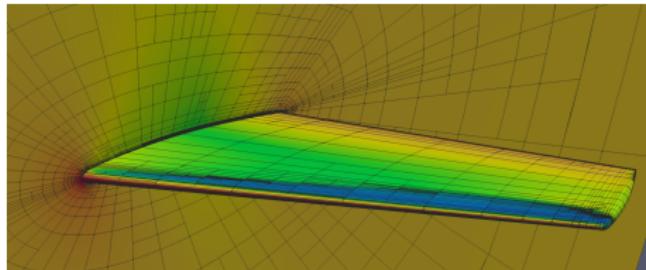
Motivation: parametrized aerodynamics problems

Goal: rapid and reliable output prediction of parametrized nonlinear PDEs in many-query/real-time scenarios.

PDEs: compressible (Reynolds-averaged) Navier-Stokes

Many-query/real-time scenarios:

- parameter & design sweep
- uncertainty quantification
- unsteady flow prediction



Mathematical problem

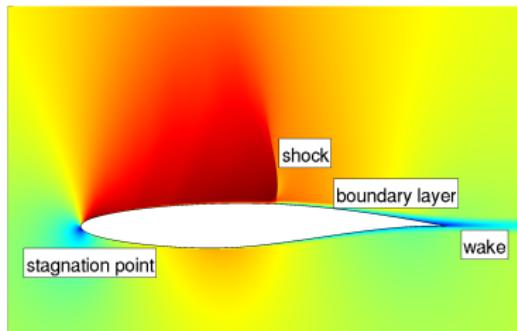
μ PDE: given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, find $u(\mu) \in \mathcal{V}$ s.t.

$$\nabla \cdot (\underbrace{F(u(\mu); \mu)}_{\text{advection flux}} + \underbrace{K(u(\mu); \mu) \nabla u(\mu)}_{\text{diffusion flux}}) = \underbrace{S(u(\mu); \mu)}_{\text{source}}$$

and evaluate output $s(\mu) \equiv \underbrace{q(u(\mu); \mu)}_{\text{output functional}} .$

Challenges: aerodynamic flows are “complex”

- nonlinearity
- convection dominance
- wide range of scales
- limited regularity



Objective

Goal: model reduction for “complex” PDEs:

$$\underbrace{\mu \in \mathcal{D}}_{\text{parameter}} \mapsto \underbrace{\tilde{u}(\mu)}_{\text{state}} \mapsto \underbrace{\tilde{s}(\mu) \pm \Delta^s(\mu)}_{\text{output + err. est.}}.$$

1. **rapid**: *orders of magnitude* online computational reduction
and *efficient* offline training
2. **reliable**: *quantitative* online error estimate in predictive setting
and *adaptive* error control in offline training
3. **automated**: minimal user intervention in training

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Q: can we bring to complex problems the level of rapidness,
reliability, and autonomy that reduced basis method achieves for
“textbook” linear problems?

Goal-oriented model reduction of nonlinear PDEs

- Overview: FE, RB, and hyperreduction (EQP)
- FE: error estimation and adaptation
- RB-EQP: error control
- RB-EQP: error estimation
- Greedy algorithm
- Example: ONERA M6 RANS
- Related work

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Discontinuous Galerkin (DG) method

[Reed & Hill; Cockburn & Shu; ...]

DG space: N_h -dim discontinuous \mathbb{P}^p space \mathcal{V}_h .

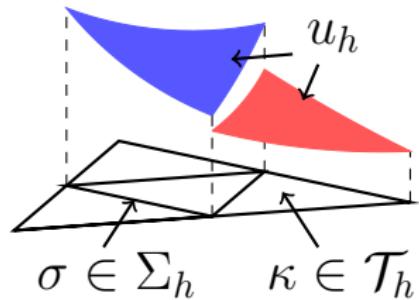
DG-FEM: given $\mu \in \mathcal{D}$, find $u_h(\mu) \in \mathcal{V}_h$ s.t., $\forall v_h \in \mathcal{V}_h$,

$$r_\mu(u_h(\mu), v_h) = \sum_{\kappa \in \mathcal{T}_h} \underbrace{\int_{\kappa} -\nabla v_h \cdot F_\mu(u_h(\mu)) \cdots dx}_{\text{element integral}} + \sum_{\sigma \in \Sigma_h} \underbrace{\int_{\sigma} \cdots ds}_{\text{facet integral}} = 0,$$

and evaluate output $s_h(\mu) \equiv q_\mu(u_h(\mu))$.

Features:

- stability for conservation laws
- unstructured meshes
- hp flexibility



DG reduced basis (RB) method

RB space: $N \ll N_h$ -dim space

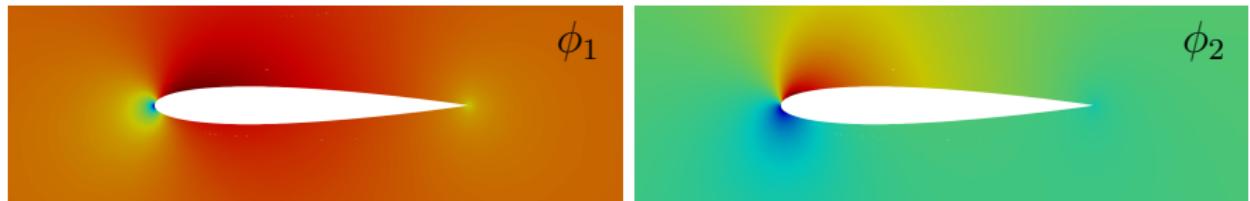
$$\mathcal{V}_N = \text{span} \underbrace{\{u_h(\mu_i)\}_{i=1}^N}_{\text{snapshots}} = \text{span} \underbrace{\{\phi_i\}_{i=1}^N}_{\text{orth. basis}} \subset \mathcal{V}_h.$$

RB: given $\mu \in \mathcal{D}$, find $u_N(\mu) \in \mathcal{V}_N$ s.t.

$$r_\mu(u_N(\mu), v_N) = 0 \quad \forall v_N \in \mathcal{V}_N$$

and evaluate output $s_N(\mu) = q_\mu(u_N(\mu))$.

Caveat: $N \ll N_h$ but computation of $r_\mu(\cdot, \cdot)$ requires $\mathcal{O}(N_h)$ ops.



Hyperreduction: empirical quadrature procedure (EQP)

Hyperreduction: find

[cf. EIM, MPE, GNAT, ECSW, ...]

$$\underbrace{\tilde{r}_\mu(\cdot, \cdot)}_{\text{hyperreduced residual}} \approx \underbrace{r_\mu(\cdot, \cdot)}_{\text{residual}} \quad \text{that admits } \mathcal{O}(N) \text{ evaluation}$$

RB-EQP hyperreduced residual:

[w/ Patera for non-DG]

$$\tilde{r}_\mu(\cdot, \cdot) \equiv \sum_{\kappa \in \mathcal{T}_h} \underbrace{\rho_\kappa}_{\substack{\text{EQP} \\ \text{weights}}} \underbrace{r_{\mu,\kappa}(\cdot, \cdot)}_{\text{"element-wise" residual}}$$

with sparse weights $\text{nnz}\{\rho_\kappa\} = \mathcal{O}(N \ll N_h)$.



Hierarchy of approximations & errors

Approximation hierarchy:

	dim.	res. eval.	sources of error
PDE	∞	∞	—
FE	N_h	$\mathcal{O}(N_h)$	FE space: $\mathcal{V}_h \subset \mathcal{V}$
RB	$N \ll N_h$	$\mathcal{O}(N_h)$	RB space: $\mathcal{V}_N \subset \mathcal{V}_h$
RB-EQP	$N \ll N_h$	$\mathcal{O}(N)$	hyperreduction: $\tilde{r}_\mu(\cdot, \cdot) \neq r_\mu(\cdot, \cdot)$

Goal: in each level of approximation

1. estimate errors
2. adaptively control errors

$$|s - \tilde{s}_N| \leq \underbrace{|s - s_h|}_{\text{FE error}} + \underbrace{|s_h - s_N|}_{\text{RB error}} + \underbrace{|s_N - \tilde{s}_N|}_{\text{hyperred error}} \lesssim \delta$$

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FE dual-weighted residual (DWR) error estimate

[Becker & Rannacher; Prudhomme & Oden; ...]

