PECOS

Predictive Engineering and Computational Sciences

ERROR DECOMPOSITION AND ADAPTIVE REFINEMENT FOR STOCHASTIC DIFFERENTIAL EQUATIONS

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General model problem

Forward problem:
Strong form:

$$-\nabla\cdot(\boldsymbol{a}(\boldsymbol{\lambda})\nabla u)+\boldsymbol{b}(\boldsymbol{\lambda})\cdot\nabla u=f(\boldsymbol{\lambda}) \quad \text{in } D=(0,1)^2$$
$$u=0 \quad \text{on } \partial D$$

Weak form: find $u(\cdot,\boldsymbol{\lambda})\in V=H_0^1(D)$ such that

$$B(u,v)=F(v) \quad \forall v\in V.$$

Where

$$B(u,v)=\int_D a(\boldsymbol{\lambda})\nabla u\cdot\nabla v\,d\boldsymbol{x}+\int_D \boldsymbol{b}(\boldsymbol{\lambda})\cdot\nabla u\,v\,d\boldsymbol{x},$$
$$F(v)=\int_D f(\boldsymbol{\lambda})\,v\,d\boldsymbol{x},$$

and $\boldsymbol{\lambda}$ represents the uncertain parameters.

Adjoint problem:
Quantity of interest (QoI):

$$Q(u)=\int_D q(\boldsymbol{x})\cdot u(\boldsymbol{x},\boldsymbol{\lambda})\,d\boldsymbol{x}.$$

Weak form: find $\phi\in V$ such that

$$B(v,\phi)=Q(v) \quad \forall v\in V.$$

Error representation:

$$\begin{aligned}Q(u)-Q(u^h)&=B(e,\phi)\\&=F(\phi)-B(u^h,\phi)\\&:=R(u^h;\phi)\end{aligned}$$

Physical discretization and parametrization

Physical discretization
The forward problem is initially discretized using piecewise linear finite elements on a uniform triangulation. The discrete forward problem is: Find $u^h\in V^h$ such that

$$B(u^h,v)=F(v) \quad \forall v\in V^h,$$

The adjoint problem is discretized using piecewise quadratic finite elements on the same triangulation. Find $\phi^+\in V^+$ such that

$$B(v,\phi^+)=Q(v) \quad \forall v\in V^+$$

Parameter space
Pseudospectral projection is used in parameter space. Let $\mathcal{I}_N=\{\boldsymbol{k}\in\mathbb{N}^d : k_1+\cdots+k_d\le N\}$ and let $\mathbb{P}^N$ denote the space of polynomials defined by $\mathbb{P}^N=\text{span}\{\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda}):\boldsymbol{k}\in\mathcal{I}_N\}$. Where $\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda})=\Psi_{k_1}(\lambda_1)\cdots\Psi_{k_d}(\lambda_d)$ and Ψ_{k_i} is the 1D Legendre polynomial of order k_i.
Solutions are expanded in the basis $\Psi_{\boldsymbol{k}}$

$$U(\boldsymbol{x},\boldsymbol{\lambda})=\sum_{\boldsymbol{k}\in\mathcal{I}_N}\underbrace{\left\langle u^h(\boldsymbol{x},\cdot),\Psi_{\boldsymbol{k}}\right\rangle}_{u^h_{\boldsymbol{k}}(\boldsymbol{x})}\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda})$$

where the coefficients, $u^h_{\boldsymbol{k}}$, are computed using quadrature.

