Lecture 2: Error Estimation and Control for Problems with Uncertain Coefficients

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Outline

- Introduction: Adaptive modeling.
- Error estimation for PDEs with uncertain coefficients.
- Adaptive scheme.
- Numerical examples.

"... It is not possible to decide (a) between h or p refinement and (b) whether one should enrich the approximation space $\mathcal{V}^h$ or S^h ... better approaches, yet to be conceived, are consequently needed."

Spectral Methods for Uncertainty Quantification,
Le Maître & Knio 2010

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Introduction

Catenary (linearized) model:

$$\boxed{\begin{aligned} -Tu'' = -\rho g, &\quad \text{in } \Omega = (0,1) \\ u = u_0, &\quad \text{at } x = 0 \\ u = u_1, &\quad \text{at } x = 1 \end{aligned}}$$

This is actually an approximation of the nonlinear catenary model:

$$\boxed{\begin{aligned} -Tu'' = -\sqrt{1+u'^2}\rho g, &\quad \text{in } \Omega = (0,1) \\ u = u_0, &\quad \text{at } x = 0 \\ u = u_1, &\quad \text{at } x = 1 \end{aligned}}$$

The linearized model may provide a poor approximation in the case of large deflections in the chain.

Base Model and Surrogate Model

1. Base model*

Find $u \in U$ s.t.

$$B(u; v) = F(v) \; \forall v \in V$$

- Is believed to capture the events of interest but is intractable.
- Is never "solved"; is only a datum for assessing other models.

2. Quantities of Interest

Given $Q : U \longrightarrow \mathbb{R}$,
find $Q(u)$

3. Surrogate models

Find $u_0 \in U_0$ s.t.

$$B_0(u_0; v) = F_0(v) \; \forall v \in V_0$$

- Must be tractable.
- Ideally captures coarser scales of the phenomena (may involve fine and coarse scale components).

4. Modeling Error

$$\mathcal{E} = Q(u) - Q(\pi u_0)$$

where $\pi : U_0 \longrightarrow U$

Error Representation

$$\boxed{\begin{aligned}\mathcal{E} = Q'(\pi u_0; u - \pi u_0) + \Delta_Q &= B'(\pi u_0; u - \pi u_0, p) + \Delta_Q \\ &= B(u;p) - B(\pi u_0; p) - \Delta_B + \Delta_Q \\ &= \underbrace{F(p) - B(\pi u_0; p)}_{\equiv \mathcal{R}(\pi u_0; p)} + \underbrace{\Delta_Q - \Delta_B}_{\equiv \Delta}\end{aligned}}$$

where “adjoint” problem is defined as:

$$\boxed{\text{Find } p \in V \text{ such that} \quad B'(\pi u_0; v, p) = Q'(\pi u_0; v), \quad \forall v \in V}$$

and

$$\Delta_B = \int_0^1 B''(\pi u_0 + se; e, e, p)(1-s)ds$$

$$\Delta_Q = \int_0^1 Q''(\pi u_0 + se; e, e)(1-s)ds$$

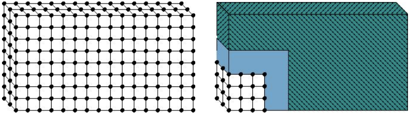
Adaptive Modeling

Adjoint Problem:

$$\boxed{B'(u;v,p) = Q'(u;v), \ \forall\, v \in U}$$

$$B'(u;v,p) = \lim_{\theta\to 0} \frac{B(u+\theta v;p) - B(u;p)}{\theta}$$

$$Q'(u;v) = \lim_{\theta\to 0} \frac{Q(u+\theta v) - Q(u)}{\theta}$$



Base (u) and surrogate models (u_0)

Theorem: If u is a solution of the base model and u_0 an arbitrary member of U, then:

$$\boxed{Q(u) - Q(\pi u_0) = \mathcal{R}(\pi u_0;p) + \Delta}$$

where Δ is a remainder involving terms of $\mathcal{O}(\|u-u_0\|^r), \ r \geq 2$ and

$$\boxed{\mathcal{R}(\pi u_0;p) = F(p) - B(\pi u_0;p)}$$

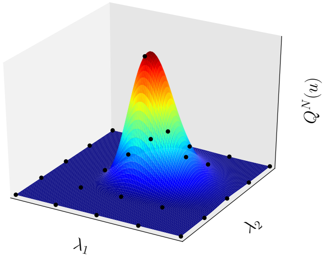
$$\boxed{B'(\pi u_0;v,p) = Q'(\pi u_0;v), \ \forall\, v \in U}$$

Oden, Prudhomme, *J. Comp. Phys.* (2002).
Oden, Prudhomme, Romkes, and Bauman, *SIAM J. Sci. Comput.* (2006).

