

Adaptive in Time Approximation of Parametric Parabolic PDEs

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Motivation

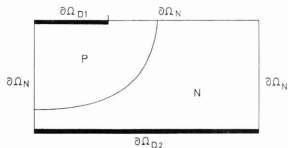


Fig. 3.1.1 P-N diode

Markowich, Ringhofer, and Schmeiser
1990

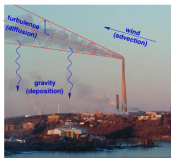


Fig. 1.1 A photograph of emissions from the Peace Superstack (in Sudbury, ON, Canada) that illustrates the three main contributions to atmospheric contaminant transport: advection from the wind, diffusion from turbulent eddy motion, and deposition owing to gravitational settling.

Stockie 2011

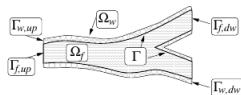


FIG. 2.1. Computational domain representing a 2D section of a vascular district featuring the lumen Ω_f and the wall Ω_w .

Quarteroni, Veneziani, and Zunino 2002

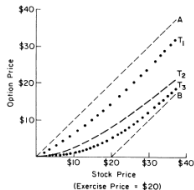


FIG. 1.—The relation between option value and stock price

Black and Scholes 1973

Problem statement

Approximate solution of

$$\frac{\partial u(\mathbf{x}, t, \mathbf{y})}{\partial t} + A(\mathbf{x}, \mathbf{y})u(\mathbf{x}, t, \mathbf{y}) = 0 \quad \rho\text{-a.s. in } \Gamma$$

(+ initial and boundary conditions) for elliptic differential operator $A(\mathbf{x}, \mathbf{y})$ with $\mathbf{y} \in \Gamma \subset \mathbb{R}^d$.

$$u^{h,l,\delta}(\mathbf{x}, t, \mathbf{y}) := \sum_{\mathbf{z} \in \mathcal{Z}^l} u^{h,\delta}(\mathbf{x}, t; \mathbf{z}) L_{\mathbf{z}}^l(\mathbf{y})$$

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Construct an approximation for use in

- ▷ Forward, Inverse Uncertainty Quantification
- ▷ Sensitivity Analysis
- ▷ Optimal Control ...

Problem Discretisation (I)

1 Spatial discretisation: Galerkin FEM

$$\frac{d}{dt} \mathbf{u}^h(t, \mathbf{y}) + A^h(\mathbf{y}) \mathbf{u}^h(t, \mathbf{y}) = \mathbf{f}^h(t, \mathbf{y})$$

¹Smolyak. 1963; Barthelmann, Novak, and Ritter. 2000; Babuška, Nobile, and Tempone. 2007.

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2 **Parametric discretisation:** Sparse Grid Interpolation¹

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2 Parametric discretisation: Sparse Grid Interpolation¹

For multi-index set $l = \{\underline{\alpha}_1, \underline{\alpha}_2, \dots\}$

$$\begin{aligned} u^{h,l}(\mathbf{x}, t, \mathbf{y}) &:= \mathcal{I}^l[u^h(\mathbf{x}, t, \mathbf{y})] \\ &= \sum_{\underline{\alpha} \in l} \bigotimes_{i=1}^d \Delta^{\alpha_i} [u^h(\mathbf{x}, t, \mathbf{y})] \\ &= \sum_{\mathbf{z} \in \mathcal{Z}^l} u^h(\mathbf{x}, t; \mathbf{z}) L_{\mathbf{z}}^l(\mathbf{y}) \end{aligned}$$

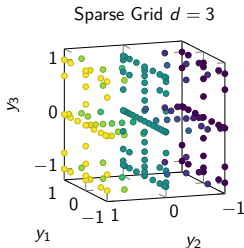
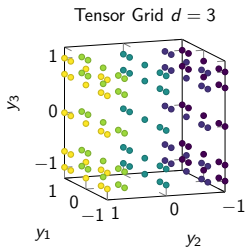
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2 Parametric discretisation: Sparse Grid Interpolation¹



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Problem Discretisation (II)

3 **ADAPTIVE** Timestepping: Implicit method with **local** error control.²

- ▷ Selects time steps $\Delta t_1, \Delta t_2, \Delta t_3, \dots$ such that

$$\|\mathbf{u}^h(t + \Delta t_k, \mathbf{z}; \mathbf{u}_k^{h,\delta}) - \mathbf{u}_{k+1}^{h,\delta}(\mathbf{z}; \mathbf{u}_k^{h,\delta})\|_{L^2(D)} \leq \delta$$

where $\mathbf{u}_k^{h,\delta} \approx \mathbf{u}^h(t_k)$.