Key: not all errors/residuals are important for output

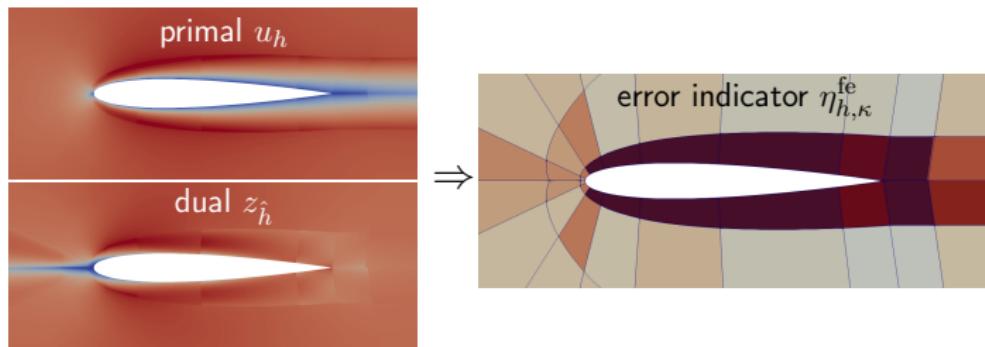
Dual problem: find $z_{\hat{h}} \in \mathcal{V}_{\hat{h}} \supset \mathcal{V}_h$ s.t.

$$r_{\mu}^{\text{du}}(u_h; w, z_N^{\text{du}}) \equiv r'_{\mu}(u_h; w, z_{\hat{h}}) - q'_{\mu}(u_h; w) = 0 \quad \forall w \in \mathcal{V}_{\hat{h}}$$

DWR error estimate:

$$\eta_h^{\text{fe}} \equiv |r_{\mu}(u_h, z_{\hat{h}})| \approx |s - s_h|$$

Elemental error indicator: $\eta_{h,\kappa}^{\text{fe}} \equiv |r_{\mu}(u_h, z_{\hat{h}}|_{\kappa})|$



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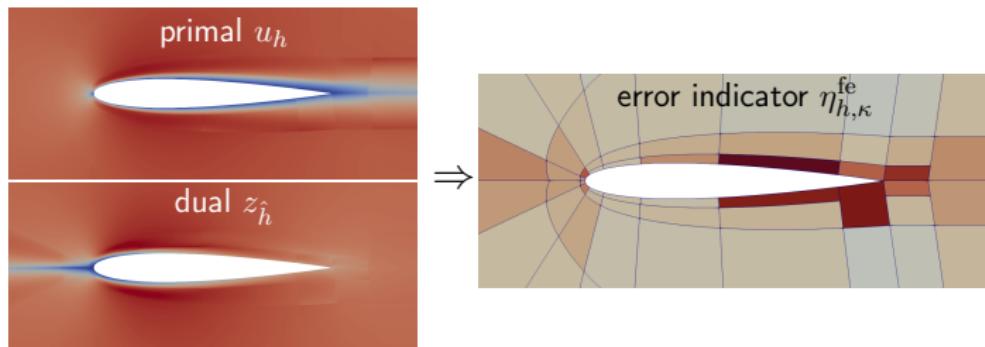
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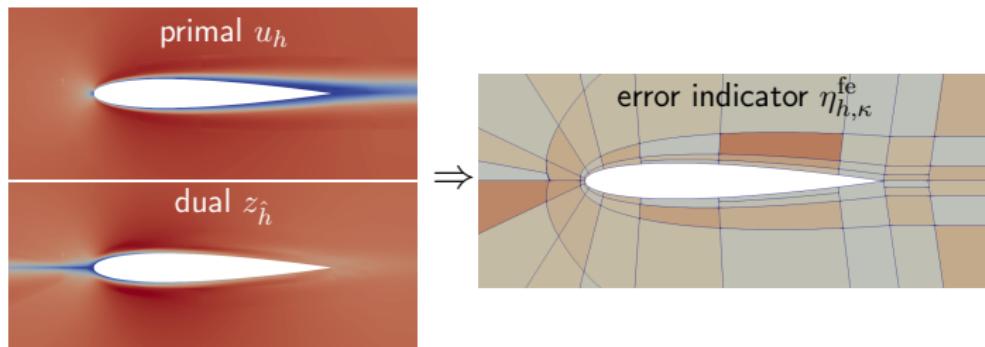
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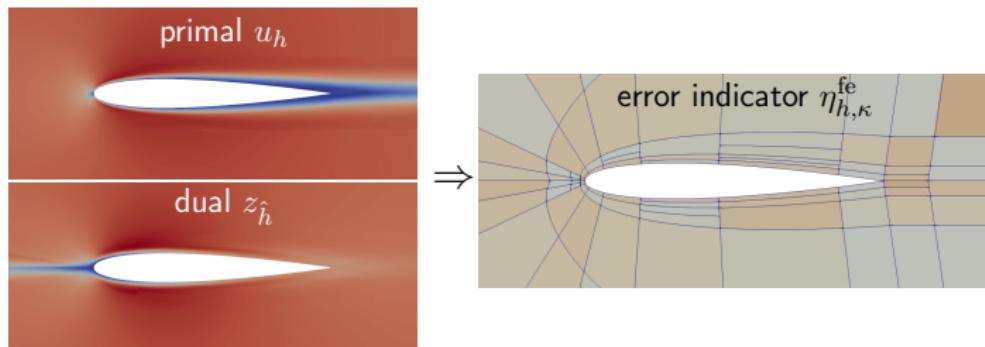
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Anisotropic adaptive mesh refinement

Employ

Solve → Estimate → Mark → Refine.

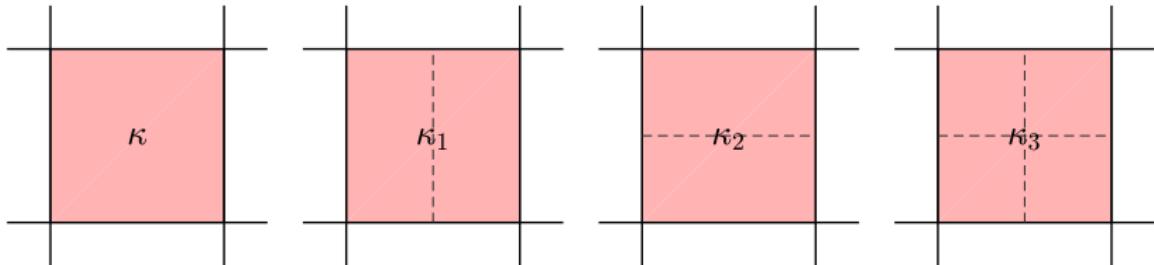
Solve: DG-FEM

Estimate: dual-weighted residual (DWR)

Mark: (i) local solve: find $u_h^{\kappa_i}$ for κ_i

(ii) anisotropic error indicator: $\eta_{h,\kappa_i}^{\text{fe}} \equiv |r_h(u_h^{\kappa_i}, z_{\hat{h}}|_{\kappa})|$

Refine: anisotropic hanging-node refinement



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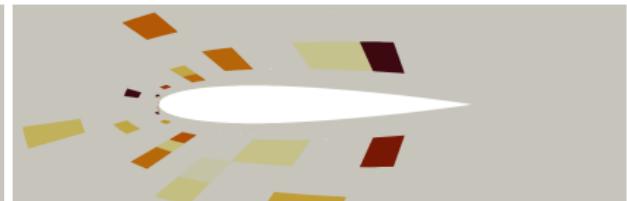
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Recap: empirical quadrature procedure (EQP)

Hyperreduction: approx. $r_\mu(\cdot, \cdot)$ by $\tilde{r}_\mu(\cdot, \cdot)$ that admits $\mathcal{O}(N)$ eval.

RB-EQP residual:

$$\tilde{r}_\mu(\cdot, \cdot) \equiv \sum_{\kappa \in \mathcal{T}_h} \underbrace{\rho_\kappa}_{\substack{\text{EQP} \\ \text{weights}}} \underbrace{r_{\mu,\kappa}(\cdot, \cdot)}_{\substack{\text{"element-wise"} \\ \text{residual}}}$$



Recap: empirical quadrature procedure (EQP)

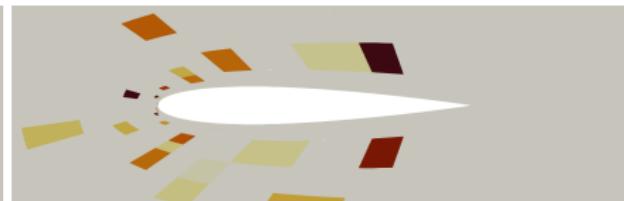
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that provides

1. energy stability
2. sparsity: $\text{nnz}\{\rho_\kappa\} = \mathcal{O}(N \ll N_h)$
3. quantitative error control: $|s_N - \tilde{s}_N| \lesssim \delta$



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that provides

1. energy stability \Rightarrow **residual redistribution**
2. sparsity: $\text{nnz}\{\rho_\kappa\} = \mathcal{O}(N \ll N_h)$ \Rightarrow **choice of $\{\rho_\kappa\}$**
3. quantitative error control: $|s_N - \tilde{s}_N| \lesssim \delta$



Hyperreduction: stability (digest)

[cf. Kalashnikova et al; Chen; ...]

Obs.: naive “elemental mask” does *not* inherit energy stability of DG

Stable decomp.: \exists DG res. localization s.t. for **any** weights $\rho_\kappa \geq 0$

$$\tilde{r}_\mu(\cdot, \cdot) \equiv \sum_{\kappa \in \mathcal{T}_h} \rho_\kappa r_{\mu,\kappa}(\cdot, \cdot)$$

is (i) energy stable for linear hyperbolic systems

(ii) symmetric and positive for linear diffusion systems

$$\underbrace{\frac{\partial}{\partial t} \left(\sum_{\kappa \in \mathcal{T}_h} \rho_\kappa \int_{\kappa} \|\tilde{u}_N\|_2^2 dx \right)}_{\text{EQP approx of change in energy}} \leq \underbrace{-2 \sum_{\kappa \in \mathcal{T}_h} \rho_\kappa \sum_{\sigma \in \partial \kappa \cap \Sigma_h^b} \int_{\sigma} \tilde{u}_N^+ (n \cdot A)^- u^b ds}_{\text{EQP approx of net energy entering } \Omega}$$

Key: linear stability is given \Rightarrow choose $\{\rho_\kappa\}$ for accuracy & sparsity

Hyperreduction output error control: DWR

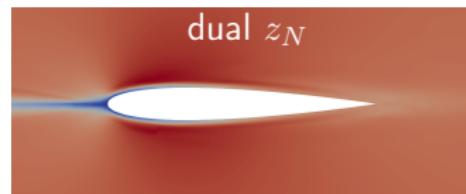
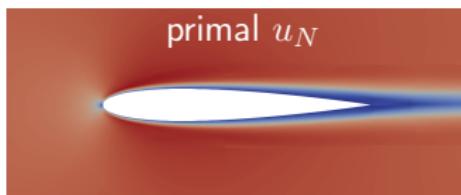
Recall: $|s - \tilde{s}_N| \leq \underbrace{|s - s_h|}_{\text{FE error } \checkmark} + \underbrace{|s_h - s_N|}_{\text{RB error}} + \underbrace{|s_N - \tilde{s}_N|}_{\text{hyperred. error}}$

Goal: hyperreduction with **quantitative error control on output**
(and not $|r_\mu(\cdot, \cdot) - \tilde{r}_\mu(\cdot, \cdot)|$)

DWR: $\underbrace{s(\mu)}_{\text{exact RB out.}} - \underbrace{\tilde{s}(\mu)}_{\text{RB-EQP out.}} \approx \underbrace{r_\mu(u_N, z_N)}_{\text{exact RB DWR}} - \underbrace{\tilde{r}_\mu(u_N, z_N)}_{\text{RB-EQP DWR}}$

where dual $z_N \in \mathcal{V}_N$ satisfies $r_\mu^{\text{du}}(u_N; w_N, z_N) = 0 \quad \forall w_N \in \mathcal{V}_N$.