Extension to UQ Modeling

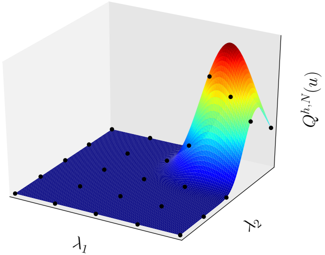
$$\boxed{\underbrace{\mathcal{A}(\lambda; u) = f(\lambda) \quad \to \quad Q(u(\lambda))}_{\mathcal{M}(\lambda)=Q(u)}}$$

$$\boxed{\underbrace{\mathcal{A}_h(\lambda; u_h) = f_h(\lambda) \quad \to \quad Q(u_h(\lambda))}_{\mathcal{M}_h(\lambda)=Q(u_h)}}$$



Surrogate model $\mathcal{M}^N$

$$\mathcal{M} \approx \mathcal{M}^N(\lambda) = Q(u_N)$$



Surrogate model $\mathcal{M}^{h,N}$

$$\mathcal{M}^h \approx \mathcal{M}^{h,N}(\lambda) = Q(u_{h,N})$$

References

Le Maître et al., 2007, 2010

- Polynomial chaos, Stochastic Galerkin, Burger's equation

Almeida and Oden, 2010

- convection-diffusion, sparse grid collocation

Butler, Dawson, and Wildey, 2011

- Stochastic Galerkin, PC representation of the discretization error (ignore truncation error)

Butler, Constantine, and Wildey, 2012

- Ignore physical discretization error, pseudo-spectral projection, improved linear functional

...

Model Problem and Discretization

Model Problem: $\mathcal{A}(\lambda; u) = f(\lambda), \quad \forall x \in D$
Assume: $\lambda = \Lambda(\theta) = \sum_{k \in \mathcal{I}_N} \lambda_k \Psi_k(\boldsymbol{\xi}(\theta))$

Non-intrusive approach ("pseudo-spectral projection method"):

$$u(\boldsymbol{x}, \boldsymbol{\xi}) \approx \sum_{k \in \mathcal{I}_N} u_k(\boldsymbol{x}) \Psi_k(\boldsymbol{\xi}) \approx \sum_{k \in \mathcal{I}_N} u_k^m(\boldsymbol{x}) \Psi_k(\boldsymbol{\xi}) := u^N(\boldsymbol{x}, \boldsymbol{\xi})$$

with

$$u_k(\boldsymbol{x}) = \langle u(\boldsymbol{x}, \cdot), \Psi_k \rangle := \int_\Omega u(\boldsymbol{x}, \boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \, \rho(\boldsymbol{\xi}) \, d\boldsymbol{\xi}$$

$$\approx \sum_{j=1}^{m(N)} u(\boldsymbol{x}, \boldsymbol{\xi}_j) \, \Psi_k(\boldsymbol{\xi}_j) \, w_j := u_k^m(\boldsymbol{x})$$

Pros: fast convergence, sampling-like $u(\boldsymbol{x}, \boldsymbol{\xi}_j)$, choice of $\boldsymbol{\xi}_j$

Model Problem and Discretization

Gaussian quadrature:

- select quadrature rule $\{\boldsymbol{\xi}_j, w_j\}_{j=1}^{m(N)}$ according to ρ_ξ
- integrand $(u^N \Psi_N)$ is at least of order $2N$ in each dimension $m(N) \geq (N+1)^n$

Parameterized discrete solution (the surrogate model):

Solve for $u^h(\boldsymbol{x}, \boldsymbol{\xi}_j) \ \rightarrow u_k^{h,m}(\boldsymbol{x}) = \sum_{j=1}^{m(N)} u^h(\boldsymbol{x}, \boldsymbol{\xi}_j) \ \Psi_k(\boldsymbol{\xi}_j) \ w_j$

$$\boxed{u^{h,N}(\boldsymbol{x}, \boldsymbol{\xi}) = \sum_{k \in \mathcal{I}_N} u_k^{h,m}(\boldsymbol{x}) \Psi_k(\boldsymbol{\xi})}$$