Error decomposition

Let $U=\sum_{\boldsymbol{k}\in\mathcal{I}_N}u^h_{\boldsymbol{k}}(\boldsymbol{x})\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda})$ and $\Phi=\sum_{\boldsymbol{k}\in\mathcal{I}_N}\phi^+_{\boldsymbol{k}}(\boldsymbol{x})\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda})$.
For a given vector of parameters $\boldsymbol{\lambda}$

$$\begin{aligned}Q\Big(u(\cdot,\boldsymbol{\lambda})\Big)-Q\Big(U(\cdot,\boldsymbol{\lambda})\Big)&=F\Big(\phi(\cdot,\boldsymbol{\lambda})\Big)-B\Big(U(\cdot,\boldsymbol{\lambda}),\phi(\cdot,\boldsymbol{\lambda})\Big)\\&=R\Big(U(\cdot,\boldsymbol{\lambda}),\phi(\cdot,\boldsymbol{\lambda})\Big)\\&=R\Big(U(\cdot,\boldsymbol{\lambda}),\phi(\cdot,\boldsymbol{\lambda})-\phi^+(\cdot,\boldsymbol{\lambda})\Big)+R\Big(U(\cdot,\boldsymbol{\lambda}),\phi^+(\cdot,\boldsymbol{\lambda})-\Phi(\cdot,\boldsymbol{\lambda})\Big)\\&\quad+R\Big(U(\cdot,\boldsymbol{\lambda}),\Phi(\cdot,\boldsymbol{\lambda})\Big)\\&\approx R\Big(U(\cdot,\boldsymbol{\lambda});\Phi(\cdot,\boldsymbol{\lambda})\Big)\end{aligned}$$

A simple manipulation gives an estimate for the error due to the approximation in each space.

$$R\Big(U(\cdot,\boldsymbol{\lambda});\Phi(\cdot,\boldsymbol{\lambda})\Big)=\underbrace{R\Big(U(\cdot,\boldsymbol{\lambda});\Phi(\cdot,\boldsymbol{\lambda})\Big)-R\Big(u^h(\cdot,\boldsymbol{\lambda});\phi^+(\cdot,\boldsymbol{\lambda})\Big)}_{\text{error due to approx in stochastic space}}+\underbrace{R\Big(u^h(\cdot,\boldsymbol{\lambda});\phi^+(\cdot,\boldsymbol{\lambda})\Big)}_{\text{error due to physical discretization}}$$

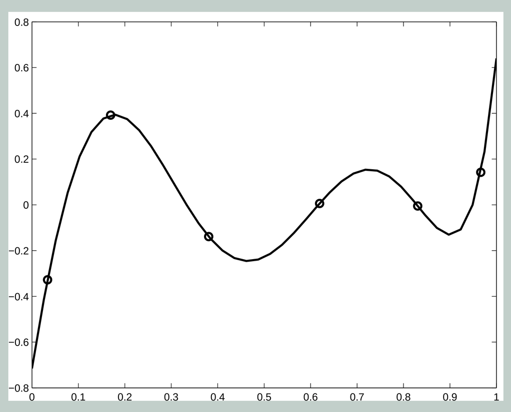
For computational efficiency we form surrogate approximations

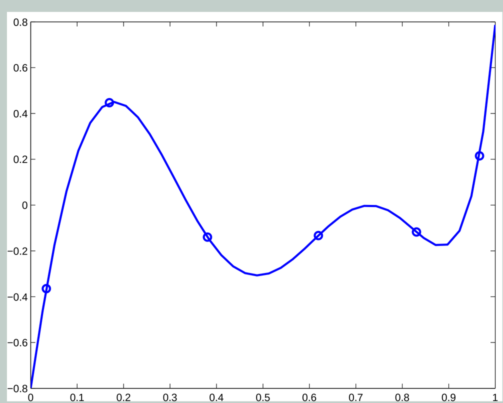
$$\mathcal{E}(\boldsymbol{\lambda})=\sum_{\boldsymbol{k}\in\mathcal{I}_M}\left\langle R\Big(U(\boldsymbol{x},\cdot);\Phi(\boldsymbol{x},\cdot)\Big),\Psi_{\boldsymbol{k}}\right\rangle\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda})$$

