

On the quantification of discretization uncertainty: comparison of two paradigms

Julien Bect^{1,*}, Souleymane Zio¹, Guillaume Perrin²,
Claire Cannamela² and Emmanuel Vazquez¹

¹ Université Paris-Saclay, CNRS, CentraleSupélec,
Laboratoire des signaux et systèmes, 91190, Gif-sur-Yvette, France.

² Commissariat à l'énergie atomique et aux énergies alternatives (CEA),
CEA/DAM/DIF, 91297, Arpajon, France.

* Corresponding/presenting author. E-mail: julien.bect@centralesupelec.fr

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- 2 The GCI (Grid Convergence Index) approach
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Computer models, discretization & UQ

mesh size

$$h > 0$$



Qol

$$z \in \mathbb{R}$$

- Consider a **PDE-based computer model**
 - mesh size $h > 0$
 - quantity of interest (Qol) $z = f(h)$
 - h and z assumed scalar for simplicity
- Ideally, we would like to know $f(0)$
(assuming a convergent numerical scheme)

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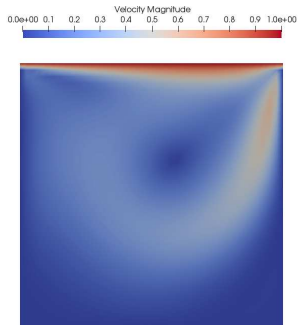
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 - mesh size $h > 0$
 - quantity of interest (QoI) $z = f(h)$
 - h and z assumed scalar for simplicity
- Ideally, we would like to know $f(0)$
(assuming a convergent numerical scheme)
- Since $f(0)$ cannot be computed, we have:

Problem

What is our **uncertainty** about $f(0)$ given a set of computation results $f(h_1), \dots, f(h_n)$?

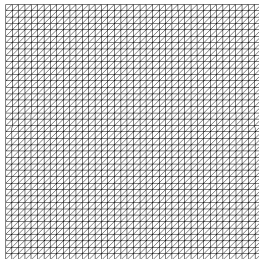
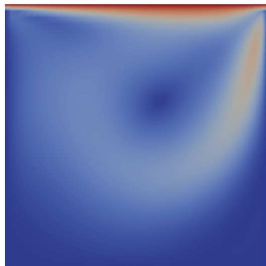
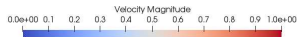
Example: lid-driven cavity problem

A classical CFD test case: **incompressible fluid** in a **rectangular cavity** ($L \times H$)
w/ horizontal velocity $u_x = 1$ imposed at the top (lid).



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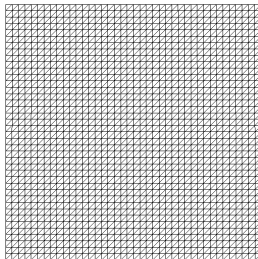
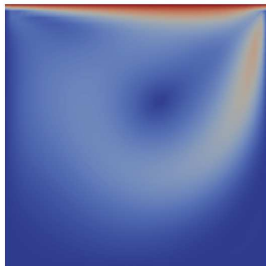
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Regular triangular grid with **mesh size $h > 0$** . Solved w/ Fenics ([Alnæs et al., 2015](#)).

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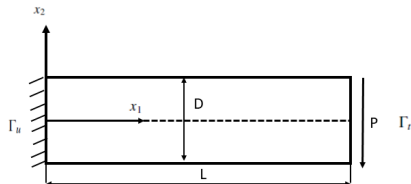


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Qol: velocity (u_x, u_y) at the center & minimum ψ of the stream function.

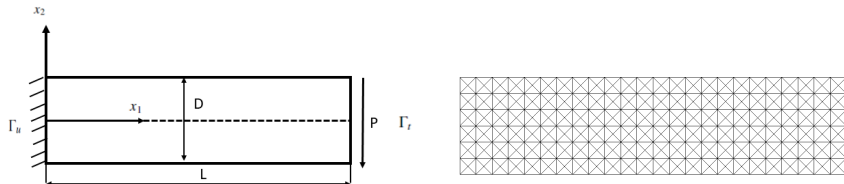
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Another classical case: quasistatic deformation of a rectangular cantilever beam w/ prescribed pressure field at the free end.