Evaluate:

$$\boxed{Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}\left(u^{h,N}\right)}$$

Goal-oriented error estimation

Weak formulation of $\mathcal{A}(\lambda(\boldsymbol{\xi}); u) = f(\boldsymbol{\xi})$

Find $u(\boldsymbol{\xi}) \in V$ such that $B_{\boldsymbol{\xi}}(u, v) = F_{\boldsymbol{\xi}}(v) \quad \forall v \in V$

Find $u^h(\boldsymbol{\xi}) \in V^h \subset V$ such that $B_{\boldsymbol{\xi}}(u^h, v^h) = F_{\boldsymbol{\xi}}(v^h) \quad \forall v^h \in V^h$

Quantity of interest (QoI):

$$Q_{\boldsymbol{\xi}}(u) = \int_D k(\boldsymbol{x}) u(\boldsymbol{x}, \boldsymbol{\xi}) \, d\boldsymbol{x}$$

Adjoint problem:

Find $p(\cdot, \boldsymbol{\xi}) \in V$ such that $B_{\boldsymbol{\xi}}(v, p) = Q_{\boldsymbol{\xi}}(v) \quad \forall v \in V$

Error representation

$$Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^h) = F_{\boldsymbol{\xi}}(p) - B_{\boldsymbol{\xi}}(u^h, p) := \mathcal{R}_{\boldsymbol{\xi}}(u^h; p)$$

[Note: $Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^h) = \mathcal{R}_{\boldsymbol{\xi}}(u^h; p) + \Delta_B \approx \mathcal{R}_{\boldsymbol{\xi}}(u^h; p)$]

Goal-oriented error estimation

Error estimator:

$$\boxed{Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^h) = \mathcal{R}_{\boldsymbol{\xi}}(u^h; p) \;\approx\; \eta(\boldsymbol{\xi})}$$

Orthogonality property: If $p^h \in V^h$ then $\mathcal{R}_{\boldsymbol{\xi}}(u^h; p^h) = 0$

Higher-order approximation of adjoint solution:

Compute $p^+(\boldsymbol{\xi}) \in V^+$, $V^h \subset V^+ \subset V$ and

$$\eta(\boldsymbol{\xi}) = \mathcal{R}_{\boldsymbol{\xi}}(u^h; p^+)$$

Other choices

- Local interpolation: $\mathcal{R}_{\boldsymbol{\xi}}(u^h; p) \approx \mathcal{R}_{\boldsymbol{\xi}}(u^h; \pi^+ p^h - p^h)$
- Residual based: $\mathcal{R}_{\boldsymbol{\xi}}(u^h; p) = B_{\boldsymbol{\xi}}(e_u, e_p) \approx \sum \eta_u(\boldsymbol{\xi}) \eta_p(\boldsymbol{\xi})$

[1] Becker & Rannacher 2001, Oden & Prudhomme, 2001

Case with Uncertain Parameters

Since $u^{h,N}(\cdot, \boldsymbol{\xi}) \in V^h \subset V$, the adjoint equation still holds

$$B_{\boldsymbol{\xi}}(u^{h,N}, p) = Q_{\boldsymbol{\xi}}(u^{h,N})$$

New error representation:

$$\begin{aligned} Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^{h,N}) \\ &= \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p) \\ &= \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p^{+}) + \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p - p^{+}) \\ &= \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p^{+,N}) + \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p^{+} - p^{+,N}) + \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p - p^{+}) \end{aligned}$$

Total Error Estimate:

$$\boxed{Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^{h,N}) \approx \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p^{+,N})}$$

[1] Butler et al., 2012, Almeida and Oden, 2010

Proposed error decomposition

$$\boxed{Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^{h,N}) = \underbrace{Q_{\boldsymbol{\xi}}(u - u^h)}_{\substack{\text{error due to}\\ \text{physical discretization}}} + \underbrace{Q_{\boldsymbol{\xi}}(u^h - u^{h,N})}_{\substack{\text{error due to approx}\\ \text{in parameter space}}} \quad [+\Delta_{Q_{\boldsymbol{\xi}}}]}$$

Total error:

$$Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^{h,N}) \approx \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p^{+,N}) := \mathcal{E}(\boldsymbol{\xi}) \qquad \begin{cases} 2 \times \text{poly. eval} \\ 1 \times \text{inner product} \end{cases}$$

