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Finite Element Method for fluid flow problems in an industrial R&D context - Motivations, theory and applications

Cenaero's intervention in UCLouvain's course *Introduction aux éléments finis (LEPL1110)*
Teacher: Vincent Legat

Pierre-Alexandre Beaufort, Margaux Boxho, David Henneaux

Contact: david.henneaux@cenaero.be

Context – Why numerical simulations matter

'Conventional' process

Simplified theory & experiments

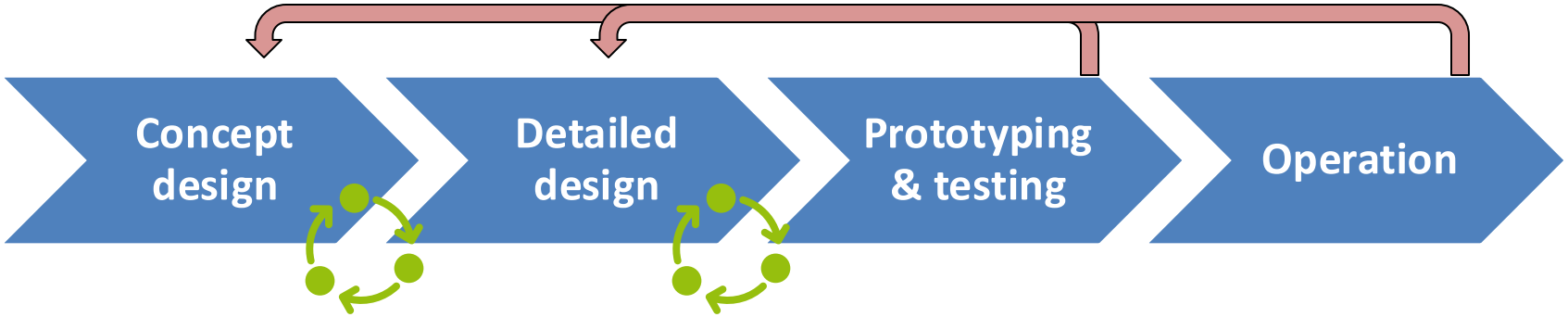
- Excessive margins -> performance degradation
- Impossibility to innovate

Verification by huge # of tests

- Possible missing of risks due to inadequate physics understanding
- Increased developed cost and time

Frequent occurrence of failures

- Possible missing of risks due to inadequate physics understanding
- Increased developed cost and time



Simulation-based process

Detailed modeling

- Optimized performance
- Allow innovative design
- Handle out-of-reach configurations for 'conventional' approach

Fast virtual tests

- Reliable outcomes combined with uncertainty quantification
- Reduced costs by accelerating R&D

Enhanced reliability

- Anticipation and mitigation strategies development
- Immediate investigation and problem resolutions

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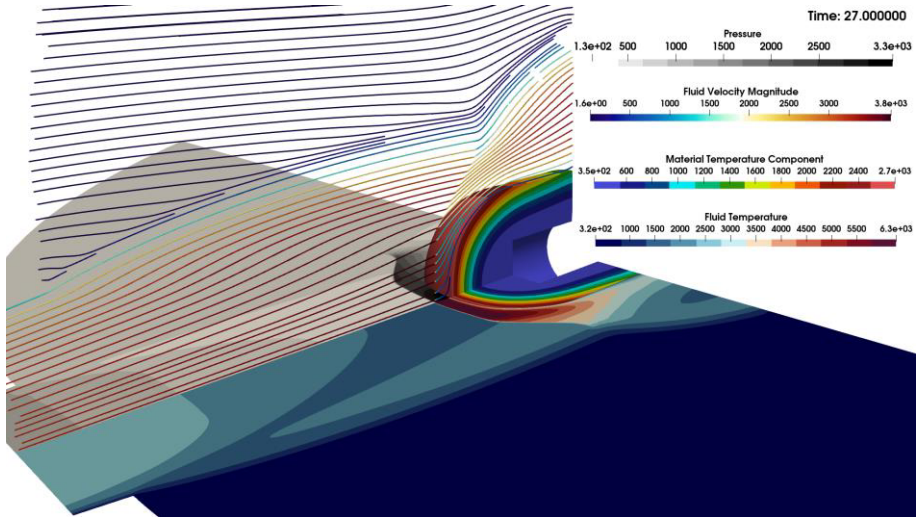
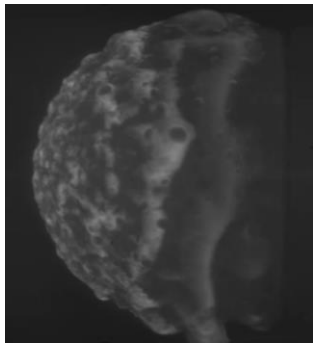
Context – Numerical simulations is one of the pillars of predictive science



Reality

Measurement techniques

Experiments



Credits: El Rassi, Helber, Fagnani

von KARMAN INSTITUTE FOR FLUID DYNAMICS

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p\mathbf{I}) = \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}$$

Simulation

Theoretical analysis

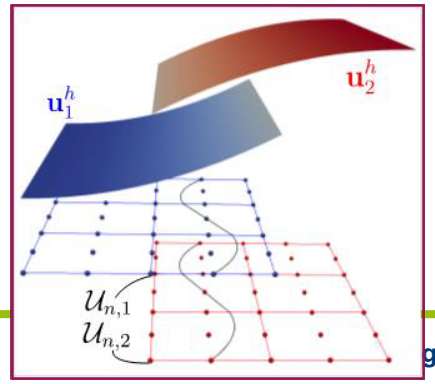
Surrogate-based models

High-fidelity database

Numerical methods

Programming

Physical models



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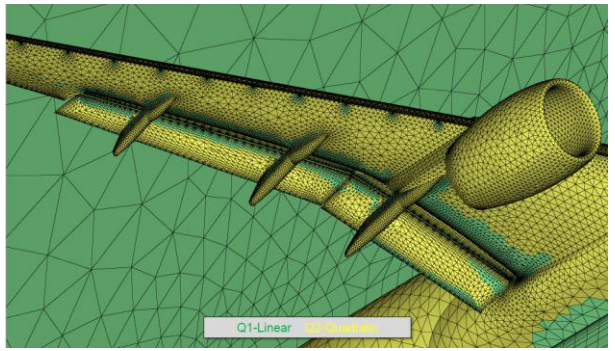
Context – Challenges and requirements for simulating fluid flows