Idea: find $\{\rho_\kappa\}$ for $\tilde{r}_\mu(\cdot, \cdot) \equiv \sum_{\kappa \in \mathcal{T}_h} \rho_\kappa r_\kappa(\cdot, \cdot)$ that controls error in dual-weighted residual.



EQP: linear program (LP)

EQP: set $\delta \in \mathbb{R}_{>0}$. Find **basic feasible solution**

$$\rho^* = \arg \min_{\rho} \sum_{\kappa \in \mathcal{T}_h} \rho_\kappa$$

subject to

$$\tilde{r}_\mu(\cdot, \cdot) \equiv \sum_{\kappa \in \mathcal{T}_h} \rho_\kappa r_\kappa(\cdot, \cdot)$$

C1. non-negativity: $\rho_\kappa \geq 0, \quad \forall \kappa \in \mathcal{T}_h$

C2. constant accuracy: $\left| |\Omega| - \sum_{\kappa \in \mathcal{T}_h} \rho_\kappa |\kappa| \right| \leq \delta$

C3. manifold accuracy: $\forall \hat{\mu} \in \Xi_J^{\text{train}}$

$$\left| \underbrace{r_{\hat{\mu}}(\hat{u}_N, z_N)}_{\text{exact RB DWR}} - \underbrace{\tilde{r}_{\hat{\mu}}(\hat{u}_N, z_N)}_{\substack{\text{RB-EQP DWR} \\ \text{linear in } \{\rho_\kappa\}}} \right| \leq \delta$$

for training sets

$$\Xi_J^{\text{train}} \equiv \{\hat{\mu}_j\}_{j=1}^J \quad \text{and} \quad U_J^{\text{train}} \equiv \{\hat{u}_N(\hat{\mu})\}_{\hat{\mu} \in \Xi_J^{\text{train}}}.$$

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C3. manifold accuracy: $\forall \hat{\mu} \in \Xi_J^{\text{train}}, i = 1, \dots, N$

$$\left| \underbrace{r_{\hat{\mu}}(\hat{u}_N, \Pi_{\phi_i} z_N)}_{\text{exact RB DWR}} - \underbrace{\tilde{r}_{\hat{\mu}}(\hat{u}_N, \Pi_{\phi_i} z_N)}_{\substack{\text{RB-EQP DWR} \\ \text{linear in } \{\rho_\kappa\}}} \right| \leq \frac{\delta}{N}$$

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EQP: properties

1. simple: linear program
2. sparse: $\text{nnz}\{\rho_\kappa\}_{\kappa \in \mathcal{T}_h} \ll |\mathcal{T}_h| \quad \Leftarrow \quad \text{intuition: } \ell_1 \text{ minimization}$
3. error control: under mild assumptions

$$|q_\mu(u_N(\mu)) - q_\mu(\tilde{u}_N(\mu))| \lesssim \delta \quad \forall \mu \in \Xi_J^{\text{train}}$$

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4. versatile: manifold accuracy constraint (C3) can be replaced to hyperreduce various forms while controlling error:
e.g., output functional $q_\mu(\cdot) \rightarrow \tilde{q}_\mu(\cdot)$ with weights $\{\rho_\kappa^q\}$

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Online-efficient *a posteriori* error estimate

Goal: estimate error $|\underbrace{s_h(\mu)}_{\text{FE}} - \underbrace{\tilde{s}_N(\mu)}_{\text{RB-EQP}}|$ in $\mathcal{O}(N)$ for any $\mu \in \mathcal{D}$

Ingredients:

1. RB approximation of DWR

(i) RB dual space: $\mathcal{V}_N^{\text{du}} = \text{span}\{z_h(\mu_i)\}_{i=1}^N \neq \mathcal{V}_N$

(ii) Dual: find $z_N^{\text{du}} \in \mathcal{V}_N^{\text{du}}$ s.t. $r_\mu^{\text{du}}(\tilde{u}_N; w, z_N^{\text{du}}) = 0 \quad \forall w \in \mathcal{V}_N^{\text{du}}$

(iii) DWR: $\eta_N^{\text{rb}} \equiv |r_\mu(\tilde{u}_N, z_N^{\text{du}})| \approx |s_h - \tilde{s}_N|$

Caveat: evaluation of z_N^{du} and $r_\mu(\cdot, \cdot)$ requires $\mathcal{O}(N_h)$ ops.

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2. EQP hyperreduction with accuracy constraints (C3) on

(i) adjoint $z_N^{\text{du}} - \tilde{z}_N^{\text{du}}$ \Rightarrow weights $\{\rho_\kappa^\eta\}$

(ii) residual $r_\mu(\cdot, \cdot) - \tilde{r}_\mu(\cdot, \cdot)$

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Simultaneous FE, RB, and EQP greedy training

Input: training set $\Xi_J^{\text{train}} \subset \mathcal{D}$; output tolerances δ^{fe} and δ^{rb}

Output: primal and dual RB; EQP weights $\{\rho_\kappa\}$, $\{\rho_\kappa^q\}$, $\{\rho_\kappa^\eta\}$

While $(\max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu) > \delta^{\text{rb}})$

1. Find $\mu^{(N)}$ that maximizes output error estimate

$$\mu^{(N)} = \arg \max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu).$$

2. Solve for $u_h(\mu^{(N)})$ and $z_h(\mu^{(N)})$;
adapt mesh as necessary s.t. $\eta_h^{\text{fe}}(\mu^{(N)}) \leq \delta^{\text{fe}}$.
3. Update primal and dual RB.
4. Update EQP weights $\{\rho_\kappa\}$, $\{\rho_\kappa^q\}$, and $\{\rho_\kappa^\eta\}$;
evaluate EQP constraints at Ξ_J^{train} .

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3. Update primal and dual RB.
4. Update EQP weights $\{\rho_\kappa\}$, $\{\rho_\kappa^q\}$, and $\{\rho_\kappa^\eta\}$; evaluate EQP constraints at Ξ_J^{train} . $\mathcal{O}(N_h)$

FE, RB, and EQP error estimation and control: summary

Approximation hierarchy:

$$|s - \tilde{s}_N| \leq \underbrace{|s - s_h|}_{\text{FE error}} + \underbrace{|s_h - s_N|}_{\text{RB error}} + \underbrace{|s_N - \tilde{s}_N|}_{\text{EQP error}}.$$

	FE	RB	RB-EQP
estimation	FE DWR (η_h^{fe})	hyperreduced DWR ($\tilde{\eta}_N^{\text{rb}}$)	
control	AMR	Greedy	output EQP

Our goal and approach:

1. rapid: EQP-hyperreduced RB
2. reliable: EQP-hyperreduced DWR
3. automated: simultaneous FE, RB, EQP greedy

Goal-oriented model reduction of nonlinear PDEs

- Overview: FE, RB, and hyperreduction (EQP)
- FE: error estimation and adaptation
- RB-EQP: error control
- RB-EQP: error estimation
- Greedy algorithm
- Example: ONERA M6 RANS
- Related work

ONERA M6 RANS

Equation: RANS equations with Spalart-Allmaras turbulence model

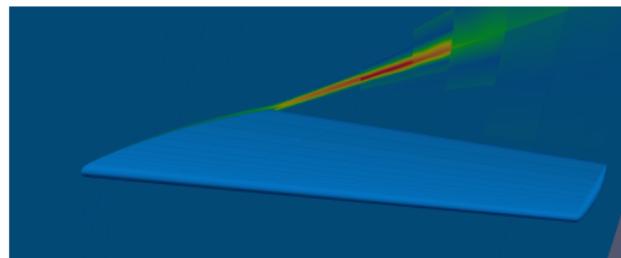
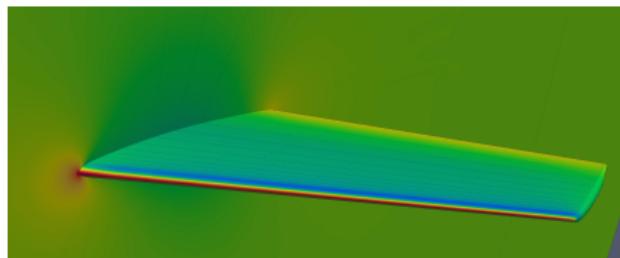
Parameters:

1. angle of attack: $\alpha \in [0^\circ, 2^\circ]$
2. Mach number: $M_\infty \in [0.3, 0.5]$
3. Reynolds number: $Re = 10^6$ (fixed)