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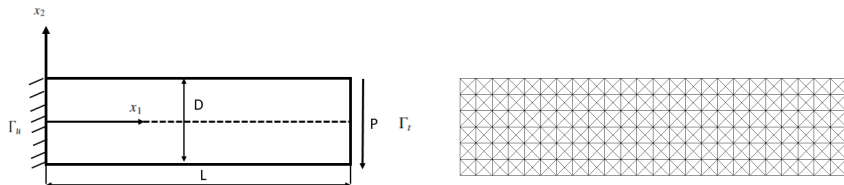
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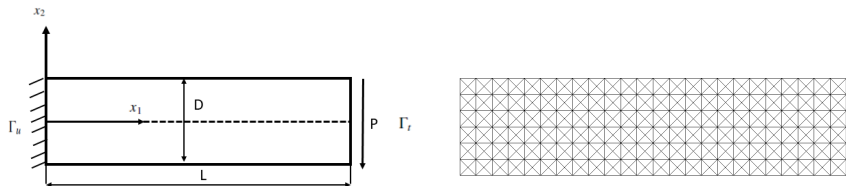


Again: regular triangular grid with mesh size $h > 0$. Solved w/ Fénics.

Qol: vertical displacement at $x_1 = 10$, $x_2 = 20$, $x_3 = 30$ and $x_4 = L = 48$.

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QoI: vertical displacement at $x_1 = 10$, $x_2 = 20$, $x_3 = 30$ and $x_4 = L = 48$.

Remark: **analytical solution** available for some particular boundary conditions

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From Richardson's extrapolation to the GCI

⇒ **Assume** that the QoI satisfies, for some $f_0, A \in \mathbb{R}$ and $p > 0$,

$$f(h) = f_0 + Ah^p + o(h^p) \quad \text{when } h \rightarrow 0.$$

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⇒ Given a triplet¹ of **solutions at mesh sizes** $h_1 < h_2 < h_3$, solve

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for f_0 , A and p .

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for f_0 , A and p . Denoting by \hat{f}_0 , \hat{A} and \hat{p} the solution:

$$f(h) \approx \hat{f}(h) = \hat{f}_0 + \hat{A}h^{\hat{p}}.$$

⇒ **Richardson extrapolation** (Richardson and Gaunt, 1927): $f(0) \approx \hat{f}_0$.

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From Richardson's extrapolation to the GCI (cont'd)

- The (fine grid) **GCI “uncertainty band”** (Roache, 1994, 1997, 1998) is:

$$UB_{GCI} = [f(h_1) - \Delta; f(h_1) + \Delta]$$

From Richardson's extrapolation to the GCI (cont'd)

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where Δ is derived from Richardson's extrapolated value:

$$\Delta = F_s \cdot \left| \hat{f}_0 - f(h_1) \right|$$

with $F_s \geq 1$ a **safety factor**.

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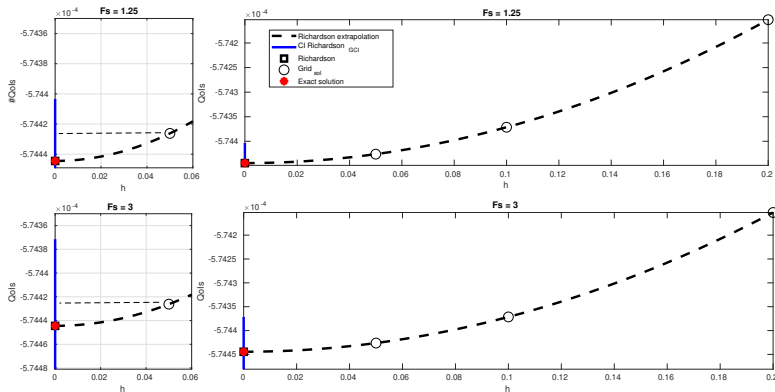
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☞ Roache recommends

- $F_s = 3$ in general (p unknown, or only two solutions used),
- $F_s = 1.25$ when p is known and $\hat{p} \approx p$.