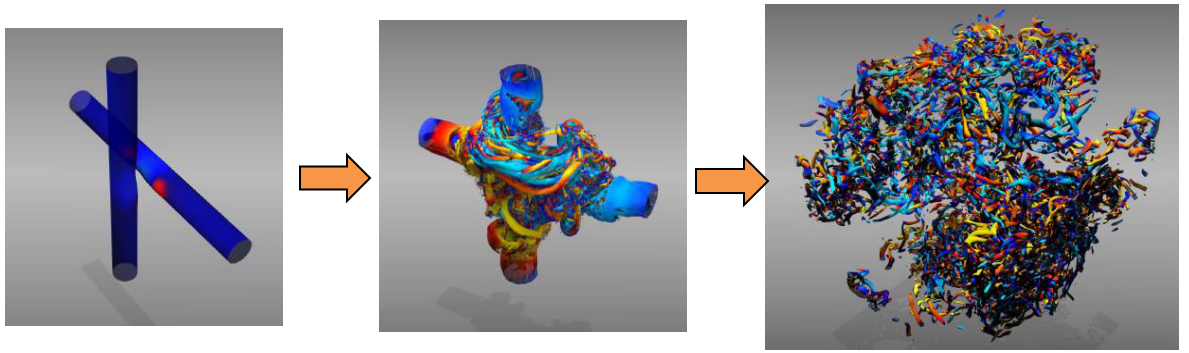
Challenges

Complex geometries



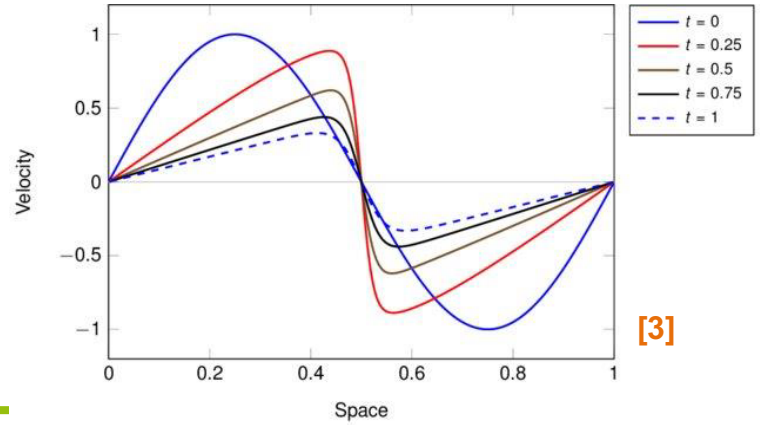
[1]

Wide range of scales



[2]

Non-linearities -> singularities



[3]

Method requirements

Flexibility

High-resolution

Stability

Credits:

[1] Cadence Poitwise

[2] Beck. PhD thesis, Univ. Stuttgart; 2015

[3] Schmitt et al., *International Conference on Computational Engineering*. 2017.

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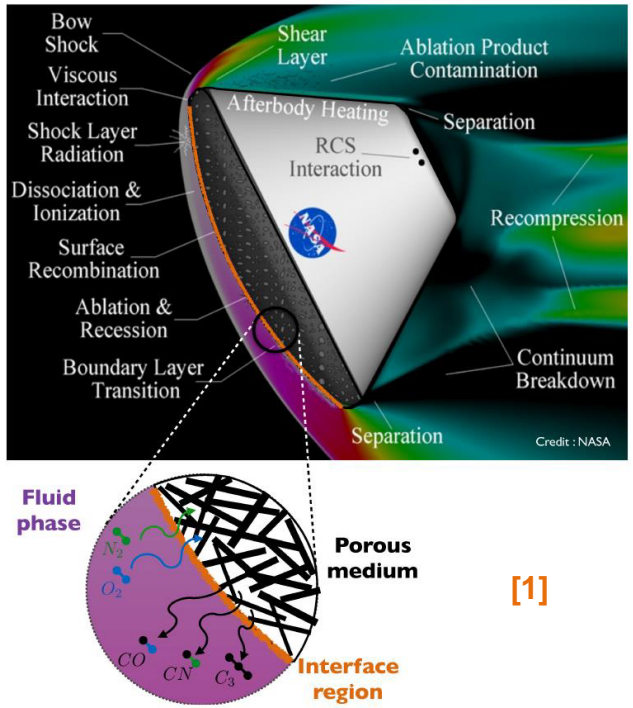
Context – Challenges and requirements for simulating fluid flows

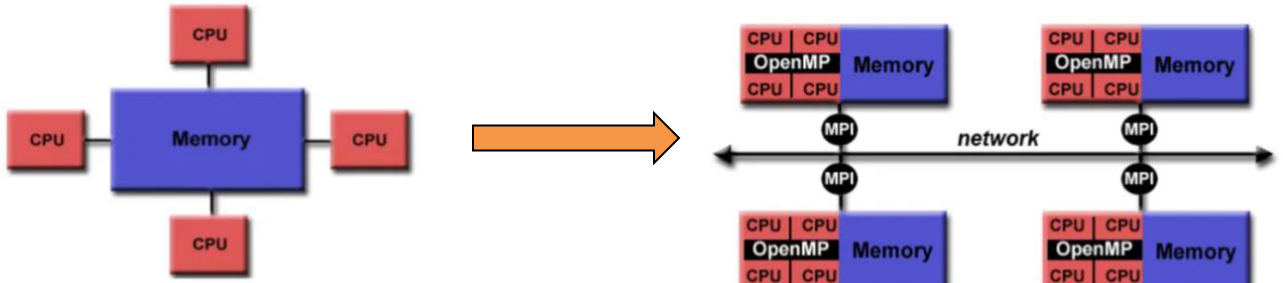
Challenges

Multiphysics nature -> stiffness



[1]

Computational cost



Method requirements

Robustness

Efficiency

Credits:

[1] Schrooyen PhD thesis, UCLouvain; 2015

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Outline

Challenges		***Method requirements***
Complex geometries	**Element-based spatial discretization**	**Flexibility**
Margaux's talk **Wide range of scales**	**High-order spatial discretization**	**High-resolution**
Non-linearities -> singularities	**FEM vs Discontinuous Galerkin**	**Stability**
Multiphysics nature + high-order operators -> stiffness	**Full discrete system solving**	**Robustness**
Computational cost	Margaux's talk **Exploitation of high-fidelity results for machine learning**	**Efficiency**

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Discretization through the weighted residual perspective

- **Prototype advection-diffusion equation – strong form**

$$\tilde{\mathbf{u}} \in \tilde{\mathcal{U}} \qquad \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \tilde{\nabla} \cdot (c\,\tilde{\mathbf{u}}) - \tilde{\nabla} \cdot (d\,\tilde{\nabla}\tilde{\mathbf{u}}) = \mathbf{0} \quad \text{on } \tilde{\Omega}$$

- **You've seen that for elliptic problem (c=0, u(x)): FEM <=> functional minimization**

$$J(\tilde{\mathbf{u}}) = \min_{\tilde{\mathbf{w}} \in \tilde{\mathcal{U}}} J(\tilde{\mathbf{w}})$$

- **But breaks down for hyperbolic equation => go for the more general weighted residual approach**

Fundamental Lemma of Variational Calculus

$$\mathcal{R}[\tilde{\mathbf{u}}] := \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \tilde{\nabla} \cdot (c\,\tilde{\mathbf{u}}) - \tilde{\nabla} \cdot (d\,\tilde{\nabla}\tilde{\mathbf{u}}) = \mathbf{0} \quad \text{on } \tilde{\Omega} \quad \Longleftrightarrow \quad \int_{\tilde{\Omega}} \tilde{\mathcal{R}}\,[\tilde{\mathbf{u}}]\ \tilde{\mathbf{w}}\ \mathrm{d}\mathbf{x} = \mathbf{0} \quad \forall \tilde{\mathbf{w}} \in C_c^{\infty}(\tilde{\Omega})$$

Pointwise condition
-> KO for non-smooth solution

Integral ("average") condition
-> OK for non-smooth solution
(derivatives in the sense of distributions)