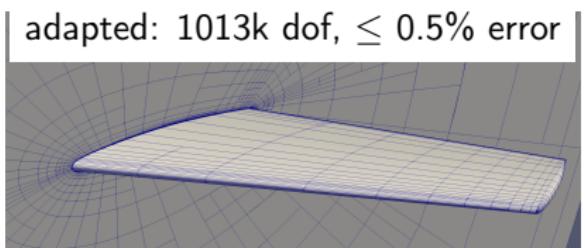
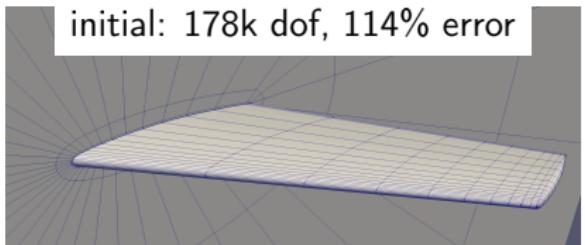
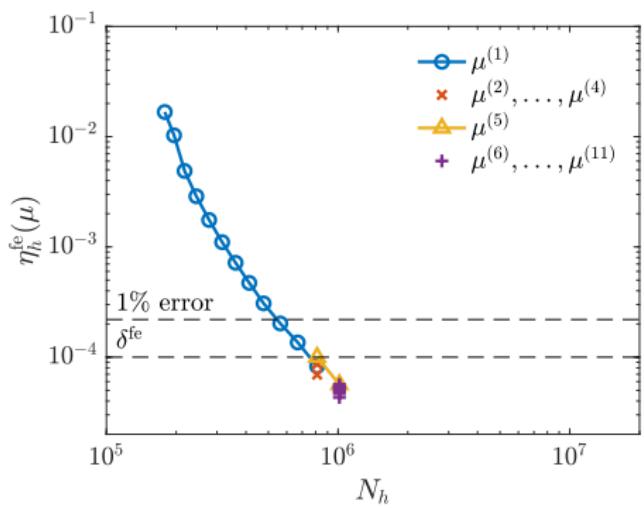
DG-RB-EQP setup:

Drag error tol.: $\delta = \delta^{\text{fe}} + \delta^{\text{rb}} = 10^{-4} + 10^{-4} \lesssim 1\%$

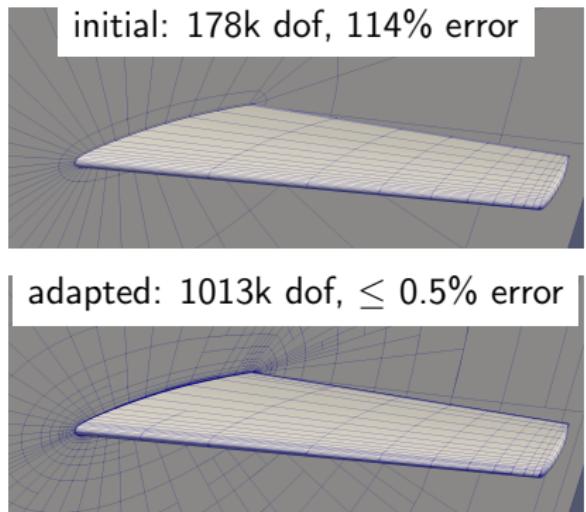
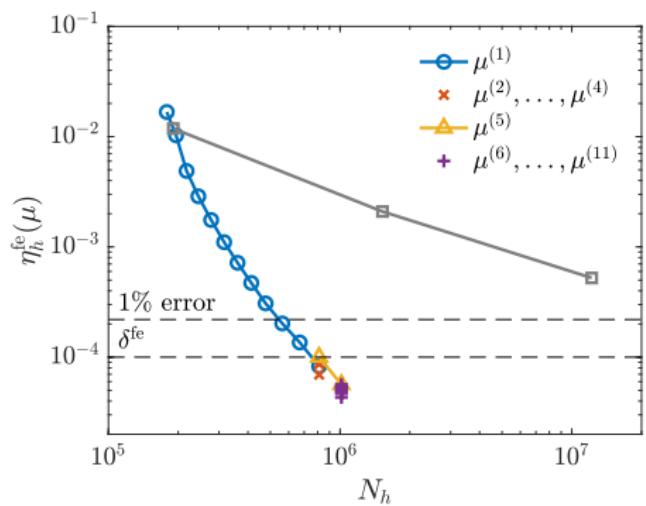
Training parameter set: $\Xi_J^{\text{train}} = 5 \times 5$ uniform grid



ONERA M6 RANS: FE convergence



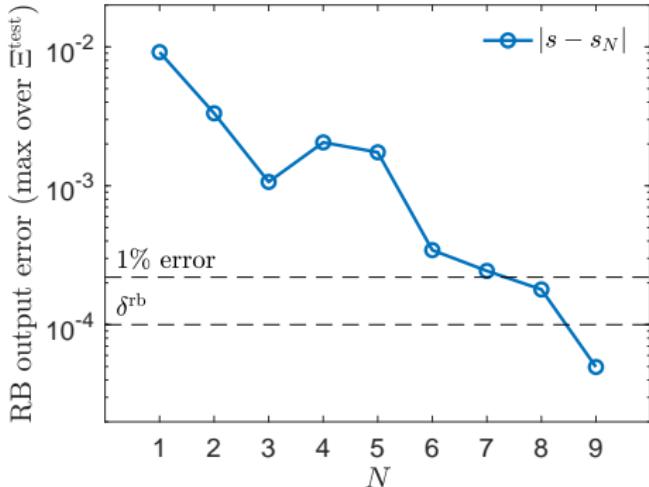
ONERA M6 RANS: FE convergence



For 1% error level,

- 2nd-order method on “best-practice” mesh: $\sim 50\text{M}$ dof
- $p = 2$ anisotropic- h adaptation: $\sim 0.56\text{M}$ dof ($\times 90$ reduction)

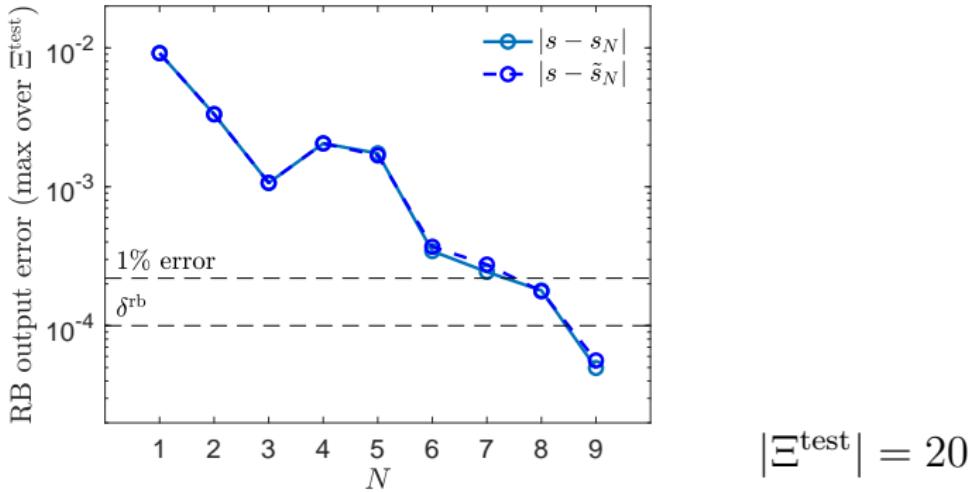
ONERA M6 RANS: RB convergence



$$|\Xi^{\text{test}}| = 20$$

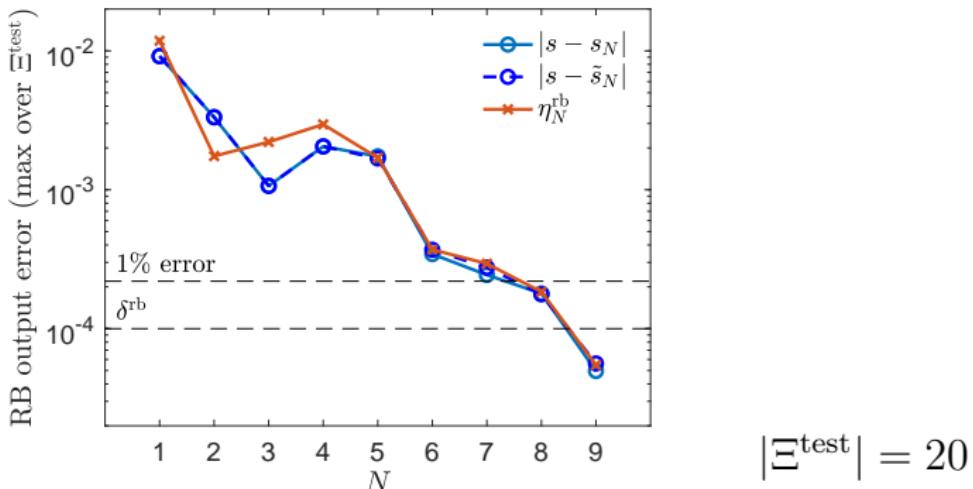
- rapid *output* convergence with N (c.f., $\|u_h - \tilde{u}_N\|_{L^2(\Omega)}$)

ONERA M6 RANS: RB convergence



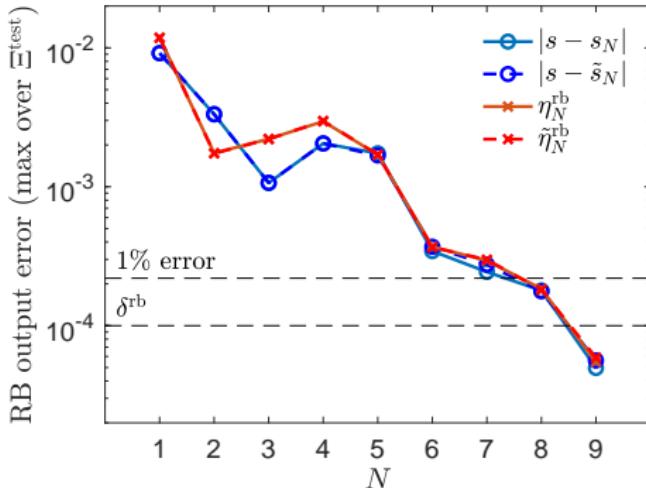
- rapid *output* convergence with N (c.f., $\|u_h - \tilde{u}_N\|_{L^2(\Omega)}$)
- EQP: $|s_N - \tilde{s}_N| < 5 \times 10^{-5}$ and $\text{nnz}\{\rho_\kappa\} \leq 75$ (0.5%).