An illustration of the GCI method



☞ Data from the Timoshenko beam problem

- QoI: vertical displacement of the beam, measured at $x = 10m$.
- Mesh sizes: $h_1 = 1/20$, $h_2 = 1/10$, and $h_3 = 1/5$.
- The GCI interval is represented for $F_s = 1.25$ (top) and $F_s = 3$ (bottom).

Some remarks on the GCI method

☞ Now a **standard tool** in VVUQ

- See, e.g., [Oberkampf and Roy \(2010\)](#), chapter 8.
- Lots of variants in the literature: choice of F_s , of \hat{p} , etc.

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✘ Does not stem from a well-founded theory of UQ

- in particular, it is **not associated with a “well-founded probability statement on the error”** ([Roache, 1994](#))

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Gaussian process emulators for computer models

Statistical inference for deterministic computer models?

☞ **Bayesian** approach (Sacks et al., 1989; Currin et al., 1991, ...)

- **prior** information about $f \rightsquigarrow$ stochastic process (prior) model
- data + Bayes theorem \rightsquigarrow **posterior** distribution

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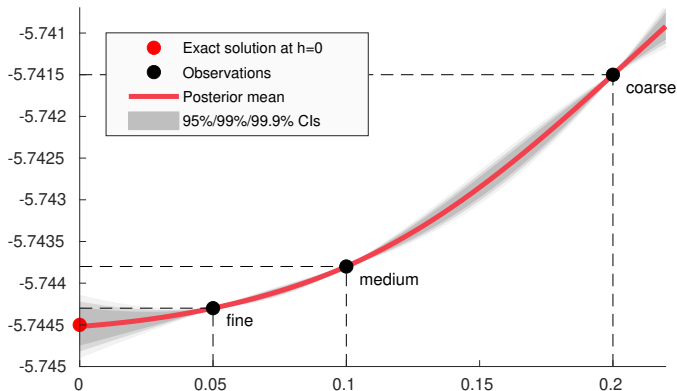
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☞ Gaussian process (GP) priors

- Commonly used for tractability, since
GP prior \Rightarrow GP posterior (a.k.a. GP “emulator”)
- Applicable to the quantif. of discretization uncertainty (Tuo et al., 2014)

Illustration of Gaussian process modelling

An example with the same data as previously (from the “beam” case):



Model: TWY2 covariance function (see next slide) w/ Matérn 3/2 stationary part
Parameters set manually (for illustration): $L = 2$, $\sigma^2 = 0.01^2$ and range $\rho = 0.8$.

Which covariance function for the discretization error?

GP model for f ? General form: $\xi(h) = \xi_0 + \varepsilon(h)$

- $\xi_0 \sim \mathcal{U}_{\mathbb{R}}$ (improper uniform distrib.), independent of ε
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☞ We investigate **several possible choices for k** :

👁 TWY1 $k(h, h') = \sigma^2 \min(h, h')^L$

👁 TWY2 $k(h, h') = \sigma^2 (hh')^{L/2} c(h - h')$

👁 STZ $k(h, h') = \sigma^2 [1 + c(h - h') - c(h) - c(h')]$

where $\sigma^2 > 0$, $L > 0$ and c a stationary correlation function

(*TWY stands for Tuo, Wu, and Yu (2014), STZ for "STationary + conditioned at Zero"*)

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Experimental methodology

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 - **3-point DoE** for the GCI method: $h_j^{\text{GCI}} = 2^{j-3} \cdot \frac{2}{9} \text{ m}$, $1 \leq j \leq 3$,
 - **n -point DoE** for the GP method: $h_j^{\text{GP}} = \frac{1}{n+1-j} \cdot 2\text{m}$, $1 \leq j \leq n$,
 - $n = 16$ chosen in order to get **similar computation times**.