Discretization through the weighted residual perspective

- **Discretization: from infinite space to 'computer-compatible' finite space**
  - **On the domain (meshing):** $\Omega \approx \tilde{\Omega}$
  - **On the test functions:**

$$\tilde{\mathbf{w}} \in \mathcal{C}_c^\infty(\tilde{\Omega}) \longrightarrow \mathbf{W} \in \mathcal{W} := \text{span}\{\mathbf{w}_1, \dots, \mathbf{w}_n, \dots, \mathbf{w}_{N_n}\}$$

$$\int_{\tilde{\Omega}} \tilde{\mathcal{R}}[\tilde{\mathbf{u}}]\ \tilde{\mathbf{w}}\, \mathrm{d}\mathbf{x} = \mathbf{0} \longrightarrow \int_{\tilde{\Omega}} \tilde{\mathcal{R}}[\tilde{\mathbf{u}}]\ \mathbf{w}_n\, \mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

  - **On the trial functions:**

$$\tilde{\mathbf{u}} \in \tilde{\mathcal{U}} \subset \mathcal{C}^2(\tilde{\Omega}) \longrightarrow \mathbf{u} \in \mathcal{U} := \text{span}\{\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_m, \dots, \boldsymbol{\phi}_{N_m}\}$$

$$\longrightarrow \int_{\Omega} \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n\, \mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

We seek an approximate solution such that the residual of the equations is made "small" in a certain integral sense (but not = 0 anymore due to discretization)

$$\mathcal{R}[\mathbf{u}] \neq \tilde{\mathcal{R}}[\tilde{\mathbf{u}}] = \mathbf{0}$$

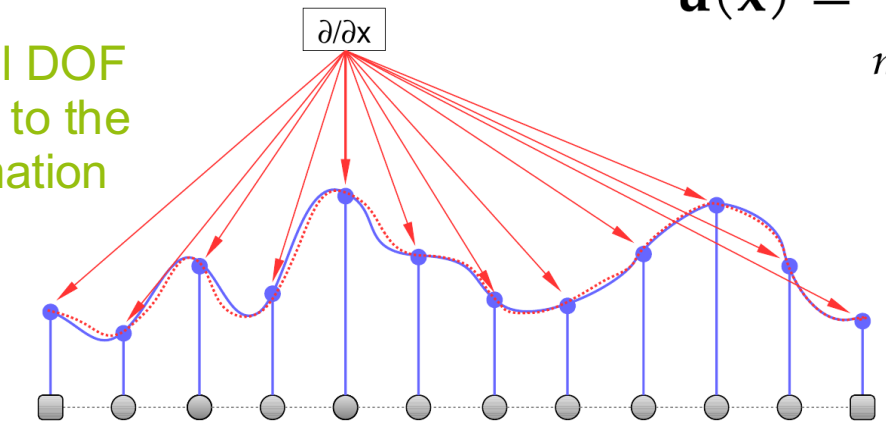
Discretization through the weighted residual perspective

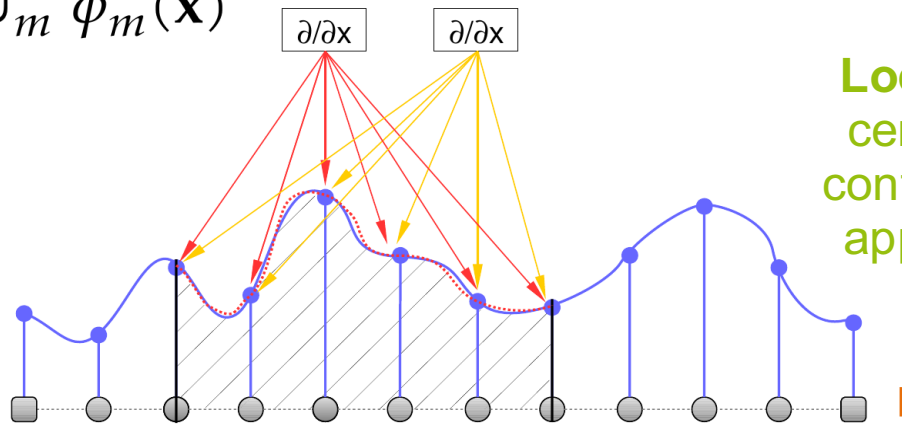
Credits:
[1] Beck. PhD thesis, Univ. Stuttgart; 2015

- **Method choice:**
  - **Solution representation**

$$\mathbf{u}(\mathbf{x}) = \sum_{m=1}^{N_m} \mathbf{U}_m \, \phi_m(\mathbf{x})$$

Global: all DOF contribute to the approximation





Local: dof in a certain stencil contribute to the approximation

[1]

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Discretization through the weighted residual perspective

- **Method choice:**
  - **Weighting of the residual**

Geometrical flexibility

$$\mathbf{w}_n(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_n)$$

Collocation

Pseudo-spectral method

Lack of geometrical flexibility due to Cartesian-like stencil or use of specific collocation points

$$\mathbf{w}_n(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x}_n \leq \mathbf{x} \leq \mathbf{x}_{n+1} \\ 0, & \text{otherwise.} \end{cases}$$

Subdomain

FVM

Lack of resolution capabilities due to enforcement of residual in a box average fashion

$$\mathbf{w}_n(\mathbf{x}) = \psi_n(\mathbf{x})$$

Petrov-Galerkin

SUPG CFEM

$$\mathbf{w}_n(\mathbf{x}) = \phi_n(\mathbf{x})$$

Galerkin

CFEM, DGFEM

Orthogonal projection of the residual on the trial space

-> error minimized in L2-norm

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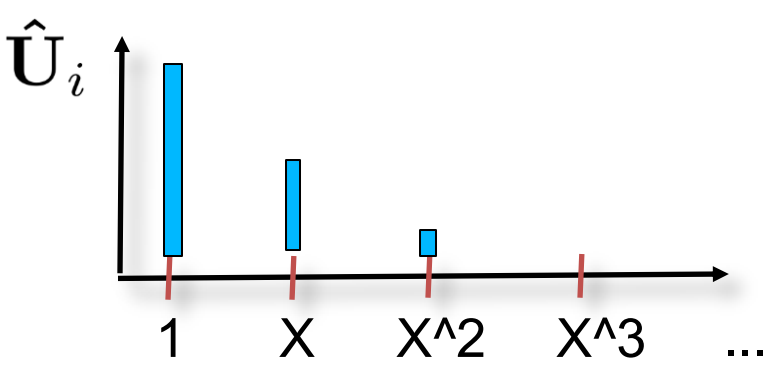
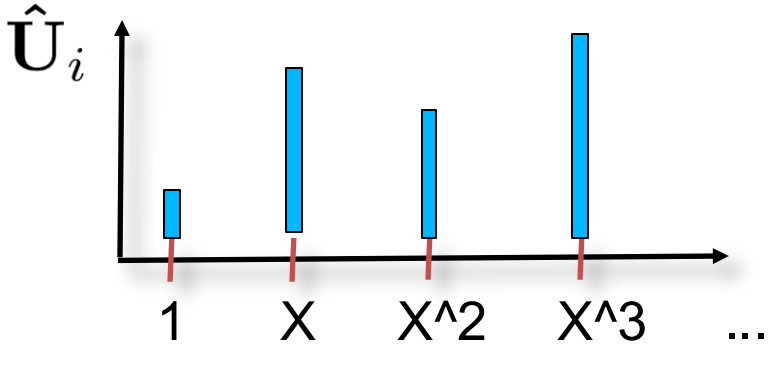
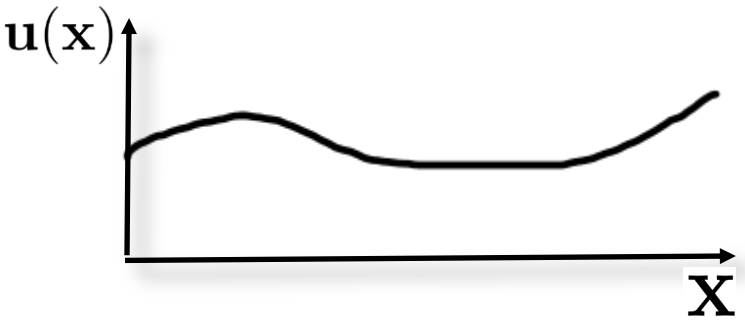
- **Expression of the solution in modal basis**