ONERA M6 RANS: RB convergence



- rapid *output* convergence with N (c.f., $\|u_h - \tilde{u}_N\|_{L^2(\Omega)}$)
- EQP: $|s_N - \tilde{s}_N| < 5 \times 10^{-5}$ and $\text{nnz}\{\rho_\kappa\} \leq 75$ (0.5%).
- effective error estimate

ONERA M6 RANS: RB convergence



$$|\Xi^{\text{test}}| = 20$$

- rapid *output* convergence with N (c.f., $\|u_h - \tilde{u}_N\|_{L^2(\Omega)}$)
- EQP: $|s_N - \tilde{s}_N| < 5 \times 10^{-5}$ and $\text{nnz}\{\rho_\kappa\} \leq 75$ (0.5%).
- effective error estimate
EQP: $|\eta_N^{rb} - \tilde{\eta}_N^{rb}| \leq 3 \times 10^{-5}$ and $\text{nnz}\{\rho_\kappa^\eta\} \leq 115$ (0.7%).

ONERA M6 RANS: computational cost

Time unit: $t^{\text{fe}} \equiv$ CPU time for single FE solve on adapted mesh

Offline cost ($N = 9$):

$$\approx 60t^{\text{fe}} \quad (\approx 6.7t^{\text{fe}} \times (N = 9 \text{ greedy iteration}))$$

major costs: snapshot & EQP training residual evaluations

Online cost ($N = 9$):

$$\approx 1/340 \times t^{\text{fe}} \text{ (for output only)}$$

$$\approx 1/290 \times t^{\text{fe}} \text{ (for output + error estimate)}$$

Remarks:

recall: adaptive DG is $\approx 90\times$ more efficient than 2nd order method at 1% error level

Goal-oriented model reduction of nonlinear PDEs

- Overview: FE, RB, and hyperreduction (EQP)
- FE: error estimation and adaptation
- RB-EQP: error control
- RB-EQP: error estimation
- Greedy algorithm
- Example: ONERA M6 RANS
- Related work

Most relevant related work (1/2)

Nonlinear ROM: “*interpolate-then-integrate*”

Gappy POD, MPE, EIM, BPIM, GNAT, ...

[Everson & Sirovich; Astrid et al; Barrault et al; Nguyen et al; Carlberg et al; ...]

Nonlinear ROM: “*direct integration*”

Hyperreduction [Ryckelynck]

Optimal cubature [An et al]

Energy-conservative sampling and weighting (ECSW) [Farhat et al]

Empirical cubature method [Hernández]

EQP for continuous Galerkin [Patera & Yano]

Most relevant related work (2/2)

Stability-aware hyperreduction:

ECSW for solids [Farhat et al]

Matrix gappy POD for solids [Carlberg et al]

Stable ROM for fluids [Barone et al; Kalashinova et al; Chen]

DWR in ROM: [Meyer & Matthies; Carlberg; Drohmann & Carlberg; ...]

ROM for *parametrized aerodynamics*:

Euler [LeGresley and Alonso; Zimmermann and Görtz]

RANS [Washabaugh et al; Zimmermann et al]

DG-RB-EQP: model reduction method that provides

1. stability for conservation laws
2. **quantitative** output error estimate and control
3. **automated** training of FE, RB, and EQP

Moderate-/high-dimensional problems

- Formulation
- High-lift RANS UQ
- NACA0012 geometry transformation (*preliminary*)

Moderate-/high-dimensional problems

- Formulation
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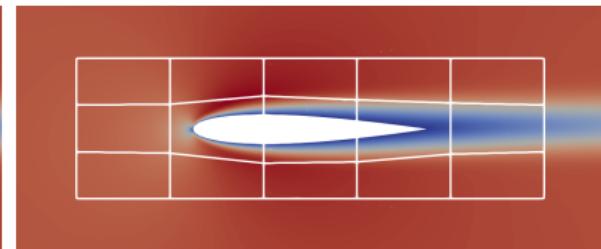
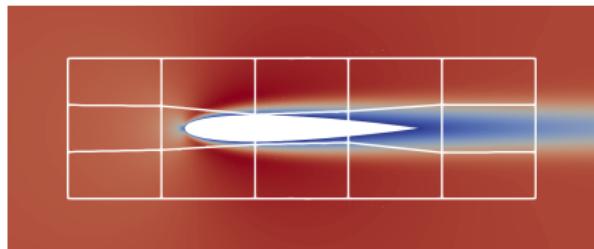
Goal: rapid and reliable solution of moderate-/high-dim. problems

- geometry transformation
- uncertainty quantification

Assumption: problem is reducible; i.e., small intrinsic dimension

Challenges:

1. ensure model is accurate for all $\mu \in \mathcal{D} \subset \mathbb{R}^{P \gg 1}$
2. control offline training cost



Recap: simultaneous FE, RB, and EQP greedy training

Input: training set $\Xi_J^{\text{train}} \subset \mathcal{D}$; output tolerances δ^{fe} and δ^{rb}

Output: primal and dual RB; EQP weights $\{\rho_\kappa\}$, $\{\rho_\kappa^q\}$, $\{\rho_\kappa^\eta\}$

While $(\max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu) > \delta^{\text{rb}})$

1. Find $\mu^{(N)}$ that maximizes the output error estimate $\mathcal{O}(JN)$

$$\mu^{(N)} = \arg \max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu).$$

2. Adaptively solve for $u_h(\mu^{(N)})$ and $z_h(\mu^{(N)})$
3. Update primal and dual RB.
4. Update EQP weights $\{\rho_\kappa\}$, $\{\rho_\kappa^q\}$, and $\{\rho_\kappa^\eta\}$ $\mathcal{O}(JN_h)$
evaluate EQP constraints at $\Xi_{J'}^{\text{EQP}} = \Xi_J^{\text{train}}$.

Adaptive Greedy and EQP training sets

[Hesthaven et al; Chen & Ghattas; Bui-Thanh et al; ...]

Goal: find (i) Ξ_J^{train} that sufficiently covers $\mathcal{D} \subset \mathbb{R}^{P \gg 1}$

(ii) minimal $\Xi_{J'}^{\text{EQP}}$ s.t. EQP error is small $\forall \mu \in \Xi_J^{\text{train}}$

Ingredients:

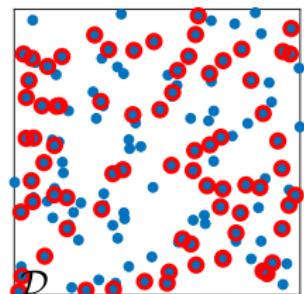
1. Online-efficient error estimate $\tilde{\eta}_N^{\text{rb}} \approx |s_h - \tilde{s}_N|$

\Rightarrow permits use of $|\Xi_J^{\text{train}}| = \mathcal{O}(10^2)$

2. Adaptive refinement of Ξ_J^{train} based on $\tilde{\eta}_N^{\text{rb}}$:

In i -th Greedy iteration, set

$$\underbrace{\Xi_J^{\text{train},i}}_{J \text{ training points}} \leftarrow \underbrace{\Xi_K^{\text{train},i-1}}_{K \text{ points w/ largest } \tilde{\eta}_N^{\text{rb}} \text{ from previous iteration}} \cup \underbrace{\Xi_L^{\text{rand}}}_{L \text{ new random points}}$$



3. Adaptive enrichment of $\Xi_{J'}^{\text{EQP}} \subset \Xi_J^{\text{train}}$ based on EQP error

Moderate-/high-dimensional problems

- Formulation
- High-lift RANS UQ
- NACA0012 geometry transformation (*preliminary*)

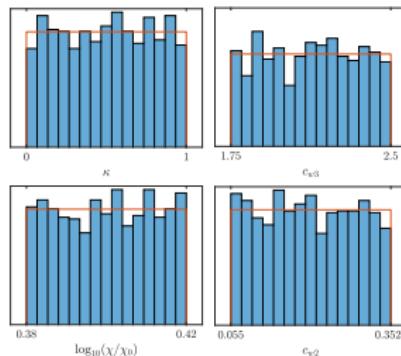
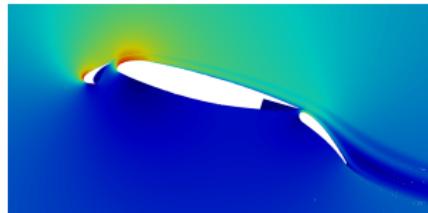
MDA high-lift RANS: turbulence model UQ

Equation: RANS equations with Spalart-Allmaras turbulence model

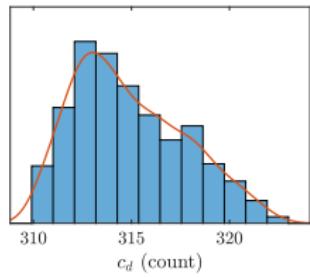
Parameters: [Spalart & Allmaras; Schaefer et al]