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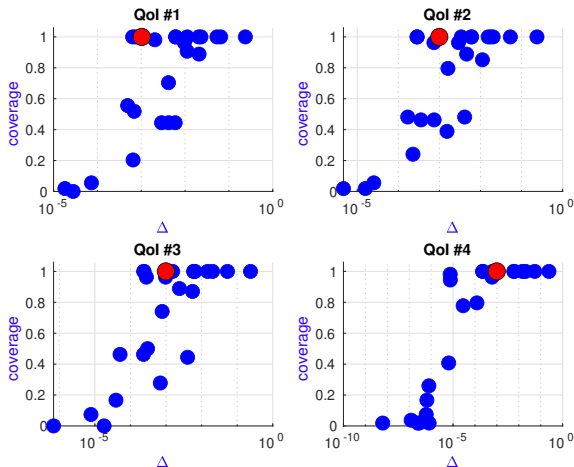
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 - GCI with $F_s = 3$,
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- ☞ Comparison of “conservative” uncertainty bands:
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- ☞ GP models: 23 different covariance models
 - Type: TWY1, TWY2 or STZ.
 - Decay parameter L (TWY1, TWY2): set to $L = 2$, $L = 4$, or estimated.
 - Correlation c (TWY2, STZ): Matérn (regularity $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$ or estim.), Gaussian.
 - Hyper-parameters (σ^2 , L , etc.) \rightsquigarrow restricted maximum likelihood (ReML).

Coverage versus interval (normalized) half-width

Average results over $6 \times 9 = 54$ instances. Interval half-widths normalized by QoI range.



Red disk: GCI with $F_s = 3$. Blue disks: GP CIs at 99.9%  STK 2.6.0 (Bect et al., 2019).

Which covariance functions lead to “good” posteriors ?

👁 Covariance functions s.t. **coverage** $\geq 90\%$ and $\Delta \leq 2 \Delta^{\text{GCI}}$:

covariance	Qol 1	Qol 2	Qol 3	Qol 4
TWY2 ($\mathcal{M}_{1/2}, L = \hat{L}$)	1.000, 0.716	1.000, 0.287	1.000, 0.239	1.000, 0.228
TWY2 ($\mathcal{M}_{1/2}, L = 4$)	1.000, 0.619	1.000, 0.289	1.000, 0.243	1.000, 0.232
TWY2 ($\mathcal{M}_{3/2}, L = \hat{L}$)	☹	☹	0.963, 0.980	0.944, 0.008
TWY2 ($\mathcal{M}_{3/2}, L = 4$)	0.981, 1.989	0.963, 0.739	0.963, 0.284	0.981, 0.008
TWY2 ($\mathcal{M}_{3/2}, L = 2$)	☹	☹	1.000, 1.543	1.000, 0.637
STZ ($\mathcal{M}_{5/2}$)	☹	☹	☹	0.963, 0.614
all the others	☹	☹	☹	☹

(left: coverage, right: $\Delta/\Delta^{\text{GCI}}$; \mathcal{M}_ν : Matérn corr. w/ regularity ν)

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👉 What works wells: **TWY2 with c not “too regular”**

- $L = 4$ makes sense (quadratic convergence observed); \hat{L} works well too ☺
- Similar observations on another DoE (coarser grids)
- Similar observations on the cavity case as well (w/ $L = 2$ instead of $L = 4$)

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- ☞ Two approaches for the **quantification of discretization uncertainty**:
 - Roache's GCI approach, based on Richardson extrapolation,
 - the statistical (Bayesian) approach, using Gaussian processes.

²To make them *really* well-founded, a fully Bayesian treatment of the hyper-parameters would be required.

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- ☞ Two approaches for the quantification of discretization uncertainty:
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 - the statistical (Bayesian) approach, using Gaussian processes.
- ☞ Some **strengths** of the (younger) Bayesian approach
 - **Prior knowledge** about f can be encoded in the prior.
 - “**well-founded² probability statement** on the error” (Roache, 1994)
 - **Tighter uncertainty bands** *if a suitable prior is used* !
(which, however, do not always contain the fine-grid solution)

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 - Tighter uncertainty bands *if a suitable prior is used* !
(which, however, do not always contain the fine-grid solution)
- ☞ Future work
 - Understand better **how to choose a suitable prior**.
 - Benchmark the method on a larger variety of problems.
 - Consider additional input parameters (as, e.g., Tuo et al., 2014).

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Thank you

Everything is in the title

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