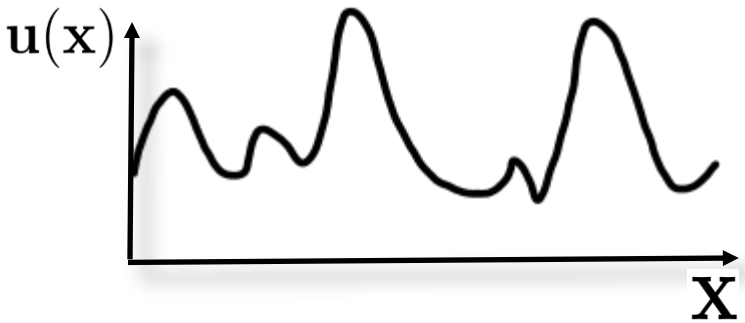




$$\mathbf{u}(\mathbf{x}) = \sum_{i=0}^{N} \hat{\mathbf{U}}_i \, \xi_i(\mathbf{x})$$



Smooth flow



Multiscale flow

Sources of numerical errors

- **Approximation error: truncation of expansion**

$$\tilde{\mathbf{u}}(\mathbf{x}) = \sum_{i=0}^{\infty} \hat{\tilde{\mathbf{U}}}_i \, \xi_i(\mathbf{x}) \longrightarrow \mathbf{u}(\mathbf{x}) = \sum_{i=0}^{N} \hat{\mathbf{U}}_i \, \xi_i(\mathbf{x})$$

$$\epsilon_1 = \sum_{i=N+1}^{\infty} \hat{\tilde{\mathbf{U}}}_i \, \xi_i(\mathbf{x})$$

- **PDE discretization error: discrete weighted residual formulation**

$$\mathcal{R}[\mathbf{u}] \neq \tilde{\mathcal{R}}[\tilde{\mathbf{u}}] = \mathbf{0} \longrightarrow \epsilon_{2,i} = |\hat{\tilde{\mathbf{U}}}_i - \hat{\mathbf{U}}_i| \quad i = 0, \ldots, N$$

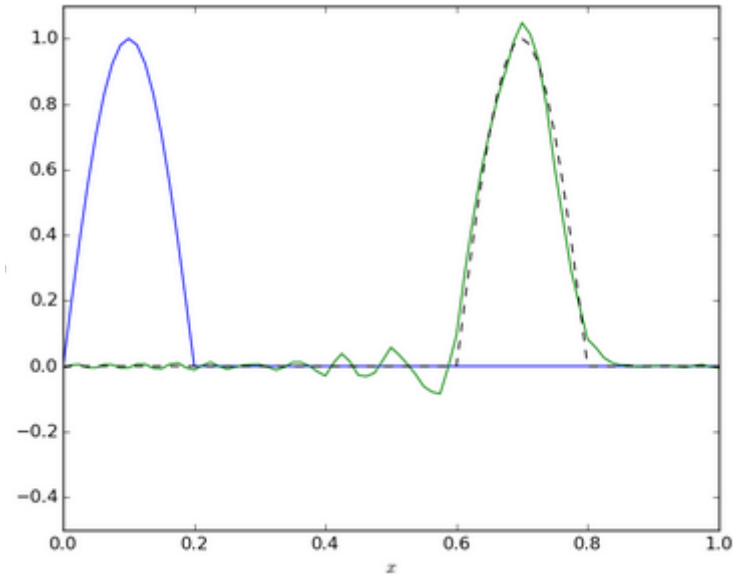
For non-linear problem, those discretization errors interact across the scales -> aliasing errors may accumulate energy in the high modes and affect the lower modes

Manifestations of numerical errors

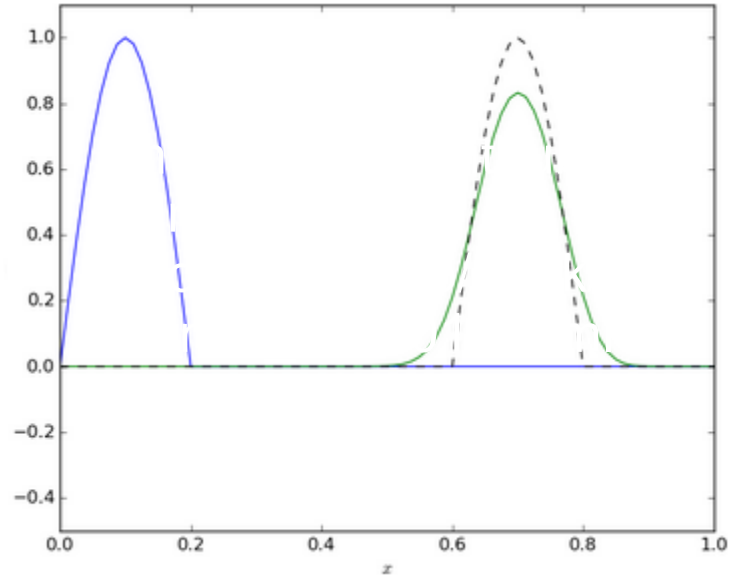
- **Approximation and discretization errors lead to alterations of phase (dispersion) and amplitude (dissipation) of the signal (solution)**

$$\epsilon_1 = \sum_{i=N+1}^{\infty} \hat{\tilde{\mathbf{U}}}_i \, \xi_i(\mathbf{x})$$

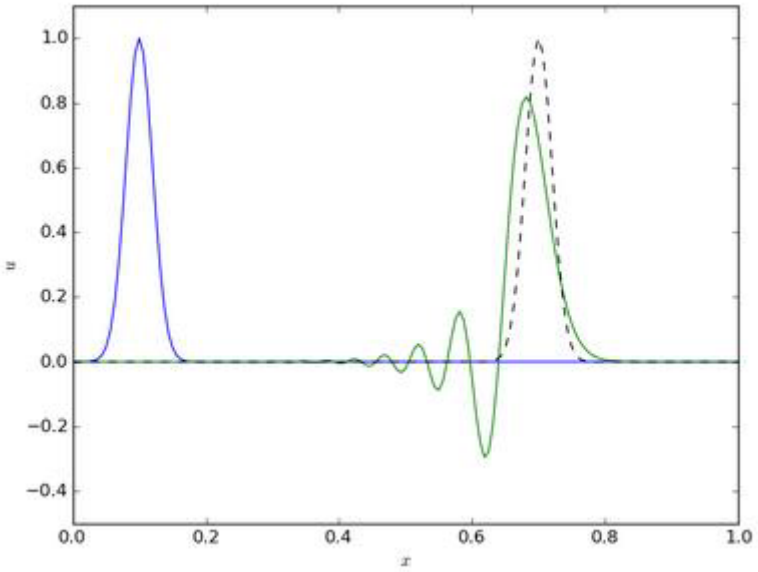
$$\epsilon_{2,i} = |\hat{\tilde{\mathbf{U}}}_i - \hat{\mathbf{U}}_i| \quad i = 0, \ldots, N$$