1. Kármán constant: $\kappa \in [0.38, 0.42]$
2. freestream turbulence intensity $\chi \equiv \tilde{\nu}/\nu \in [3, 30]$
3. 2nd wall parameter $c_{w_3} \in [1.75, 2.5]$
4. 3rd wall parameter $c_{w_2} \in [0.055, 0.3525]$

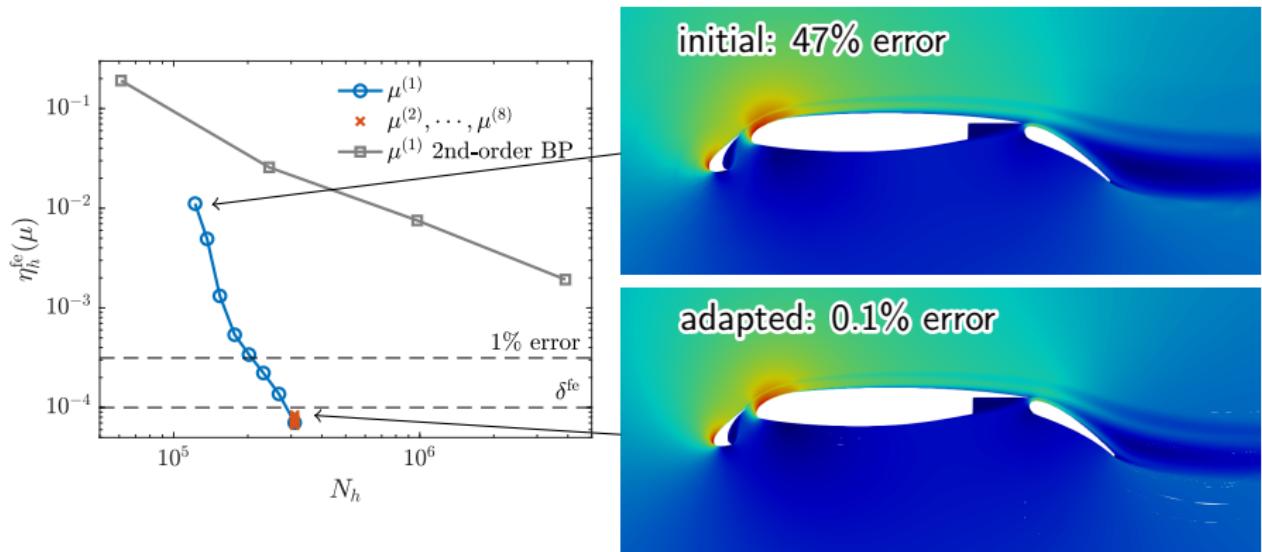
Condition: $M_\infty = 0.2$, $Re_c = 9 \times 10^6$, $\alpha = 16^\circ$



\Rightarrow



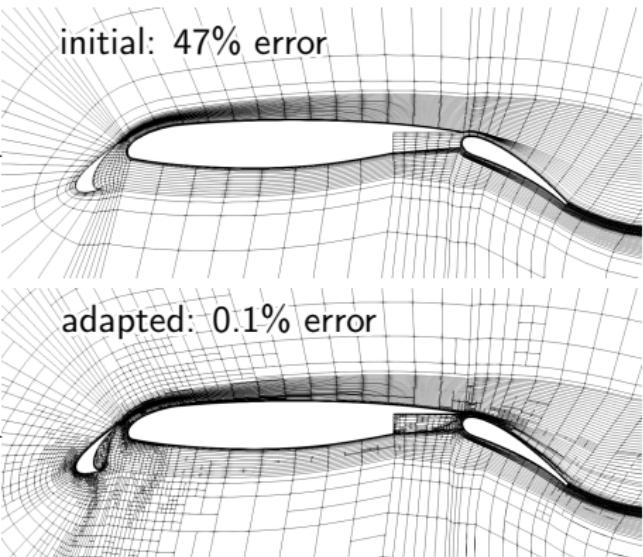
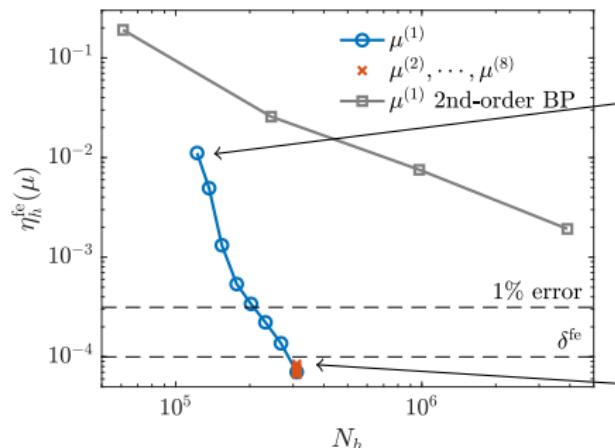
MDA high-lift RANS UQ: FE convergence



For 1% error level

- 2nd-order method on “best-practice” mesh: $\approx 25\text{M}$ dof
- high-order anisotropic adaptation: $\approx 0.25\text{M}$ dof

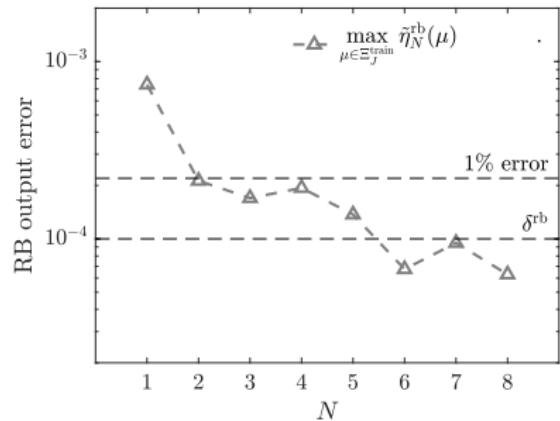
MDA high-lift RANS UQ: FE convergence



For 1% error level

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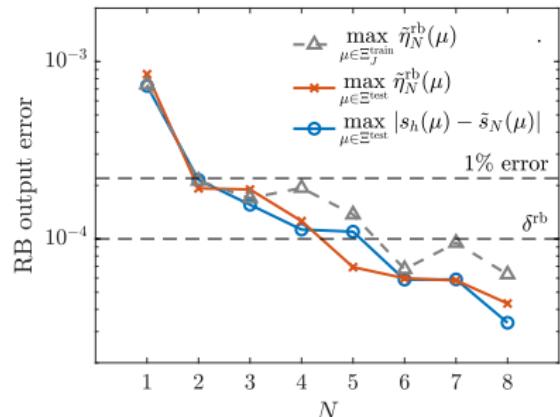
MDA high-lift RANS UQ: RB convergence



Offline:

training set: $|\Xi_J^{\text{train}}| = 75$ & mean $|\Xi_{J'}^{\text{EQP}}| = 20$

MDA high-lift RANS UQ: RB convergence



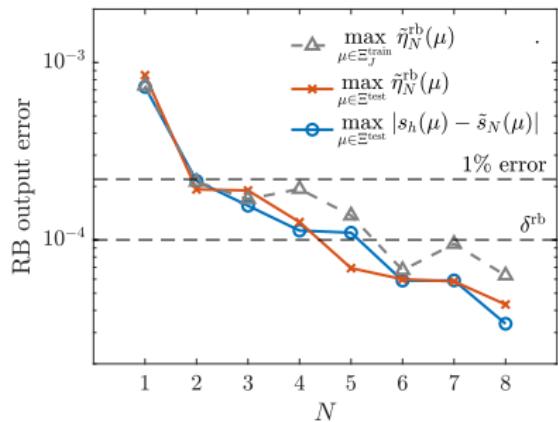
$$|\Xi^{\text{test}}| = 20$$

Offline:

training set: $|\Xi_J^{\text{train}}| = 75$ & mean $|\Xi_{J'}^{\text{QP}}| = 20$

coverage: $\max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu) > \max_{\mu \in \Xi^{\text{test}}} \tilde{\eta}_N^{\text{rb}}(\mu)$ for $N > 3$

MDA high-lift RANS UQ: RB convergence



$$|\Xi^{\text{test}}| = 20$$

Offline:

training set: $|\Xi_J^{\text{train}}| = 75$ & mean $|\Xi_{J'}^{\text{EQP}}| = 20$

coverage: $\max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu) > \max_{\mu \in \Xi^{\text{test}}} \tilde{\eta}_N^{\text{rb}}(\mu)$ for $N > 3$

Online ($N = 8$):

EQP: $\text{nnz}\{\rho_\kappa\} \leq 140$ (1.3%) and $\text{nnz}\{\rho_\kappa^\eta\} \leq 160$ (1.5%)

cost: $\approx 1/180 \times t^{\text{fe}}$ (for output + error estimate)

Moderate-/high-dimensional problems

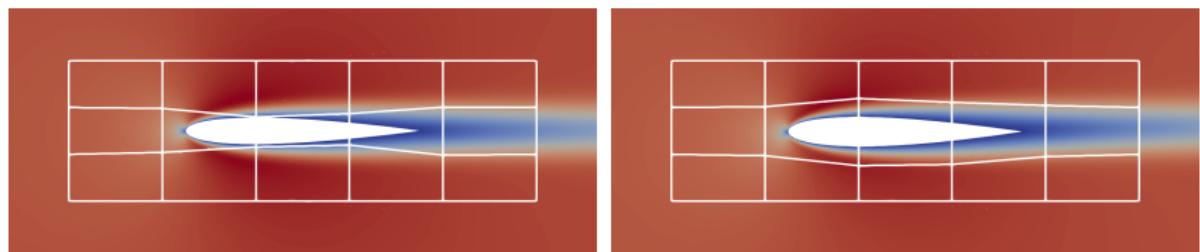
- Formulation
- High-lift RANS UQ
- NACA0012 geometry transformation (*preliminary*)