Physical space discretization error:

$$Q_{\boldsymbol{\xi}}(u) - Q_{\boldsymbol{\xi}}(u^{h}) \approx \mathcal{R}_{\boldsymbol{\xi}}(u^{h}; p^{+}) := \mathcal{E}^D(\boldsymbol{\xi}) \qquad \begin{cases} 2 \times \text{pde solve} \\ 1 \times \text{inner product} \end{cases}$$

Parameter space discretization error:

$$Q_{\boldsymbol{\xi}}(u^h) - Q_{\boldsymbol{\xi}}(u^{h,N}) \approx \mathcal{R}_{\boldsymbol{\xi}}(u^{h,N}; p^{+,N}) - \mathcal{R}_{\boldsymbol{\xi}}(u^{h}; p^{+}) := \mathcal{E}^\Omega(\boldsymbol{\xi})$$

Summary of the procedure

- Solve forward and adjoint problems at quadrature points,

$$\boxed{\begin{array}{c}\left\{u^{h}(\boldsymbol{x},\boldsymbol{\xi}_j)\right\}_{j=1}^{m(N)} \\ \left\{p^{+}(\boldsymbol{x},\boldsymbol{\xi}_j)\right\}_{j=1}^{m(N)}\end{array}} \quad \rightarrow \quad \mathcal{R}_{\boldsymbol{\xi}_j}\left(u^{h};p^{+}\right)$$

- Construct fully discrete solutions and PC expansion for $\mathcal{E}^D$

$$\boxed{\begin{array}{l} u^{h,N}(\boldsymbol{x},\boldsymbol{\xi}) = \sum_{k\in\mathcal{I}_N} u_k^{h,m}(\boldsymbol{x})\Psi_k(\boldsymbol{\xi}) \\ p^{+,N}(\boldsymbol{x},\boldsymbol{\xi}) = \sum_{k\in\mathcal{I}_N} p_k^{+,m}(\boldsymbol{x})\Psi_k(\boldsymbol{\xi})\end{array}} \qquad \mathcal{E}^D(\boldsymbol{\xi}) = \sum_{k\in\mathcal{I}_{\boldsymbol{N}}} e_k^D\Psi_k(\boldsymbol{\xi})$$

- Construct $\mathcal{E}$ and $\mathcal{E}^\Omega$

$$\mathcal{E}(\boldsymbol{\xi}) = \sum_{k\in\mathcal{I}_{\boldsymbol{M}}} e_k\Psi_k(\boldsymbol{\xi}) \qquad \mathcal{E}^\Omega(\boldsymbol{\xi}) = \mathcal{E}(\boldsymbol{\xi}) - \mathcal{E}^D(\boldsymbol{\xi})$$

Adaptivity Strategy

if $\left\|\mathcal{E}^D\right\| > \left\|\mathcal{E}^\Omega\right\|$

  Refine physical approximation space V^h $(h \leftarrow \frac{h}{2})$

else

  Refine random approximation space S^N $(N \leftarrow N+1)$

end

- for a given physical mesh, refine approximation in Ω to the level of physical discretization error
- use error indicator to guide h refinement in parameter space
- anisotropic p-refinement in higher dimensions

Example 1: Smooth response surface in 2D

Convection-diffusion problem in 2D:

$$\boxed{\begin{array}{rl} -\nabla \cdot (2\nabla u) + \begin{bmatrix} 10\sin\left(\frac{\pi}{2}\xi_1\right) \\ 10\cos\left(\pi\xi_2\right) \end{bmatrix} \cdot \nabla u = f(\boldsymbol{\xi}) & \text{in } D = (0,1)^2 \\ u = 0 & \text{on } \partial D \end{array}}$$

Loading f is chosen such that, with ξ_1, $\xi_2 \sim U(0,1)$:

$$\boxed{u(x,y,\boldsymbol{\xi}) = 400\left[\xi_1(x-x^2)e^{-\frac{20}{\xi_1}(x-\xi_1)^2}\right]\left[\xi_2(y-y^2)e^{-\frac{20}{\xi_2}(y-\xi_2)^2}\right]}$$

Quantity of interest:

$$\boxed{Q(u(\cdot,\boldsymbol{\xi})) = \frac{1}{4}\int_{0.5}^{1}\int_{0.5}^{1} u(x,y,\boldsymbol{\xi})\,dxdy \approx \int_D q(x,y)\,u(x,y,\boldsymbol{\xi})\,dxdy}$$