Dispersion error



Dissipation error



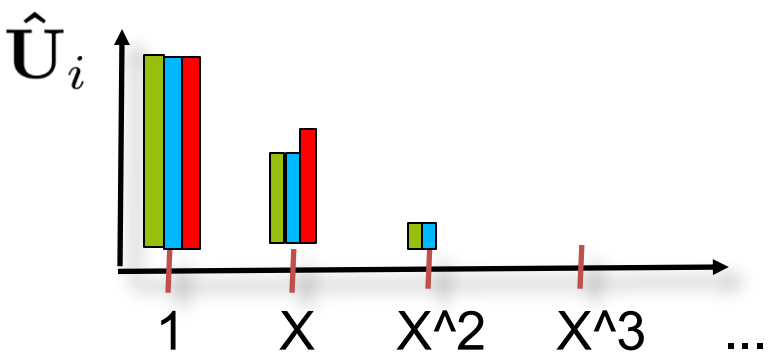
Dispersion + Dissipation errors

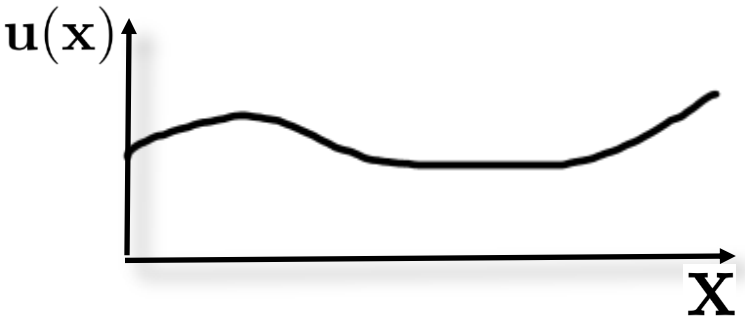
Credits:

[1] https://hplgit.github.io/fdm-book/doc/pub/book/sphinx/._book012.html

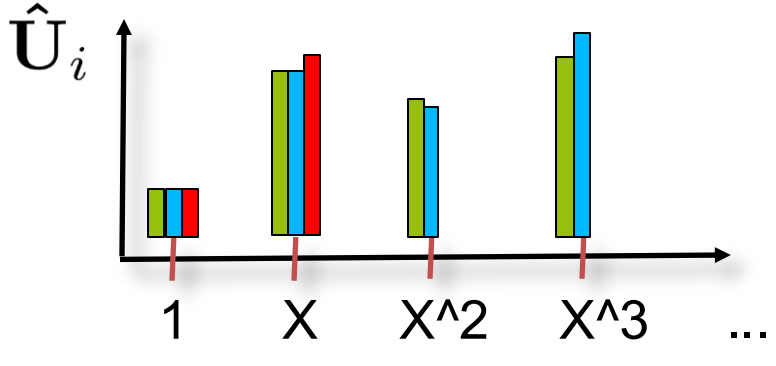
Interest of high-order discretization for multiscale problem

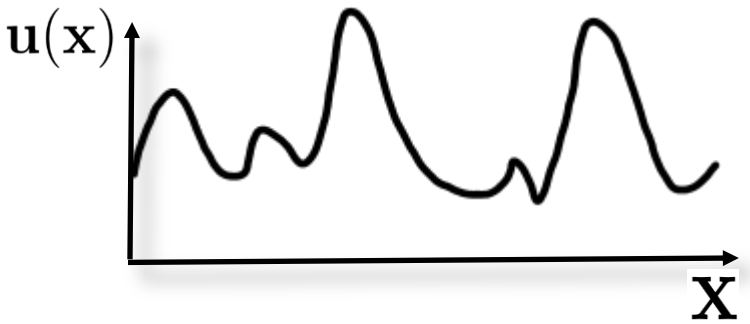
- **Increasing the scheme order reduces dispersion and dissipation errors -> increased resolution capabilities at higher modes**



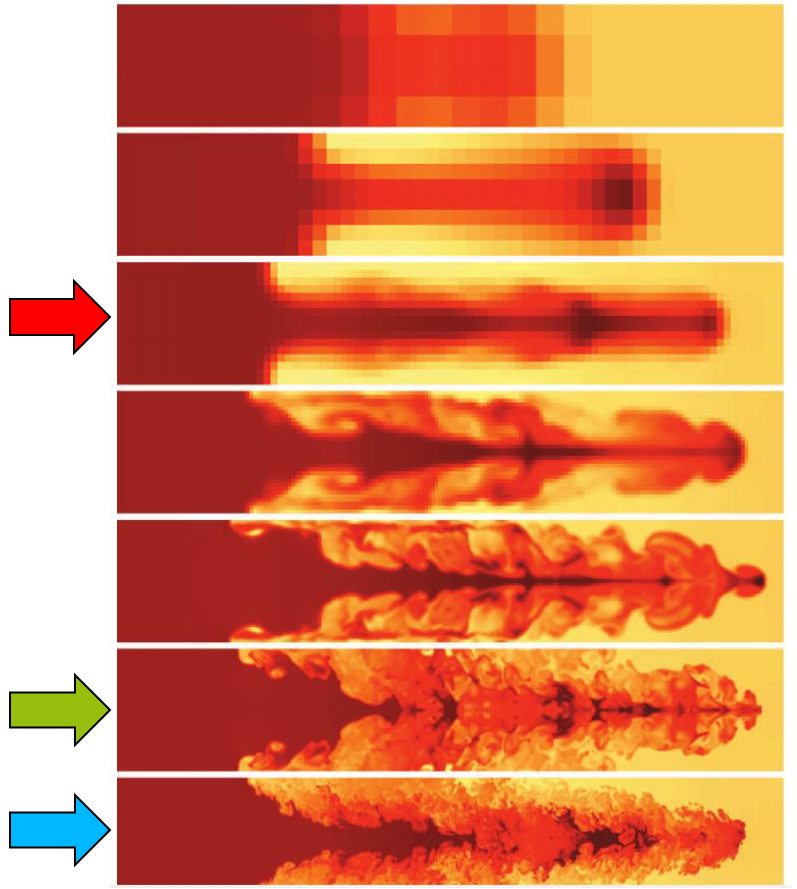


Smooth flow





Multiscale flow



Credits:

[1] Kadanoff, Leo P. "Excellence in computer simulation. " *Computing in Science & Engineering* 6.2 (2004): 57-67.