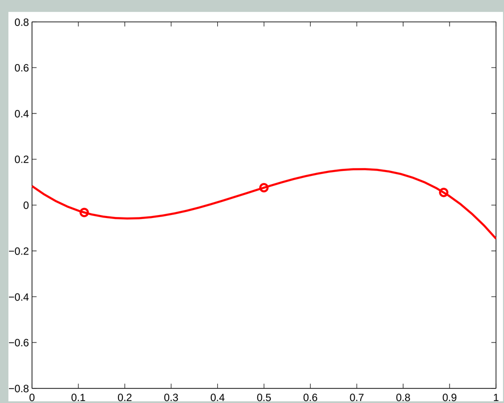
$$\mathcal{E}^{\Omega}(\boldsymbol{\lambda})=\mathcal{E}(\boldsymbol{\lambda})-\mathcal{E}^D(\boldsymbol{\lambda}) \qquad \mathcal{E}^D(\boldsymbol{\lambda})=\sum_{\boldsymbol{k}\in\mathcal{I}_N}\left\langle R\Big(u^h(\boldsymbol{x},\cdot);\phi^+(\boldsymbol{x},\cdot)\Big),\Psi_{\boldsymbol{k}}\right\rangle\Psi_{\boldsymbol{k}}(\boldsymbol{\lambda})$$

and obtain computable error estimates for the error in each space as well as an estimator of the total error in the QoI.

$$\mathcal{E}(\boldsymbol{\lambda})=\mathcal{E}^{\Omega}(\boldsymbol{\lambda})+\mathcal{E}^D(\boldsymbol{\lambda})$$







Adaptive algorithms

Global approximation

Choose N $(M=2N)$, h
while $\|\mathcal{E}\|>$ tol **do**
construct $U,\Phi,\mathcal{E}^D(\boldsymbol{\lambda}),\mathcal{E}(\boldsymbol{\lambda})$
calculate $\|\mathcal{E}-\mathcal{E}^D\|$, and $\|\mathcal{E}^D\|$.
if $\|\mathcal{E}-\mathcal{E}^D\|\le\|\mathcal{E}^D\|$ **then**
refine physical mesh
else
refine polynomial approximation
$(N\leftarrow N+1)$
end if
end while

Piecewise approximation

refine physical mesh

for $\mathcal{E}_i>TOL/|\{\mathcal{E}_i\}|$ **do**
estimate sub element errors
$\{e_j\}_{j=1}^{2^d}$
if $\exists e_j>\alpha_h\mathcal{E}_i^D$ **then**
split element into 2^d elements
refine **dominate** element(s)
else
refine **existing** element's physical mesh
end if
end for

refine polynomial approximation

for $\mathcal{E}_i>TOL/|\{\mathcal{E}_i\}|$ **do**
estimate sub element errors
$\{e_j\}_{j=1}^{2^d}$
if $\exists e_j>\alpha_N\mathcal{E}_i^\Omega$ **then**
split element into 2^d elements
else
for **existing** element $N\leftarrow N+1$
end if
end for

References

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[BDW11] T. Butler, C. Dawson, and T. Wildey.
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SIAM J. Sci. Comput., 33(3):1267–1291, 2011.

[WK05] X. Wan and G.E. Karniadakis.
An adaptive multi-element generalized polynomial chaos method for stochastic differential equations.
J. Comput. Phys., 209(2):617–642, 2005.

Smooth response surface

Let

$$a(\boldsymbol{\lambda})=2 \qquad \boldsymbol{b}(\boldsymbol{\lambda})=\begin{bmatrix}10\sin\left(\frac{\pi}{2}\lambda_1\right)\\10\cos\left(\pi\lambda_2\right)\end{bmatrix}$$

and f be chosen so that

$$u(x,y,\boldsymbol{\lambda})=400\Big[\lambda_1(x-x^2)e^{-\frac{20}{\lambda_1}(x-\lambda_1)^2}\Big]\cdot\Big[\lambda_2(y-y^2)e^{-\frac{20}{\lambda_2}(y-\lambda_2)^2}\Big].$$