Example 1: Effectivity indices

$\|\mathcal{E}^{\Omega}\|_{L^2_\Omega}$	$\|\mathcal{E}^{D}\|_{L^2_\Omega}$	$\|\mathcal{E}\|_{L^2_\Omega}$	$\frac{\|\mathcal{E}\|_{L^2_\Omega}}{\|Q(u)-Q(u^{h,p,N})\|_{L^2_\Omega}}$
5.12427e-01	3.28574e-03	4.34727e-01	.851
1.79962e-01	3.48349e-03	1.95149e-01	.782
5.23817e-02	6.59002e-03	4.25596e-02	.921
2.30547e-02	3.77558e-03	2.85842e-02	.949
6.17006e-03	5.77325e-03	8.41438e-03	.998
2.21929e-03	4.48790e-03	7.25161e-03	.987
2.20458e-03	**3.98680e-04**	2.80610e-03	.984
7.00606e-04	4.31703e-04	9.24221e-04	.990
3.58282e-04	4.13817e-04	8.06397e-04	1.01
3.58118e-04	1.47612e-04	5.17592e-04	1.03
1.38497e-04	1.49756e-04	2.71081e-04	1.11
8.78811e-05	2.61145e-05	1.06502e-04	1.02
5.10997e-05	2.59334e-05	7.73100e-05	1.00
1.34534e-05	2.59640e-05	3.87553e-05	.985
1.33674e-05	1.22096e-05	2.57607e-05	.981

Example 2: Response surface with discontinuity

Convection-diffusion model in 2D:

$$\boxed{\begin{aligned} -2\Delta u + \begin{bmatrix} \sin(\frac{3\pi}{2}\xi_1) \\ 4\lfloor \xi_2 - \xi_1 \rfloor \end{bmatrix} \cdot \nabla u = f(\boldsymbol{\xi}) \quad & \text{in } D = (0,1)^2 \\ u = 0 \quad & \text{on } \partial D \end{aligned}}$$

Loading f is chosen so that

$$\boxed{u(x, y, \boldsymbol{\xi}) = 10 \sin\left(\frac{3\pi}{2}\xi_1\right)\left(4\lfloor \xi_2 - \xi_1 \rfloor\right) \cdot (x - x^2)(y - y^2)}$$

where

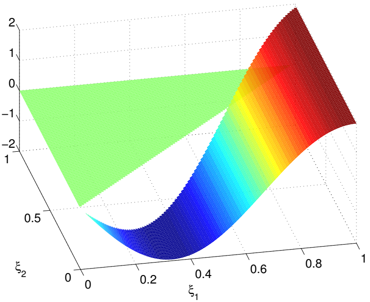
$$\lfloor \xi_2 - \xi_1 \rfloor = \begin{cases} 0 & \xi_1 \leq \xi_2 \\ -1 & \xi_1 > \xi_2 \end{cases}$$

with ξ_1, $\xi_2 \sim U(0, 1)$.

Example 2: Response surface with discontinuity

$$Q(u(\cdot,\boldsymbol{\xi})) = u\left(\frac{1}{3},\frac{1}{3},\boldsymbol{\xi}\right) \approx \int_D q(x,y)\; u(x,y,\boldsymbol{\xi})\; dxdy$$

$$q(x,y) = \frac{100}{\pi}\exp\Big(-100(x-1/3)^2 - 100(y-1/3)^2\Big)$$



True response for QoI over parameter space.

Adaptive scheme:

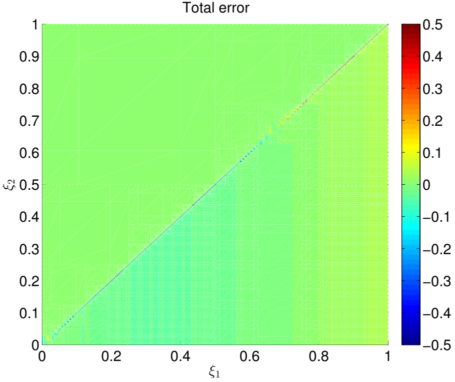
If $\|\mathcal{E}_{\Omega_i}\|_{L^2_{\Omega_i}} > 0.75\ \max_j \left\|\mathcal{E}_{\Omega_j}\right\|_{L^2_{\Omega_j}}$