NACA0012 geometry transform

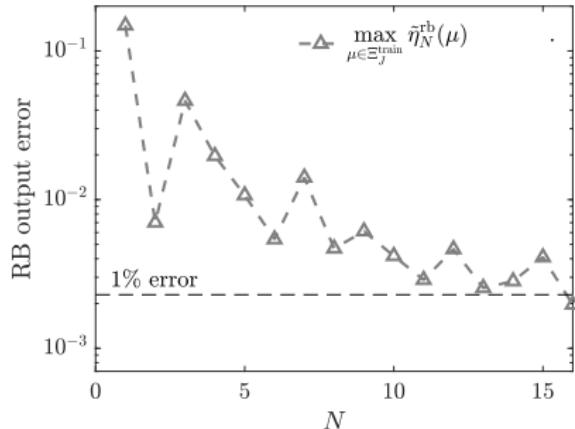
Equation: laminar Navier-Stokes equations

Parameters: $\mathcal{D} \subset \mathbb{R}^{10}$

1. angle of attack: $\alpha \in [0^\circ, 2^\circ]$
2. Mach number: $M_\infty \in [0.2, 0.5]$
3. free-form deformation (FFD): 8 parameters



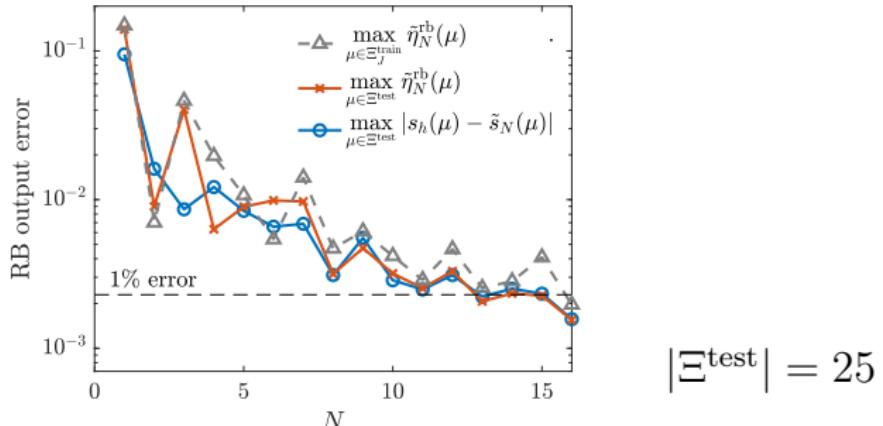
NACA0012 geom. transform: RB convergence (*preliminary*)



Offline:

training set: $|\Xi_J^{\text{train}}| = 150$ & mean $|\Xi_{J'}^{\text{EQP}}| \approx 34$

NACA0012 geom. transform: RB convergence (*preliminary*)

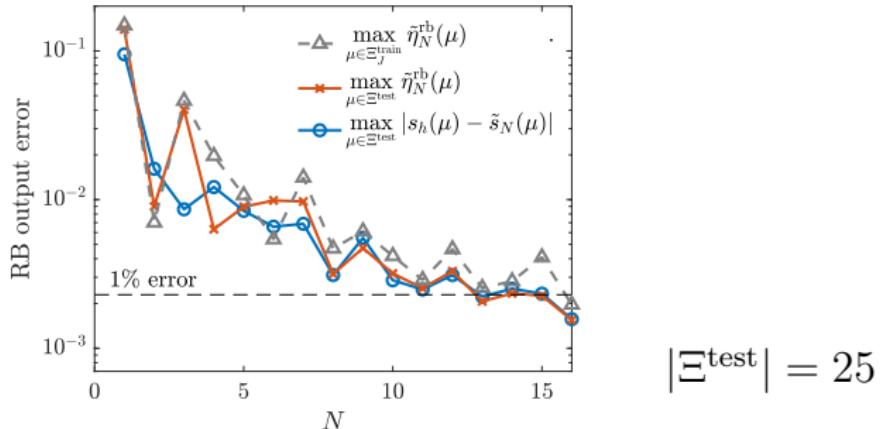


Offline:

training set: $|\Xi_J^{\text{train}}| = 150$ & mean $|\Xi_{J'}^{\text{EQP}}| \approx 34$

coverage: $\max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu) > \max_{\mu \in \Xi^{\text{test}}} \tilde{\eta}_N^{\text{rb}}(\mu)$ for $N > 6$

NACA0012 geom. transform: RB convergence (*preliminary*)



Offline:

training set: $|\Xi_J^{\text{train}}| = 150$ & mean $|\Xi_{J'}^{\text{EQP}}| \approx 34$

coverage: $\max_{\mu \in \Xi_J^{\text{train}}} \tilde{\eta}_N^{\text{rb}}(\mu) > \max_{\mu \in \Xi^{\text{test}}} \tilde{\eta}_N^{\text{rb}}(\mu)$ for $N > 6$

Online:

EQP: $\text{nnz}\{\rho_\kappa\} \leq 160$ (13%) and $\text{nnz}\{\rho_\kappa^\eta\} \leq 260$ (21%)

Time-dependent problems

- Formulation
- NACA0012 separated flow (*preliminary*)

Time-dependent problems

- Formulation
- NACA0012 separated flow (*preliminary*)

Semi-discrete DG: find $u_h(t) \in \mathcal{V}_h$ s.t., $\forall v \in \mathcal{V}_h$,

$$\underbrace{r_\mu^{\text{td}}(u_h, v_h)}_{\text{time-dep. residual}} = \underbrace{m_\mu(\partial_t u_h, v_h)}_{\text{mass term}} + \underbrace{r_\mu(u_h, v_h)}_{\text{steady residual}} = 0$$

Example: separated flow past NACA0012

DG reduced basis (RB) method

RB space:

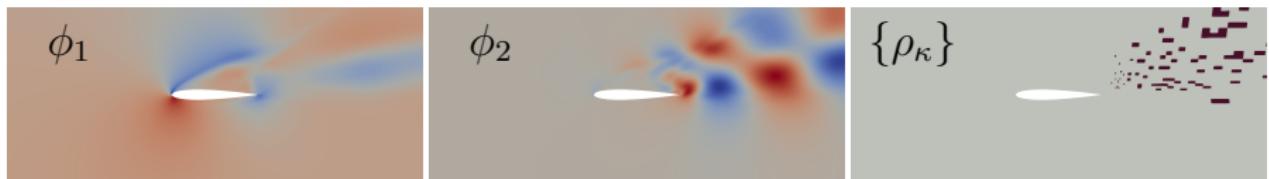
$$\mathcal{V}_N = \text{POD}_N\{u_h(t^j)\}_{j=1}^{N_t} = \text{span}\{\phi_i\}_{i=1}^N$$

RB: find $u_N(t) \in \mathcal{V}_N$ s.t.,

$$r_\mu^{\text{td}}(u_N(t), v_N) = 0 \quad \forall v_N \in \mathcal{V}_N$$

RB-EQP: find $\tilde{u}_N(t) \in \mathcal{V}_N$ s.t.,

$$\tilde{r}_\mu^{\text{td}}(\tilde{u}_N(t), v_N) \equiv \sum_{\kappa \in \mathcal{T}_h} \underbrace{\rho_\kappa}_{\substack{\text{EQP} \\ \text{weights}}} \underbrace{r_{\mu,\kappa}^{\text{td}}(u_N, v_N)}_{\substack{\text{"element-wise"} \\ \text{residual}}} = 0 \quad \forall v \in \mathcal{V}_N$$



Hyperreduction output error control: DWR

Dual: find $z_N(t) \in \mathcal{V}_N$ s.t. "backward integration"

$$r_\mu^{\text{td}, \text{du}}(u_N; w_N, z_N) = 0 \quad \forall w_N \in \mathcal{V}_N$$

DWR:

$$\int_I [\underbrace{q_\mu(u_N)}_{\text{exact RB out.}} - \underbrace{q_\mu(\tilde{u}_N)}_{\text{RB-EQP out.}}] dt \approx \int_I [\underbrace{r_\mu^{\text{td}}(u_N, z_N)}_{\text{exact RB DWR}} - \underbrace{\tilde{r}_\mu^{\text{td}}(u_N, z_N)}_{\text{RB-EQP DWR}}] dt$$

Hyperreduction output error control: DWR

Dual: find $z_N(t) \in \mathcal{V}_N$ s.t.

“backward integration”

$$r_\mu^{\text{td}, \text{du}}(u_N; w_N, z_N) = 0 \quad \forall w_N \in \mathcal{V}_N$$

DWR:

$$\int_I [\underbrace{q_\mu(u_N)}_{\text{exact RB out.}} - \underbrace{q_\mu(\tilde{u}_N)}_{\text{RB-EQP out.}}] dt \approx \int_I [\underbrace{r_\mu^{\text{td}}(u_N, z_N)}_{\text{exact RB DWR}} - \underbrace{\tilde{r}_\mu^{\text{td}}(u_N, z_N)}_{\text{RB-EQP DWR}}] dt$$

EQP manifold accuracy (C3): for $I^j \equiv [t^j, t^{j+1}], j = 1, \dots, J-1$,

$$\left| \int_{I^j} [\underbrace{r_{\hat{\mu}}^{\text{td}}(\hat{u}_N(t), \Pi_{\phi_i} z_N(t))}_{\text{exact RB DWR}} - \underbrace{\tilde{r}_{\hat{\mu}}^{\text{td}}(\hat{u}_N(t), \Pi_{\phi_i} z_N(t))}_{\substack{\text{RB-EQP DWR} \\ \text{linear in } \{\rho_\kappa\}}}] dt \right| < \delta$$

Key: space-time analysis \Rightarrow inherits EQP error control properties

Online-efficient *a posteriori* error estimate

PDE-to-FE error estimate: FE DWR

FE-to-RB-EQP error estimate:

1. RB approximation of DWR

- (i) RB dual space: $\mathcal{V}_N^{\text{du}} = \text{POD}_N\{z_h(t^j)\}_{j=1}^{N_t} \neq \mathcal{V}_N$
- (ii) Dual: find $z_N^{\text{du}} \in \mathcal{V}_N^{\text{du}}$ s.t. $r_\mu^{\text{td}, \text{du}}(\tilde{u}_N; w, z_N^{\text{du}}) = 0 \quad \forall w \in \mathcal{V}_N^{\text{du}}$
- (iii) DWR: $\eta_N^{\text{rb}} \equiv |\int_I r_\mu^{\text{td}}(\tilde{u}_N, z_N^{\text{du}}) dt| \approx |s_h - \tilde{s}_N|$

Caveat: evaluation of z_N^{du} and $r_\mu(\cdot, \cdot)$ requires $\mathcal{O}(N_h)$ ops.