For the QoI we define

$$q(x,y)=\Big[1+\tanh[1000(x-0.5)]\Big]\cdot\Big[1+\tanh[1000(y-0.5)]\Big].$$

$$\lambda_1\sim U(0,1) \qquad \lambda_2\sim U(0,1)$$

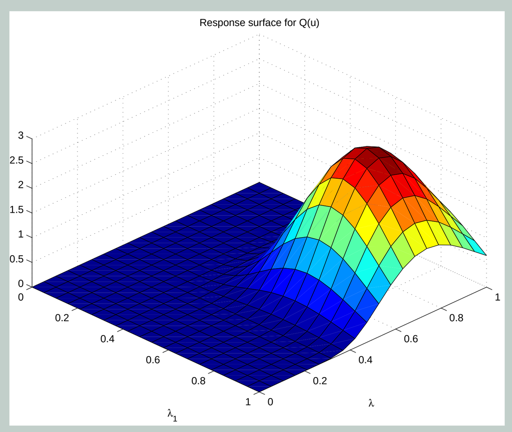


Figure: Exact quantity of interest

	$\left\|\mathcal{E}^{\Omega}\right\|^2_{L^2(\Omega)}$	$\left\|\mathcal{E}^{D}\right\|^2_{L^2(\Omega)}$	$\left\|\mathcal{E}\right\|^2_{L^2(\Omega)}$	$\frac{\|\mathcal{E}\|^2_{L^2(\Omega)}}{\|Q(u)-Q(U)\|^2_{L^2(\Omega)}}$
Global	2.2379e-03	3.7513e-04	2.7582e-03	1.0023
	7.3117e-04	4.6532e-04	9.4083e-04	1.0044
	3.7186e-04	4.1253e-04	8.1932e-04	1.0518
	3.8743e-04	1.1014e-04	4.9064e-04	1.0865
	1.6523e-04	1.1142e-04	2.5706e-04	1.2042
	1.0446e-04	1.1062e-04	2.1730e-04	1.2744
PW	4.0316e-03	4.0316e-03	4.6410e-03	0.9803
	5.8767e-04	5.8767e-04	1.2772e-03	1.0276
	5.9570e-04	5.9570e-04	6.8116e-04	1.0157
	3.0194e-04	3.0194e-04	3.5404e-04	0.9935
	3.9369e-05	3.9369e-05	8.9687e-05	0.9991
	3.9178e-05	3.9178e-05	6.1090e-05	0.9936

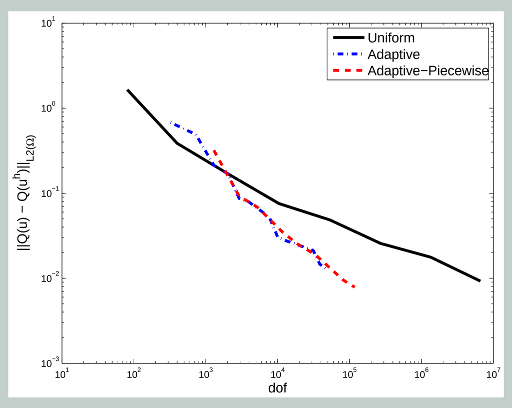


Figure: Convergence of true error

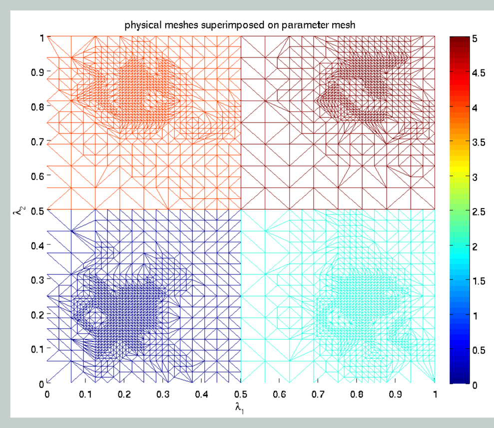


Figure: Physical mesh superimposed on parameter space.