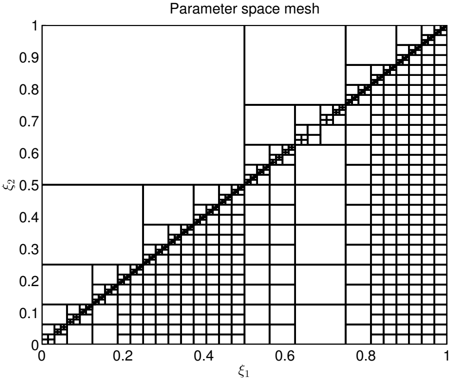
split Ω_i into 2^n new elements by bisection in each stochastic direction

end

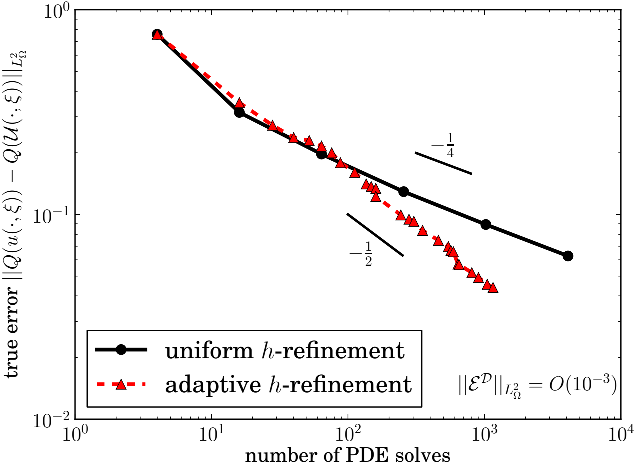
Example 2: Response surface with discontinuity

Adaptive h_Ω refinement





Example 2: Convergence of true error

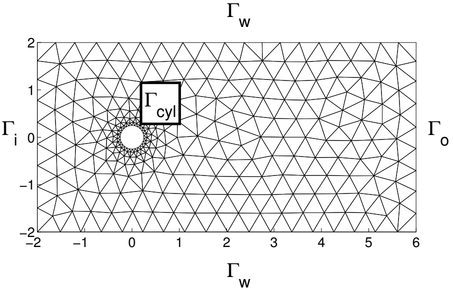


Example 3: Flow at low Reynolds numbers

Navier-Stokes equations:

$$\boxed{\begin{aligned} -\nu\Delta\boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p &= \boldsymbol{0} \\ \nabla\cdot\boldsymbol{u} &= 0 \end{aligned}}$$

$$\begin{aligned} \boldsymbol{u} &= \boldsymbol{u}_{\text{in}}, & \boldsymbol{x} &\in \Gamma_{\text{in}} \\ \boldsymbol{u} &= 0, & \boldsymbol{x} &\in \Gamma_{\text{w}} \cup \Gamma_{\text{cyl}} \\ \boldsymbol{\sigma}\cdot\boldsymbol{n} &= \boldsymbol{0}, & \boldsymbol{x} &\in \Gamma_{\text{o}} \end{aligned}$$



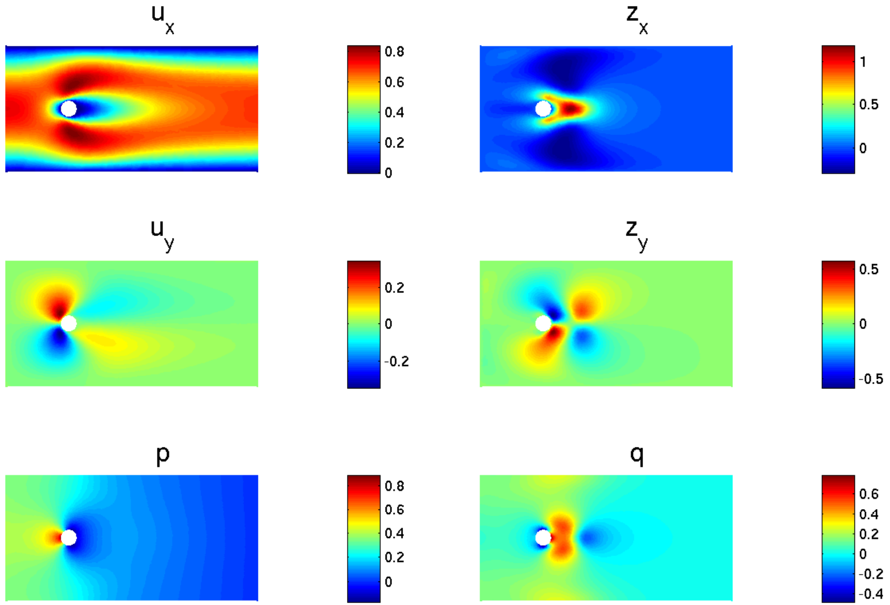
$$\boxed{\text{QoI: } Q_{\boldsymbol{\xi}}(\boldsymbol{u}) = u_x(\boldsymbol{x}_0, \boldsymbol{\xi})}$$