Online-efficient *a posteriori* error estimate

PDE-to-FE error estimate: FE DWR

FE-to-RB-EQP error estimate:

1. RB approximation of DWR

(i) RB dual space: $\mathcal{V}_N^{\text{du}} = \text{POD}_N\{z_h(t^j)\}_{j=1}^{N_t} \neq \mathcal{V}_N$

(ii) Dual: find $\tilde{z}_N^{\text{du}} \in \mathcal{V}_N^{\text{du}}$ s.t. $\tilde{r}_\mu^{\text{td}, \text{du}}(\tilde{u}_N; w, \tilde{z}_N^{\text{du}}) = 0 \quad \forall w \in \mathcal{V}_N^{\text{du}}$

(iii) DWR: $\tilde{\eta}_N^{\text{rb}} \equiv |\int_I \tilde{r}_\mu^{\text{td}}(\tilde{u}_N, \tilde{z}_N^{\text{du}}) dt| \approx |s_h - \tilde{s}_N|$

2. EQP hyperreduction with accuracy constraints (C3) on

(i) adjoint $z_N^{\text{du}} - \tilde{z}_N^{\text{du}}$

(ii) residual $r_\mu^{\text{td}}(\cdot, \cdot) - \tilde{r}_\mu^{\text{td}}(\cdot, \cdot)$

Time-dependent problems

- Formulation
- NACA0012 separated flow (*preliminary*)

NACA0012 separated flow

Equation: laminar Navier-Stokes equations

Flow condition: separated flow (*fixed parameter*)

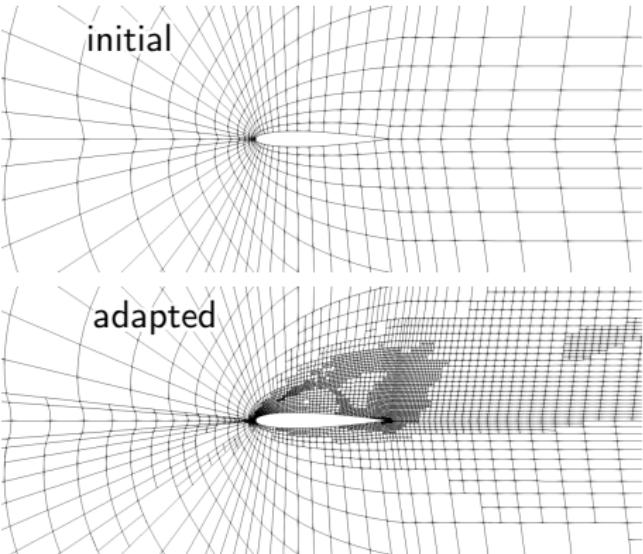
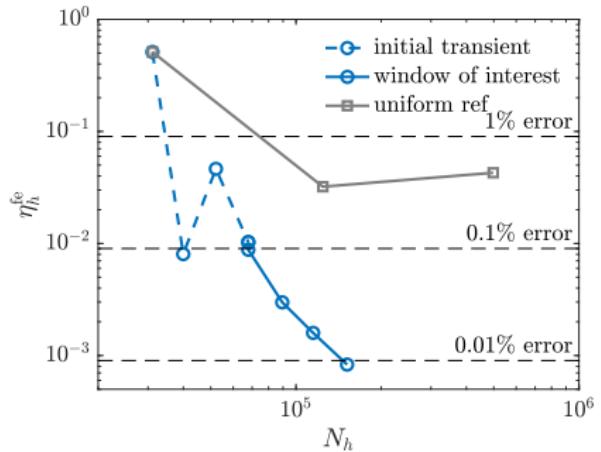
$$\alpha = 20^\circ, M_\infty = 0.3, Re_c = 1000$$

Output: time-averaged drag

primal

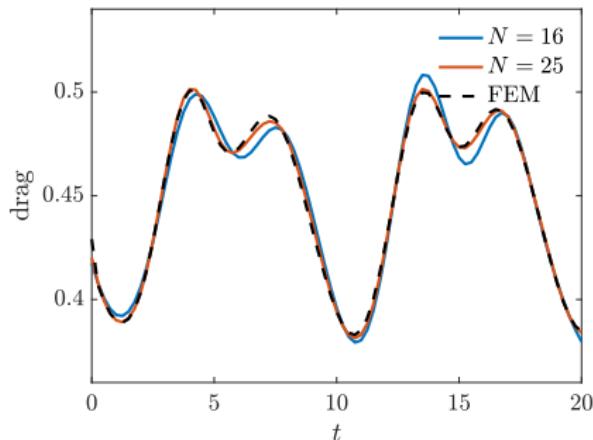
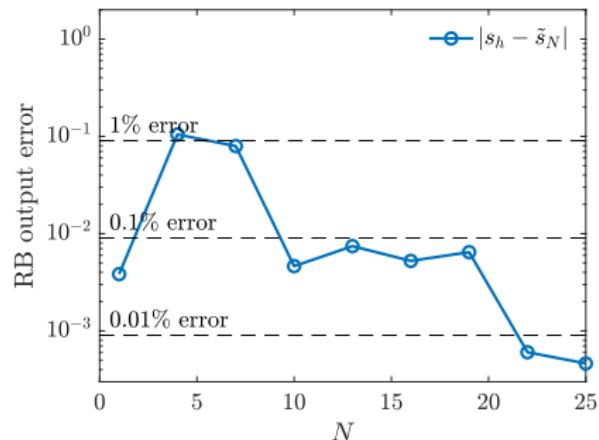
dual

NACA0012 separated flow: FE error convergence



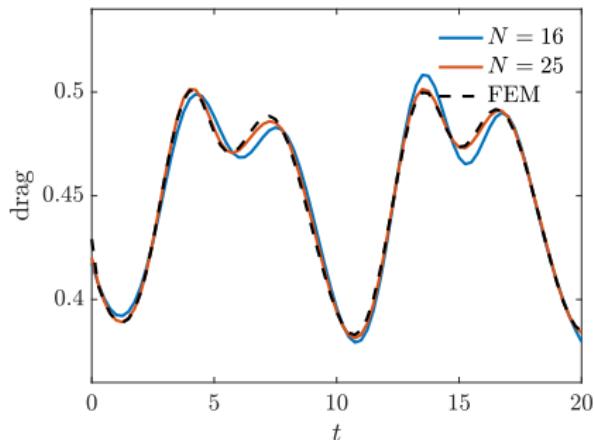
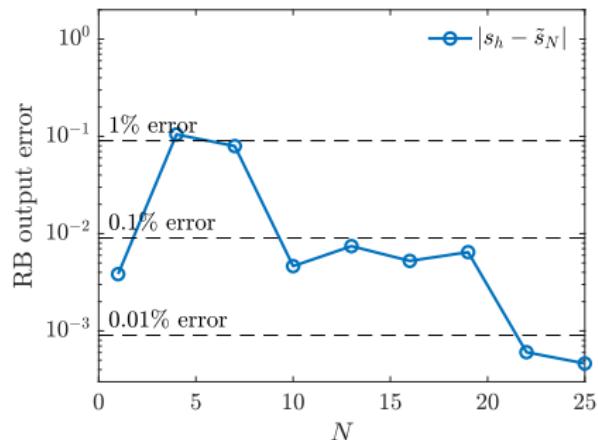
- static adapted mesh s.t. $\mathcal{V}_N \subset \mathcal{V}_h$ is fixed.
- error control on time-averaged (not instantaneous) output

NACA0012 separated flow: RB convergence (*preliminary*)



- Output: rapid convergence with N
EQP: $\text{nnz}\{\rho_\kappa\} \leq 380$ (6%)

NACA0012 separated flow: RB convergence (*preliminary*)



- Output: rapid convergence with N
EQP: $\text{nnz}\{\rho_\kappa\} \leq 380$ (6%)
- Error est.: slower convergence with $N \Leftarrow$ dual not as reducible

Summary

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DG-RB-EQP: goal-oriented ROM for **nonlinear PDEs** based on
DG-FEM + RB + DWR err. est. + EQP hyperreduction
that provides **quantitative** and **automated** output error control:

$$|s - \tilde{s}_N| \leq \underbrace{|s - s_h|}_{\text{FE error}} + \underbrace{|s_h - s_N|}_{\text{RB error}} + \underbrace{|s_N - \tilde{s}_N|}_{\text{EQP error}} \lesssim \delta$$

offline: $\eta_h^{\text{fe}} \lesssim \delta^{\text{fe}}$ online: $\tilde{\eta}_N^{\text{rb}} \lesssim \delta^{\text{rb}}$

with applications in

parameter & design sweep

uncertainty quantification

unsteady flows