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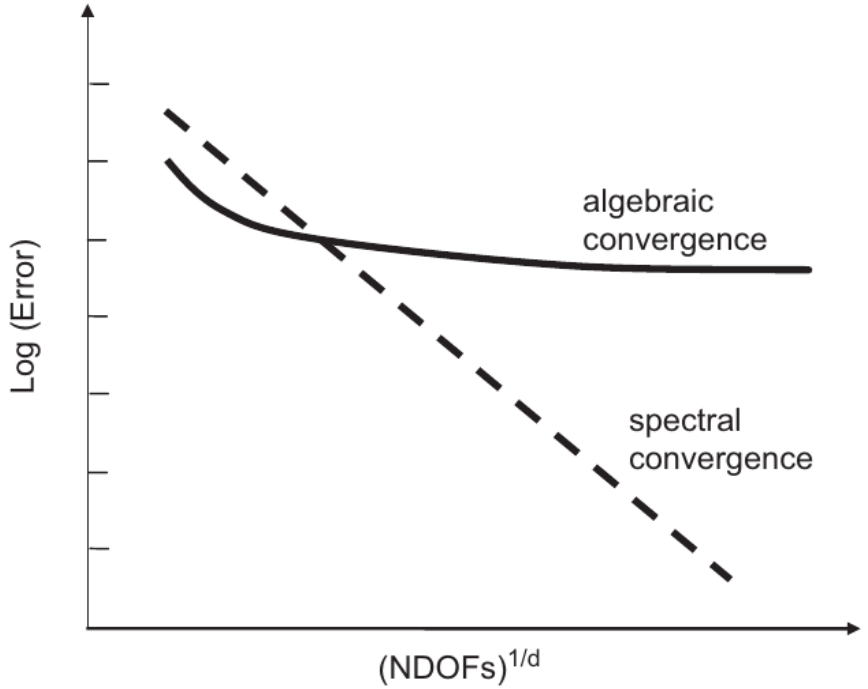
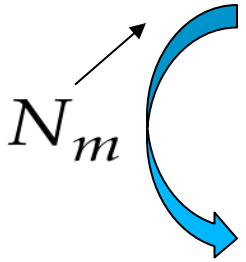
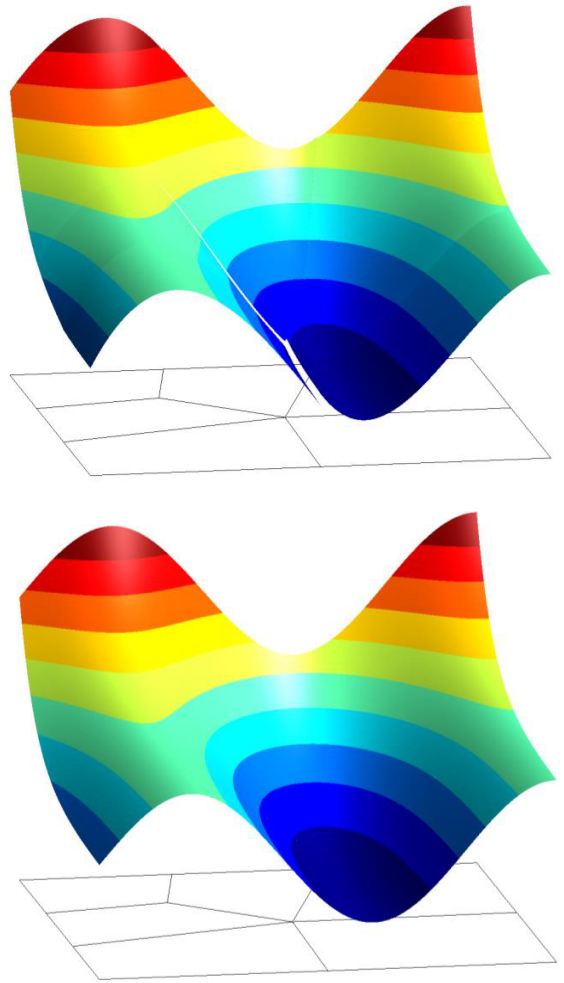
Why going high-order can pay off

- **FE-type element-based methods offer a natural way to improve subcell resolution by locally increasing the interpolation order (i.e. without stencil extension)**
- **For the same # DOF, increasing the order quickly leads to errors levels (far) below what can mesh refinement reaches**

$$\mathbf{u}(\mathbf{x}) = \sum_{m=1}^{N_m} \mathbf{U}_m \, \phi_m(\mathbf{x})$$







Credits:

[1] Wang, Zhi Jian. "High-order methods for the Euler and Navier–Stokes equations on unstructured grids." *Progress in Aerospace Sciences* 43.1-3 (2007): 1-41.

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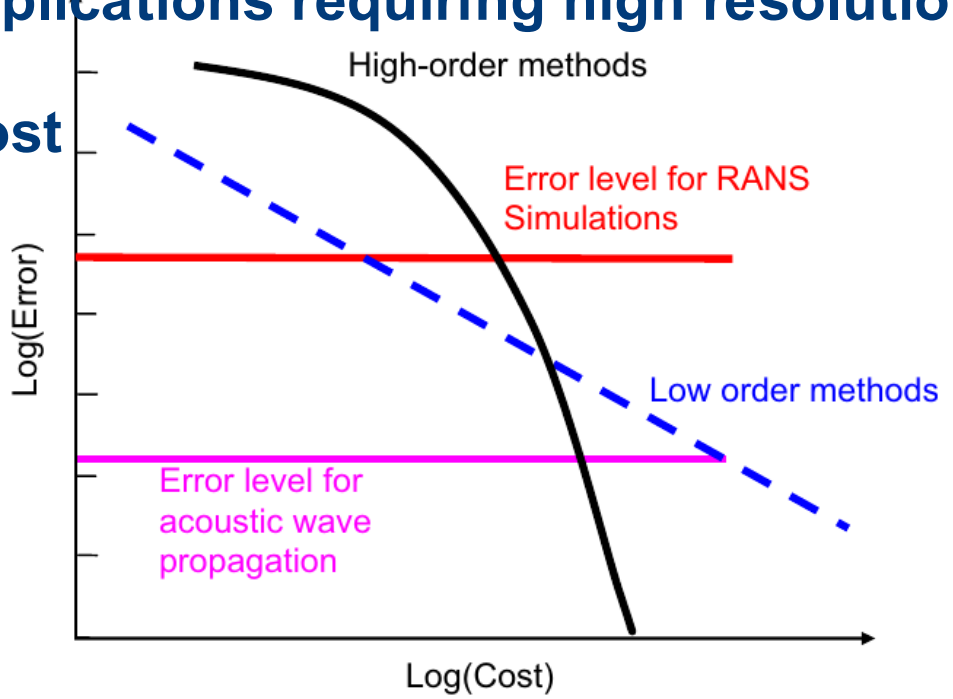
- **For the same # DOF, increasing the order quickly leads to errors levels (far) below what can mesh refinement reaches**
- **For some applications requiring high resolution, this leads to a lower cost**



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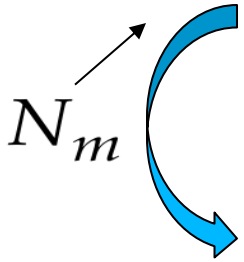