- ▷ Extend to continuous time $u^{h,\delta}(\mathbf{x}, t; \mathbf{z}) \approx u^h(\mathbf{x}, t; \mathbf{z})$.

²Gresho, Griffiths, and Silvester. 2008.

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- ▷ Extend to continuous time $u^{h,\delta}(\mathbf{x}, t; \mathbf{z}) \approx u^h(\mathbf{x}, t; \mathbf{z})$.

▷ **Final approximation:**

$$u^{h,l,\delta}(\mathbf{x}, t, \mathbf{y}) := \sum_{\mathbf{z} \in \mathcal{Z}^l} u^{h,\delta}(\mathbf{x}, t; \mathbf{z}) L_{\mathbf{z}}^l(\mathbf{y})$$

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Toy Example

Consider³ $u : D \times [0, T] \times \Gamma \rightarrow \mathbb{R}$ such that ρ -a.s.

$$\frac{\partial u(\mathbf{x}, t, \mathbf{y})}{\partial t} - \epsilon \nabla^2 u(\mathbf{x}, t, \mathbf{y}) + \mathbf{w}(\mathbf{x}, \mathbf{y}) \cdot \nabla u(\mathbf{x}, t, \mathbf{y}) = 0$$

$$\Gamma = [-1, 1]^d \subset \mathbb{R}^d. \quad \nabla \cdot \mathbf{w} \equiv 0, \quad \epsilon = 0.1.$$

³Elman, Silvester, and Wathen. 2014.

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▷ Wind field

$$\mathbf{w}(\mathbf{x}, \mathbf{y}) := \mathbf{w}_0(\mathbf{x}) + \sum_{i=1}^d \lambda_i y_i \mathbf{w}_i(\mathbf{x}).$$

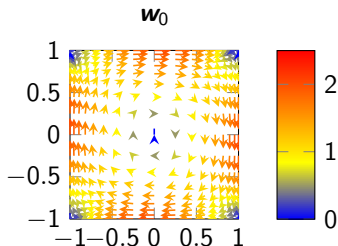
▷ Hot wall BC

$$u(\mathbf{x}, t, \mathbf{y}) = (1 - x_2^4) (1 - \exp(-t/\tau))$$

for $x_1 = 1$, zero elsewhere.

▷ Initial Condition

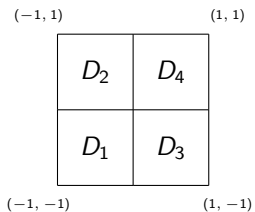
$$u(\mathbf{x}, 0, \mathbf{y}) = 0 \text{ for all } (\mathbf{x}, \mathbf{y}) \in D \times \Gamma.$$



³Elman, Silvester, and Wathen. 2014.

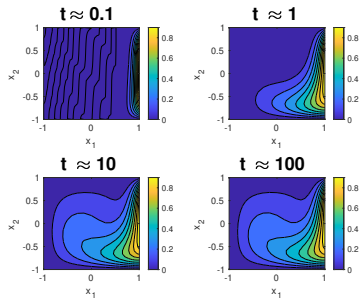
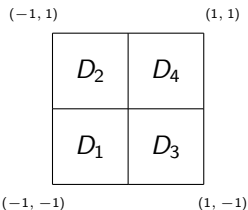
Toy Example: $d = 4$

- ▷ $\mathbf{w}_i(\mathbf{x}) := \mathbf{w}_0(2(x_1 - a_i), 2(x_2 - b_i))$ for $\mathbf{x} \in D_i$,
- ▷ $\mathbf{w}_i(\mathbf{x}) = 0$ otherwise,
- ▷ $\lambda_i = 0.5$ for $i = 1, 2, 3, 4$.