Response surface with a discontinuity

Let

$$a(\boldsymbol{\lambda})=2 \qquad \boldsymbol{b}(\boldsymbol{\lambda})=\begin{bmatrix}\sin(\frac{3\pi}{2}\lambda_1)\\2+4\lfloor\lambda_2-\lambda_1\rfloor\end{bmatrix}$$

For the QoI we define

$$q(x,y)=\frac{100}{\pi}\exp\Big(-100(x-0.33)^2-100(y-0.33)^2\Big)$$

f is chosen so that

$$u(x,y,\boldsymbol{\lambda})=10\sin\Big(\frac{3\pi}{2}\lambda_1\Big)\Big(2+4\lfloor\lambda_2-\lambda_1\rfloor\Big)\cdot(x-x^2)(y-y^2) \qquad \lambda_1,\lambda_2\sim U(0,1)$$

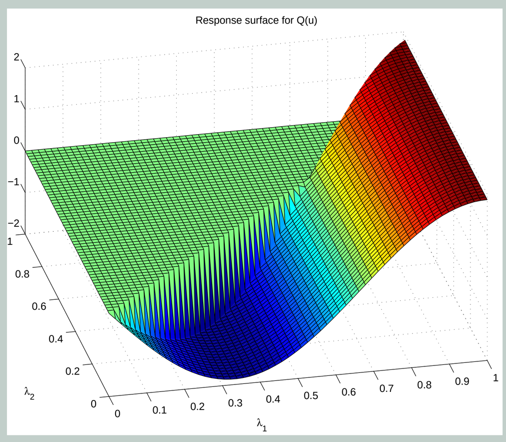


Figure: Exact response surface

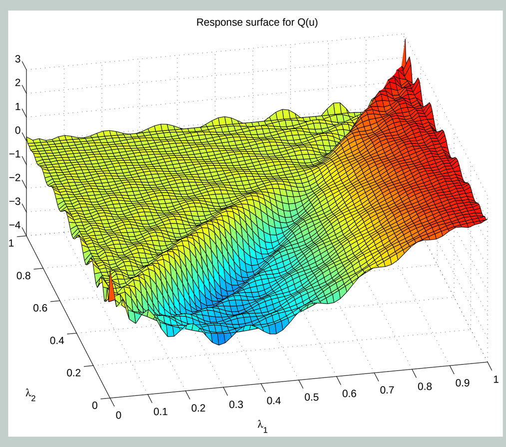


Figure: Response - global algorithm

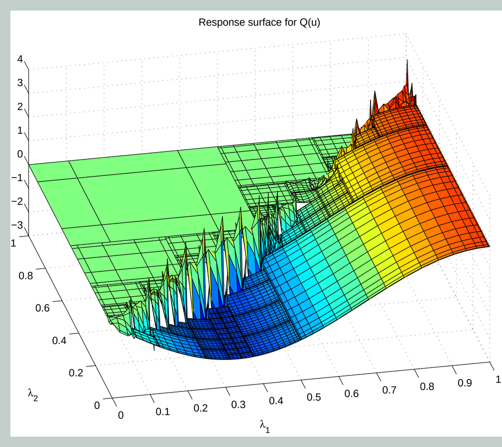
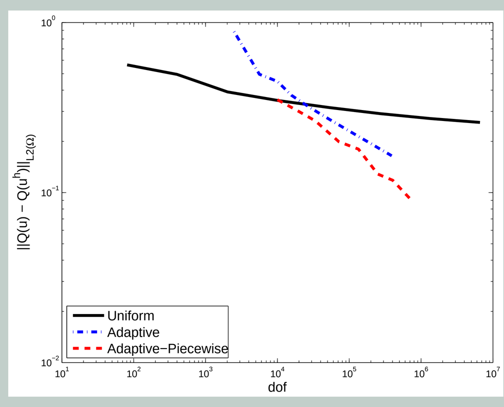


