Mathematical challenges in scientific computing

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EPEL









- Scientific computing is an enabling technology for scientific discoveries, for innovation and for digitalisation: it is a huge field of science.
- E.g., it makes it possible to simulate physical phenomena at all scales





SC & 'macroscopic' PDE models





Good results rely on error control (and robustness) !



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Conceptual map of my talk









- We solve for $\Delta \mathbf{x}_i^{-1} = 0$
- Maximum principle \Rightarrow **x** is folding free
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- $\|\mathbf{x} \mathbf{x}_h\| \lesssim \sum_{Q \in \mathcal{T}} \mathcal{E}(\mathbf{x}_h, Q)$ Error control by local quantities
- Refine elements where the estimator is large
- Iterate the process until the mapping is folding free
- Local estimators for the nonlinear quantity det(Dx) ?





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X

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Reliability is a worthy mathematical question ...

Error control in defeauturing



Error control in defeauturing



Ω

O. Chanon's work @EPFL

 Γ_D

 $\widetilde{\Gamma}_N$

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- \mathcal{L} continuous and elliptic operator w.r.t. to V
- \tilde{u}_0 cheap extension of u_0 (no meshing of features!)
- estimate the $||u \widetilde{u_0}||_V$ with a computable quantity
- As no meshing on "features" \Rightarrow only **boundary integrals of** \widetilde{u}_0 are allowed

For linear \mathcal{L} , and blue features only (reds are more complex)

$$e = u - u_0$$
, $\langle \mathcal{L}e, e \rangle = \langle (g - \gamma_N(u_0)), e \rangle_{\Gamma_-}$

From here, we deduce an error indicator, taking into account compatibility of data, the length of the features' boundary...

Sobolev type estimates are the main tool to achieve this.

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Error control in defeauturing



¹⁵ Annalisa Buffa



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SC & macroscopic PDE models



7,333.3

3,333.3

2,666.7 2,000.0 1,333.3

666.7



Simulation

Good results rely on error control (and robustness) !

Conceptual map of my talk

Design

Defeaturing

Repairing



Mesh

One example : a slender structural part of any car



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 Kirchhoff Love shell model is a singularly perturbed elliptic 4th order PDE on the mid-surface displacement

$$\mathcal{A}_t(\mathbf{u},\mathbf{v}) = \langle \mathbf{f},\mathbf{v} \rangle \quad \forall \mathbf{v} \in V_{\mathcal{KL}}$$

- On a given mesh ${\mathcal T}$, robustness is very hard to achieve for "very" slender structures...

One example : a slender structural part of any car



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Error control: find functionals $\mathcal{E}(\cdot, Q), \forall Q \in \mathcal{T}$ such that

$$\|\mathbf{u}-\mathbf{u}_h\|_{KL}^2 \lesssim \sum_{Q\in\mathcal{T}} \mathcal{E}^2(\mathbf{u}_h, Q)$$

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load



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Ground rule: we can afford computing only $\mathcal{A}_t(\mathbf{u}_h, \cdot)$ and in particular **no** residuals (high order derivatives of \mathbf{u}_h)

 $\forall Q \in \mathcal{T}, \ \mathbf{b}_h \in \mathcal{B}(Q)$ such that

$$\mathcal{A}_t(\mathbf{b}_h, \mathbf{b'}_h) = \mathcal{A}_t(\mathbf{u}_h, \mathbf{b'}_h) - \langle \mathbf{f}, \mathbf{b'}_h \rangle \quad \forall \mathbf{b'}_h \in \mathcal{B}(\mathbf{Q})$$



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- Local to each element Q
- Contains functions easy to integrate
- Provide a meaningful control on the error



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- $\mathcal{B}(Q)$ can indeed be generated via multiscale approaches
- Refine elements with large $\mathcal{E}(\mathbf{u}_h, Q)$
- Iterate the process until $\mathcal{E}(\mathbf{u}_h, Q)$ is below a tolerance



- Several level of refinements to reach tolerance
- Boundary layers around the load and the holes get numerically resolved..
 - We control the error !

EPFL

Annalisa Buffa Error control Error **Mathematics** control on and robust ╬ makes a meshing/ numerics for difference defeaturing PDES 2021 Strasbourg September **IMU** Centennial

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