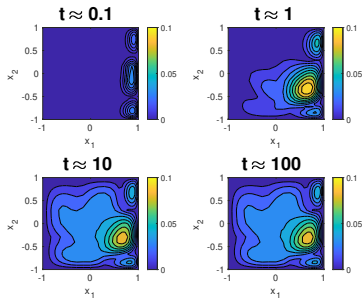


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- ▷ $\mathbf{w}_i(\mathbf{x}) = 0$ otherwise,
- ▷ $\lambda_i = 0.5$ for $i = 1, 2, 3, 4$.
- ▷ $I = \{\|\underline{\alpha}\|_1 \leq 4 + 5\}$, $\delta = 10^{-8}$.



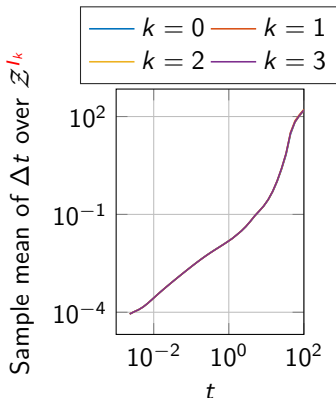
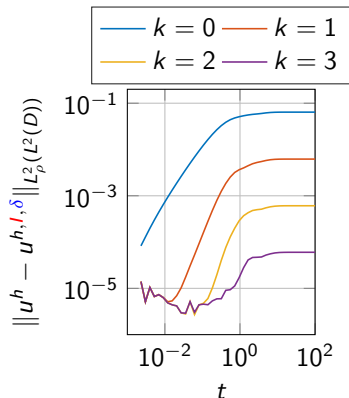
$\mathbb{E}[u^{h,I,\delta}(\mathbf{x}, t, \cdot)]$ for $t \approx 0.1, 1, 10, 100$



$\text{stddev}[u^{h,I,\delta}(\mathbf{x}, t, \cdot)]$ for $t \approx 0.1, 1, 10, 100$

Approximation Error and Timestep Evolution

Approximation of u^h with Smolyak grids with $I_k = \{\|\alpha\|_1 \leq d + k\}$ and timestepping LE tolerance $\delta = \mathcal{O}(10^{-8})$ (GE tol $\mathcal{O}(10^{-5})$).



Small t | **LoFi** parameter approximation
Large t | **HiFi** parameter approximation

HiFi time-stepping
LoFi time-stepping

Error Estimation (I)

Consider error as function of time $e(t) := \|u(\cdot, t, \cdot) - u^{h,I,\delta}(\cdot, t, \cdot)\|_{L^2_\rho(L^2(D))}$

$$e = \underbrace{\|u - u^h\|}_{\text{spatial}} + \underbrace{\|u^h - u^{h,I}\|}_{\text{interpolation}} + \underbrace{\|u^{h,I} - u^{h,I,\delta}\|}_{\text{timestepping}} \|_{L^2_\rho(L^2(D))}$$

Error Estimation (II)

- ▷ **Interpolation Error:** Choose $\mathcal{I}^{I^*} := \mathcal{I}^{I \cup \mathcal{R}_I}$. **Saturation assumption** results in constant C such that

$$\|u^h - u^{h,I}\|_{L^2_\rho(L^2(D))} \leq C \|u^{h,I^*} - u^{h,I}\|_{L^2_\rho(L^2(D))}$$

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- ▷ Split as

$$\pi_{\text{interp}}(t) \leq \sum_{\underline{\alpha} \in \mathcal{R}_I} \left\| \bigotimes_{j=1}^d \Delta^{\alpha_j} [u^{h,\delta}(\cdot, t; \mathbf{y})] \right\|_{L^2_\rho(L^2(D))} = \sum_{\underline{\alpha} \in \mathcal{R}_I} \pi_{\text{interp},\underline{\alpha}}(t)$$

Error Estimation (III)

▷ **Timestepping Error:**

$$\|u^{h,I} - u^{h,I,\delta}\|_{L^2_\rho(L^2(D))} \leq \sum_{\mathbf{z} \in \mathcal{Z}^I} \underbrace{\|e^\delta(\cdot, t; \mathbf{z})\|_{L^2(D)}}_{\text{Global timestepping error}} \|L^I_{\mathbf{z}}(\mathbf{y})\|_{L^2_\rho(\Gamma)} =: \pi_{ts}(t).$$

⁴Skeel. 1986.

⁵Shampine. 1994.