Figure: Response - piecewise

	$\left\|\mathcal{E}^{\Omega}\right\|^2_{L^2(\Omega)}$	$\left\|\mathcal{E}^{D}\right\|^2_{L^2(\Omega)}$	$\left\|\mathcal{E}\right\|^2_{L^2(\Omega)}$	$\frac{\|\mathcal{E}\|^2_{L^2(\Omega)}}{\|Q(u)-Q(U)\|^2_{L^2(\Omega)}}$
Global	4.4533e-02	1.2871e-05	4.4575e-02	0.5321
	3.8879e-02	1.3086e-05	3.8924e-02	0.5236
	3.4536e-02	1.3260e-05	3.4582e-02	0.5170
	3.1087e-02	1.3404e-05	3.1134e-02	0.5118
	2.8276e-02	1.3524e-05	2.8323e-02	0.5076
	2.5940e-02	1.3627e-05	2.5986e-02	0.5041
PW	3.5460e-02	1.3016e-05	3.5442e-02	0.5094
	2.7707e-02	1.3732e-05	2.7708e-02	0.6991
	1.6752e-02	1.4030e-05	1.6766e-02	0.5170
	9.7675e-03	1.4373e-05	9.7873e-03	0.5937
	6.7371e-03	1.4491e-05	6.7576e-03	0.4851
	4.9759e-03	1.4630e-05	4.9945e-03	0.5817



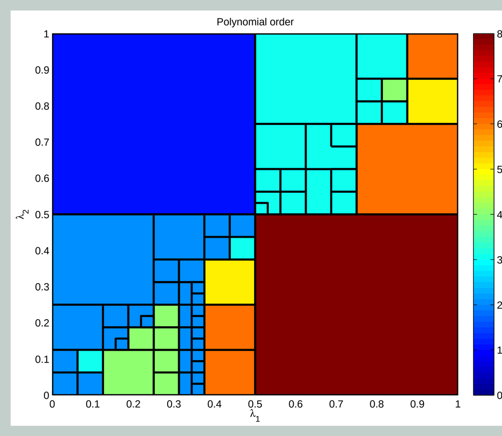
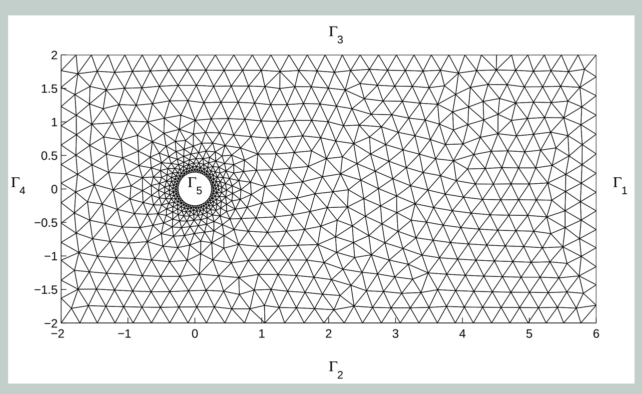
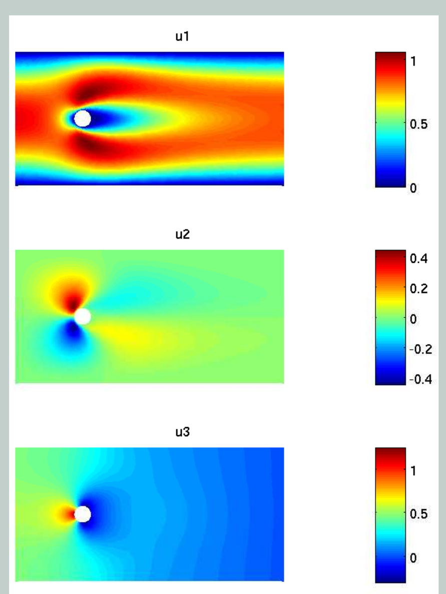
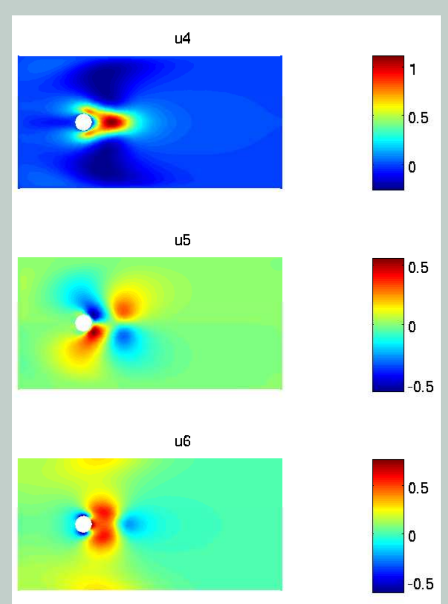