Parameterization of uncertainty:

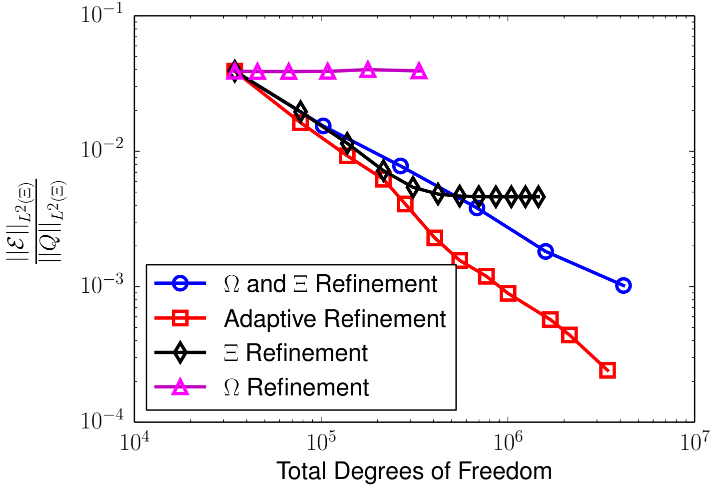
$$\begin{cases} \nu = \xi_1 \\ u_{\text{in},x} = \xi_2 \dfrac{3}{32}(4 - y^2) \end{cases}$$

Let $\xi_1 \sim U(0.01, 0.1)$, $\xi_2 \sim U(1, 3)$

s.t. $\text{Re} = \dfrac{\xi_2}{8\xi_1} \in [1.25, 37.5]$


u_x
0.8
0.6
0.4
0.2
0
z_x
1
0.5
0
u_y
0.2
0
-0.2
z_y
0.5
0
-0.5
p
0.8
0.6
0.4
0.2
0
q
0.6
0.4
0.2
0
-0.2
-0.4

Example 3: Flow at low Reynolds numbers



Statistical quantities of interest (sQoI)

Which features of $Q(u)$ are we interested in?

- Moments:

$$\mathcal{S}(u) = \langle Q(u) \rangle$$
$$\mathcal{S}(u) = \text{Var}\left[Q(u)\right]$$

- Probability of failure:

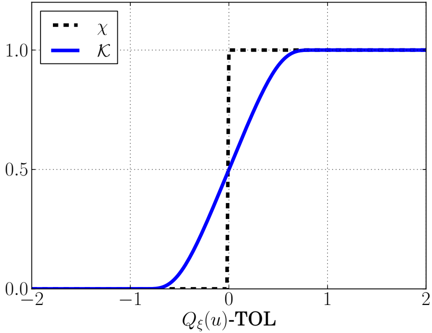
$$\mathcal{S}(u) = P\left[Q(u) > \text{tol}\right] = \int_\Omega \mathbf{1}_{\{Q(u)>\text{tol}\}} \rho(\xi)\, d\xi$$

If $\mathcal{S}$ is nonlinear, e.g. variance

$$\boxed{\mathcal{E}^{\mathcal{S}} = \text{Var}\left[Q(u)\right] - \text{Var}\left[Q(u^{h,N})\right] \neq \text{Var}\left[Q(u) - Q(u^{h,N})\right] \approx \text{Var}\left[\mathcal{E}^{Q}\right]}$$

Statistical quantities of interest (sQoI)

$$\begin{aligned} P\left(\{Q_\xi(u) > \text{tol}\}\right) \\ &= \int_\Omega \chi_{\{Q_\xi(u)>\text{tol}\}}\rho(\xi)d\xi \\ &\approx \int_\Omega \mathcal{K}\left(Q_\xi(u)\right)\rho(\xi)d\xi \\ &:= \mathcal{S}(u) \end{aligned}$$



Concluding remarks and future work

- Error representation for the total error in surrogate models and contributions from each approximation space.
- Development of adaptive refinement strategies based on error decomposition.
- Extension to statistical QoI (sQoI), such as probabilities of failure.