Error Estimation (III)

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- ▷ Need strategy to compute an estimate $\pi_{ge}(t; \mathbf{z}) \approx \|e^\delta(\cdot, t; \mathbf{z})\|_{L^2(D)}$.
- ▷ Use two different **local error** tolerances⁴ and scaling argument⁵

$$\pi_{ge}(t) = \left(\frac{\delta}{\delta_0}\right)^{p/p+1} \pi_{ge}^{\delta_0}(t).$$

- ▷ Using π_{ge} , we have a computable bound

$$\pi := \pi_{\text{interp}} + \pi_{\text{corr}} + \pi_{ts}.$$

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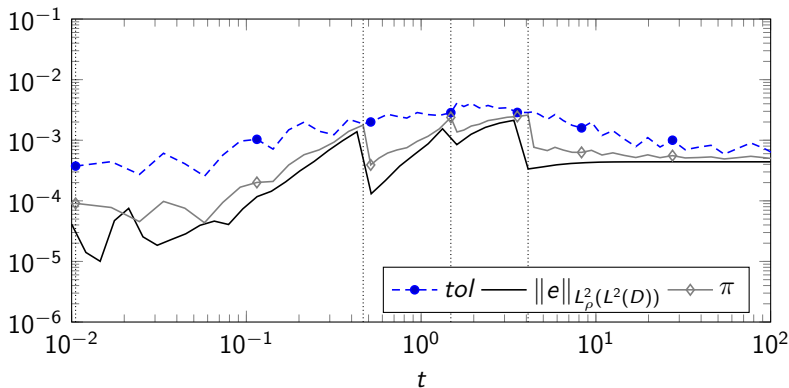
Adaptive SC Algorithm

... \rightarrow SOLVE \rightarrow ESTIMATE \rightarrow MARK \rightarrow REFINE \rightarrow ...

- 1 Initialise time $t = 0$, $\mathcal{Z} = \{\mathbf{0}\}$.
- 2 Solve linear systems associated with each collocation point $\mathbf{z} \in \mathcal{Z}^*$ to time $t + \Delta t$.
- 3 Estimate π_{interp} , π_{corr} , π_{ts} , $\{\pi_{\text{interp}, \underline{\alpha}}\}_{\underline{\alpha} \in \mathcal{R}_I}$
- 4a If $\pi_{\text{interp}} \geq \text{tol} \propto \pi_{\text{corr}}$, then mark $\mathcal{J} \subset \mathcal{R}_I$ and refine I .
- 4b Else accept timestep $t \leftarrow t + \Delta t$.
- 5 Return to step 2 and repeat until $t = T$.

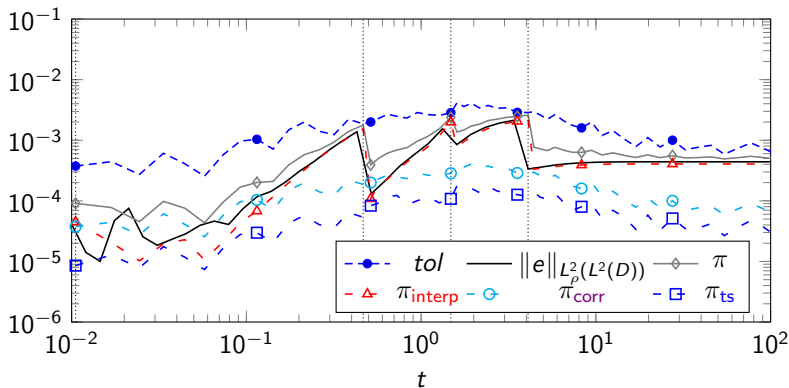
Adaptive Approximation $d = 4$

$\pi, \pi^{\text{interp}}, \pi^{\text{corr}}, \pi^{\text{ts}}$ for the parametric $d = 4$ double glazing problem
(vertical dotted lines denote parametric refinement)



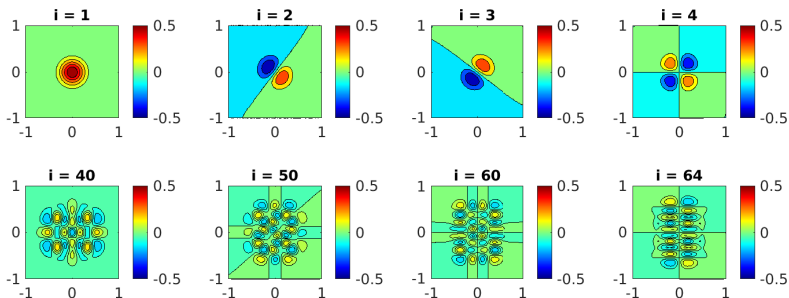
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Extension to higher dimensions ($d = 64$)

$$w(\mathbf{x}, \mathbf{y}) := w_0(\mathbf{x}) + \sum_{i=1}^{64} (\nabla \times \phi_i(\mathbf{x})) y_i$$