Figure: Parameter space mesh

Navier Stokes flow past a cylinder





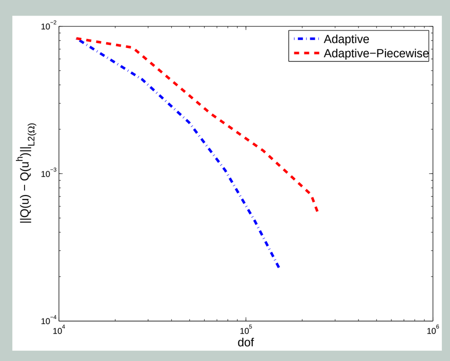


$$\begin{aligned}-\lambda_1\nabla\boldsymbol{u}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}+\nabla p&=\boldsymbol{f}\\\nabla\cdot\boldsymbol{u}&=0\\\boldsymbol{u}(\Gamma_4)&=\begin{bmatrix}\lambda_2\cdot\frac{3}{32}(4-y^2)\\0\end{bmatrix}\\\boldsymbol{u}&=0, \quad \boldsymbol{x}\in\Gamma_2\cup\Gamma_3\cup\Gamma_5\\(\nu\nabla\boldsymbol{u}-p\boldsymbol{I})&=0, \quad \boldsymbol{x}\in\Gamma_1\end{aligned}$$

$$q(\boldsymbol{x})=\begin{bmatrix}\frac{100}{\pi}\exp\Big(-100(x-1)^2-100(y-0)^2\Big)\\0\end{bmatrix}$$

$$\lambda_1\sim U(0.01,0.1) \qquad \lambda_2\sim U(1,4)$$

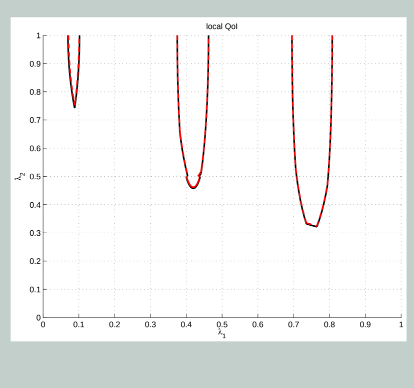
	$\left\|\mathcal{E}^{\Omega}\right\|^2_{L^2(\Omega)}$	$\left\|\mathcal{E}^{D}\right\|^2_{L^2(\Omega)}$	$\left\|\mathcal{E}\right\|^2_{L^2(\Omega)}$
Global	4.8969e-06	1.1054e-08	4.9729e-06
	1.0774e-06	1.1351e-08	1.1082e-06
	2.1222e-07	1.1170e-08	2.2771e-07
	3.8686e-08	1.0974e-08	5.0287e-08
PW	6.4097e-06	1.1083e-08	6.4647e-06
	2.0061e-06	1.0825e-08	2.0454e-06
	4.9921e-07	1.1004e-08	5.1946e-07
	2.6232e-07	1.0852e-08	2.7677e-07



Conclusions and future work

- proposed decomposition successfully quantifies error from each space
- the ability to adapt physical meshes to different regions of parameter space allows computational resources to be used more efficiently
- if a fixed physical mesh is used the decomposition provides a computable threshold for minimum obtainable error

⇒ apply a similar technique to intrusive methods such as stochastic Galerkin
⇒ apply to probabilistic quantities of interest (exceedance probabilities and the determination of the limit state surface)



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