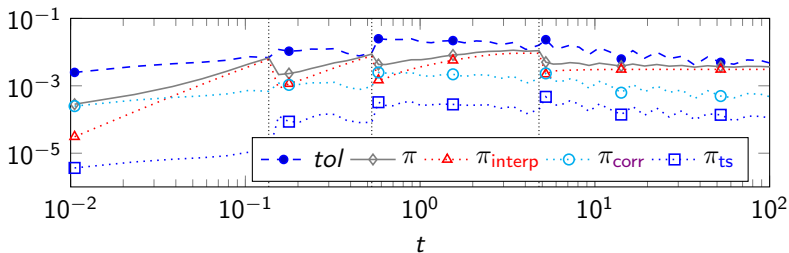


Stream functions of perturbations

Numerical Results ($d = 64$)

Benjamin M. Kent et al. (2022). *Efficient Adaptive Stochastic Collocation Strategies for Advection-Diffusion Problems with Uncertain Inputs*. URL: <https://arxiv.org/abs/2210.03389>

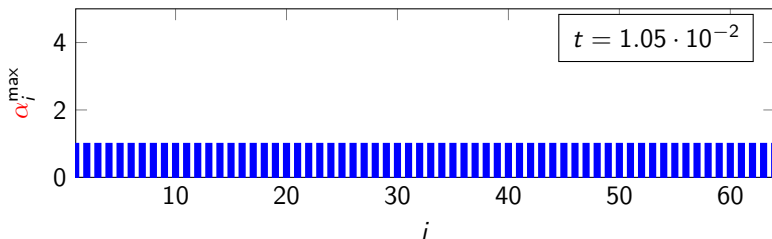
$\pi, \pi^{\text{interp}}, \pi^{\text{corr}}, \pi^{\text{ts}}$ for the parametric $d = 64$ double glazing problem



Numerical Results ($d = 64$)

Benjamin M. Kent et al. (2022). *Efficient Adaptive Stochastic Collocation Strategies for Advection-Diffusion Problems with Uncertain Inputs*. URL: <https://arxiv.org/abs/2210.03389>

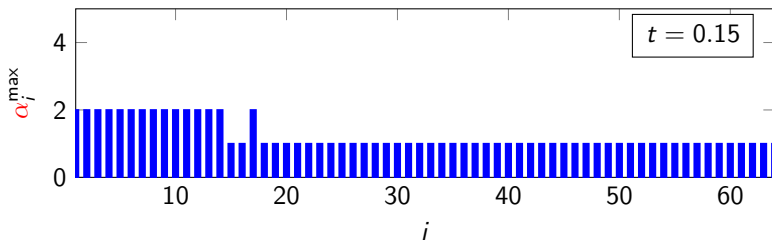
Maximum interpolant level $\alpha_i^{\max} := \max_{\underline{\alpha} \in I} \alpha_i$ for each parameter dimension i at snapshots in time



Numerical Results ($d = 64$)

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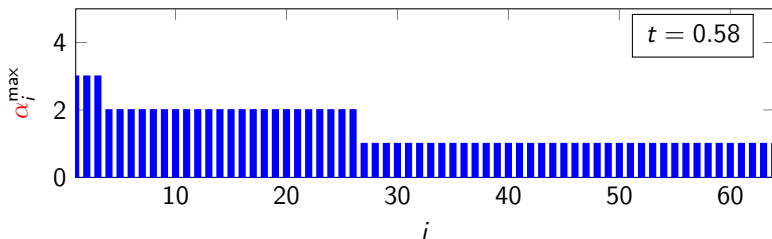
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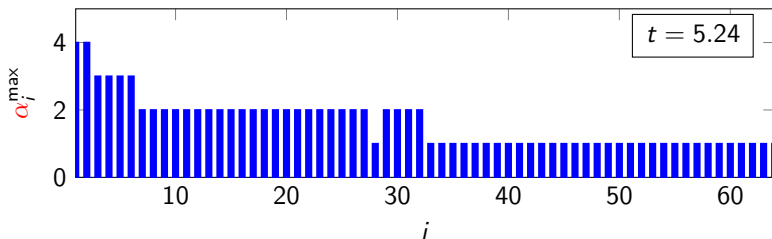
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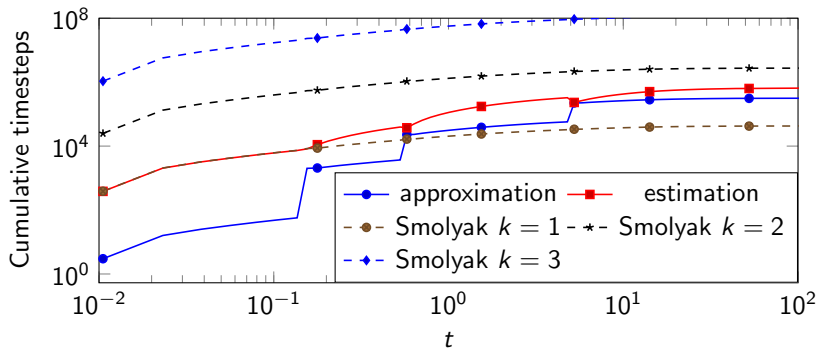
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Computational cost (total number of timesteps)











Numerical Results ($d = 64$)

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Adaptive approximation for parametric problems is **ESSENTIAL!**

-  Babuška, Ivo, Fabio Nobile, and Raúl Tempone (2007). “A Stochastic Collocation Method for Elliptic Partial Differential Equations with Random Input Data”. In: *SIAM Journal on Numerical Analysis* 45.3, pp. 1005–1034. DOI: 10.1137/050645142. eprint: <https://doi.org/10.1137/050645142>. URL: <https://doi.org/10.1137/050645142>.
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-  Black, Fischer and Myron Scholes (1973). “The pricing of options and corporate liabilities”. In: *Journal of political economy* 81.3, pp. 637–654.
-  Elman, Howard, David J. Silvester, and Andy Wathen (2014). *Finite Elements and Fast Iterative Solvers: with Applications in Incompressible Fluid Dynamics*. Second. Oxford, UK: Oxford University Press. ISBN: 9780191523786. DOI: 10.1093/acprof:oso/9780199678792.001.0001.

-  Gresho, Philip M., David F. Griffiths, and David J. Silvester (2008). “Adaptive Time-Stepping for Incompressible Flow Part I: Scalar Advection-Diffusion”. In: *SIAM Journal on Scientific Computing* 30.4, pp. 2018–2054. DOI: [10.1137/070688018](https://doi.org/10.1137/070688018).
-  Kent, Benjamin M. et al. (2022). *Efficient Adaptive Stochastic Collocation Strategies for Advection-Diffusion Problems with Uncertain Inputs*. URL: <https://arxiv.org/abs/2210.03389>.
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-  Shampine, Lawrence F. (1994). *Numerical solution of ordinary differential equations*. English. Chapman & Hall mathematics. New York, NY; London: Chapman & Hall. ISBN: ISBN: 0412051516.

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Stream function based expansion $d = 64$

- ▷ Use $\mathbf{w}(\mathbf{x}, \mathbf{y}) = \nabla \times \psi(\mathbf{x}, \mathbf{y})$ for $\psi(\mathbf{x}, \mathbf{y}) = \psi_0(\mathbf{x}) + \sum_{i=1}^d \sqrt{\lambda_i} \psi_i(\mathbf{x}) y_i$.
- ▷ $\mathbf{w}_0 = \nabla \times (-(1 - x_1^2)(1 - x_2^2))$
- ▷ Approximate eigenpairs (λ_i, ψ_i) of $C(\mathbf{x}_1, \mathbf{x}_2) = \prod_{i,j=1}^2 (1 - x_{i,j}^2) \sigma_0^2 \exp\left(-\frac{\|\mathbf{x}_1 - \mathbf{x}_2\|_2^2}{L}\right)$
- ▷ Choose $\sigma_0^2 = 5$, $L = 1$, $d = 64$.

$\pi, \pi_{\text{interp}}, \pi_{\text{corr}}, \pi_{\text{ts}}$ for the parametric $d = 64$ double glazing problem