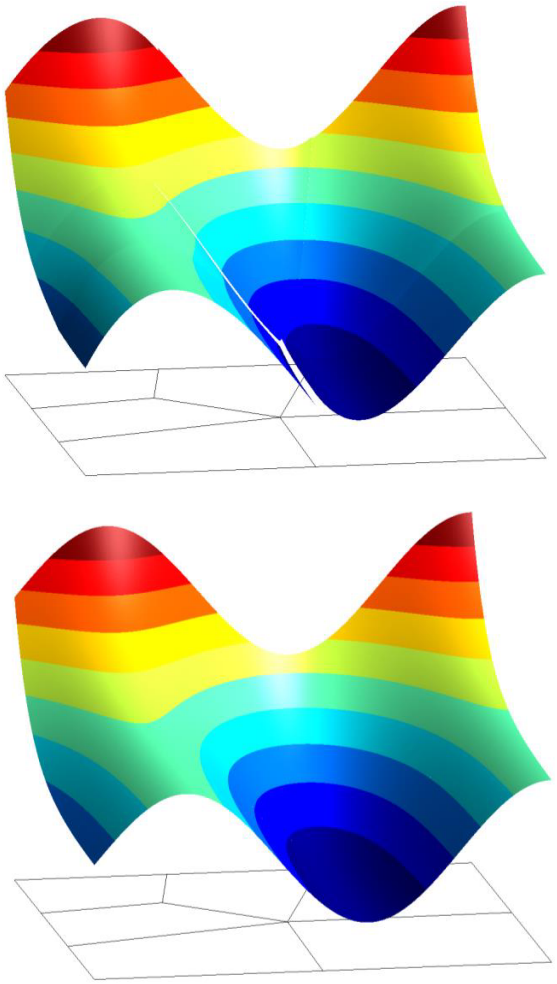

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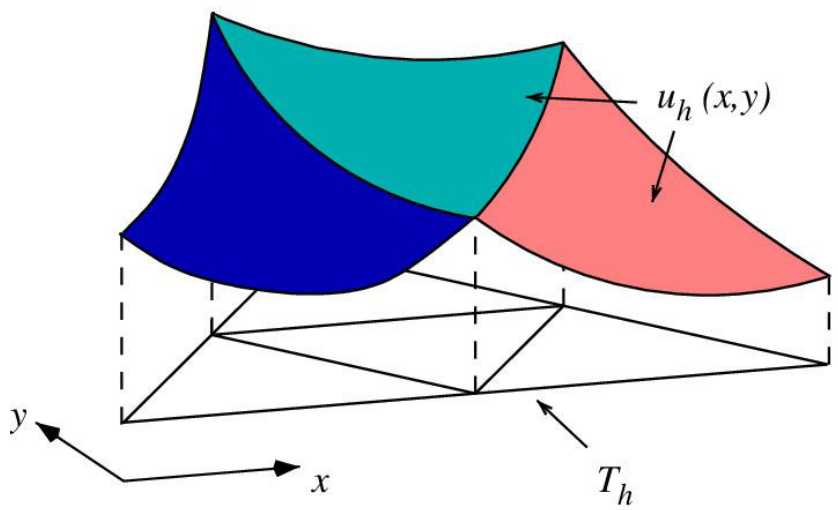
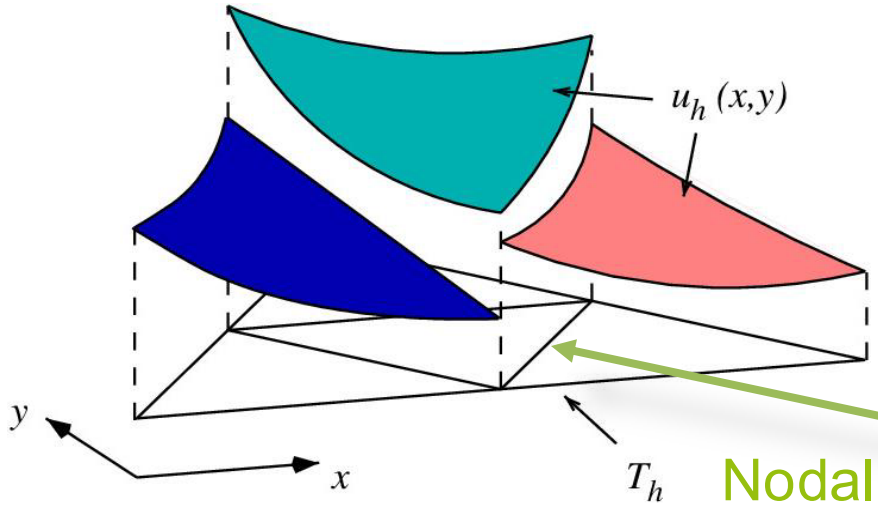
Continuous Finite Element vs Discontinuous Galerkin

- You've seen that the coercivity (hence stability) of the continuous FE discretized form is ensured for pure elliptic problem.
- But it's note the case for hyperbolic problem -> let's consider that case:

$$\mathcal{R}[\tilde{\mathbf{u}}] := \tilde{\nabla} \cdot (c\,\tilde{\mathbf{u}}) = \mathbf{0} \quad \text{on } \tilde{\Omega} \quad \Rightarrow \quad \int_{\Omega} \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n \,\mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \ldots N_n$$

- Different choices of function space between FEM and DGM:

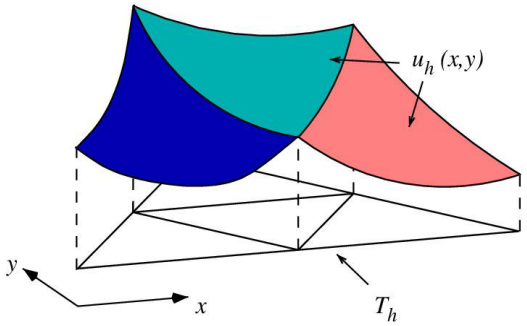


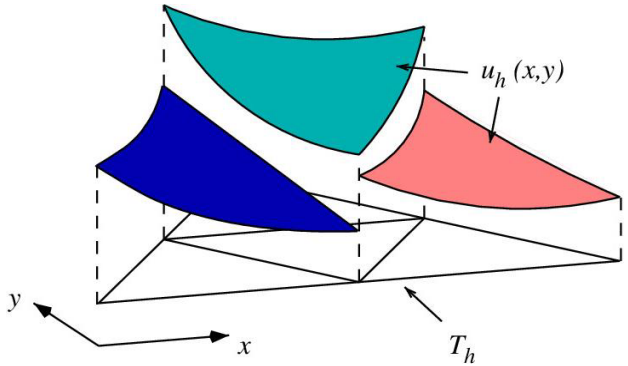


Nodal unknows doubled at the element interfaces

Continuous Finite Element vs Discontinuous Galerkin

- **Different choices of function space between FEM and DGM:**

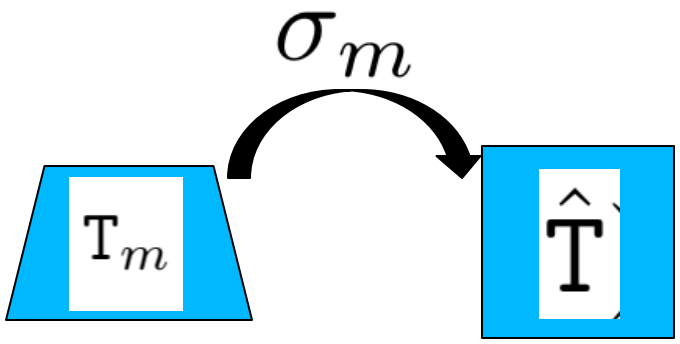


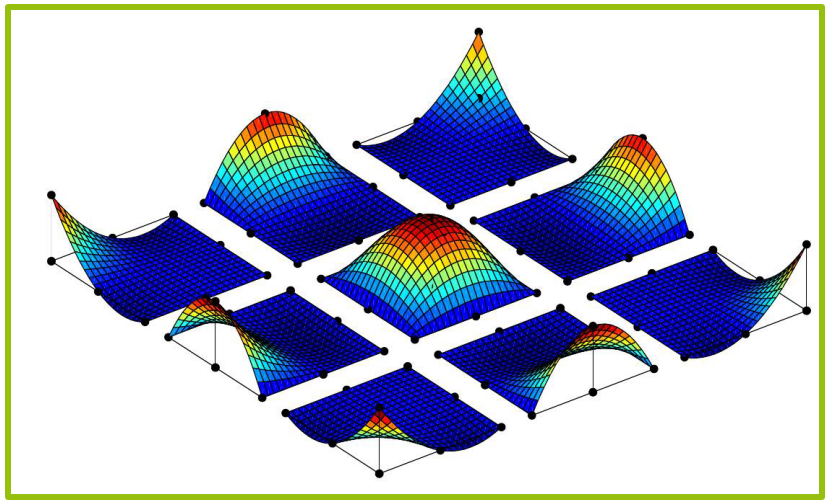


$$\mathcal{W}_p^c = \left\{ w \in \mathcal{C}^0(\Omega) : w_{|\mathtt{T}_m} \circ \sigma_m \in \mathcal{P}_p(\hat{\mathtt{T}}) \right\}$$

$$\mathcal{W}_p^d = \left\{ w \in L^2(\Omega) : w_{|\mathtt{T}_m} \circ \sigma_m \in \mathcal{P}_p(\hat{\mathtt{T}}) \right\}$$

$$\Omega = \bigcup_m \mathtt{T}_m$$





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Continuous Finite Element vs Discontinuous Galerkin

$$\int_\Omega \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n\,\mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

- **Galerkin continuous FE (with weak essential boundary condition enforcement)**

$$\int_\Omega [\nabla \cdot (c\,u)]\, w\,\mathrm{d}x + \int_{\partial\Omega} c(u - u_B) w\,\mathrm{d}s = 0\,, \quad \forall w \in \mathcal{W}_p^c$$

- **The form is coercive... but not in the norm defining the function space -> no control leading to oscillatory solution as the mesh is refined**

$$B(v,v) \geq \gamma_0 \int_\Omega w^2\,\mathrm{d}x + \frac{1}{2}\int_{\partial\Omega} b\,w^2\,\mathrm{d}s$$

Continuous Finite Element vs Discontinuous Galerkin

$$\int_\Omega \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n\,\mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

- **Petrov-Galerkin continuous FE (with weak essential boundary condition enforcement)**

$$\int_\Omega [\nabla\cdot(c\,u)]\,[w + c\,\zeta\,\nabla w]\,\mathrm{d}x + \int_{\partial\Omega} c(u-u_B)w\,\mathrm{d}s = 0\,, \quad \forall w \in \mathcal{W}_p^c$$

- **Artificial diffusion in streamline direction "c" gives now control on the previously unbounded directional derivative of the solution**

$$\zeta \int_\Omega (c\,\nabla u)(c\,\nabla w)\,\mathrm{d}x + \zeta \int_\Omega (\nabla c\,u)(c\,\nabla w)\,\mathrm{d}x$$

Continuous Finite Element vs Discontinuous Galerkin

$$\int_\Omega \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n\,\mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

- **Discontinuous Galerkin FE**

$$\int_{\mathrm{T}_m} [\nabla \cdot (c\,u)]\, w\,\mathrm{d}x = 0$$

Integration by part

$$- \int_{\mathrm{T}_m} (c\,u)\nabla w\,\mathrm{d}x + \int_{\partial \mathrm{T}_m} c\,u\,w\,\mathrm{d}s = 0$$

$$- \int_\Omega (c\,u)\nabla w\,\mathrm{d}x + \sum_{\mathrm{T}_m} \int_{\partial \mathrm{T}_m} \underbrace{c\,u}_{\mathcal{F}}\, w\,\mathrm{d}s = 0\,, \quad \forall w \in \mathcal{W}_p^d$$

Sum over elements

Continuous Finite Element vs Discontinuous Galerkin

$$\int_\Omega \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n\,\mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

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Sum over elements

- **Because of solution jump at element interfaces, definition of a numerical flux function based on left and right states**

$$\mathcal{F} = b(u^+ + u^-) + b_0(u^+ - u^-)$$

- **Control on the solution jump in the DG norm only if b 0 != 0. In particular, upwind stabilization is ensured by**

$$b_0 = \frac{1}{2}|b| \qquad \mathcal{F} = \begin{cases} b\,u^- & \text{if } b < 0 \\ b\,u^+ & \text{if } b \geq 0 \end{cases}$$

Continuous Finite Element vs Discontinuous Galerkin

$$\int_\Omega \mathcal{R}[\mathbf{u}]\ \mathbf{w}_n\,\mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \dots N_n$$

- **Discontinuous Galerkin FE exploits weak imposition of inter-element continuity, in contrast to strong continuity in continuous FEM. This has a stabilizing effect (if numerical flux properly chosen) and lead to improved order of convergence.**

$$\int_\Omega [\nabla \cdot (c\,u)]\,w\,\mathrm{d}x - \sum_{\mathrm{T}_m \setminus \partial\Omega} \int_{\partial \mathrm{T}_m} c(u^+ - u^-) w\,\mathrm{d}s + \int_{\partial\Omega} c(u - u_B) w\,\mathrm{d}s = 0\,, \quad \forall w \in \mathcal{W}_p^c$$

- **What about elliptic operator with DGM? Contrary to continuous FEM, well-posedness via the Lax-Milgram theorem cannot be invoked since we're considering non-conforming FE -> need to prove it for every discrete function space (i.e. stability conditions depending on element type and order).**

Outline

Challenges		***Method requirements***
Complex geometries	**Element-based spatial discretization**	**Flexibility**
Margaux's talk **Wide range of scales**	**High-order spatial discretization**	**High-resolution**
Non-linearities -> singularities	**FEM vs Discontinuous Galerkin**	**Stability**
Multiphysics nature + high-order operators -> stiffness	**Full discrete system solving**	**Robustness**
Computational cost	**Exploitation of high-fidelity results for machine learning** Margaux's talk	**Efficiency**

Application of DG spatial discretization to Navier-Stokes fluid equations

- **Also an advection-diffusion-reaction equation on which we apply weighted residual approach**

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \underline{\boldsymbol{F}}^c(\mathbf{u}) = \nabla \cdot \underline{\boldsymbol{F}}^d(\mathbf{u}, \nabla \mathbf{u}) + \mathbf{S}(\mathbf{u}, \nabla \mathbf{u}) \Rightarrow \tilde{\mathcal{R}}[\tilde{\mathbf{u}}] \triangleq \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \tilde{\nabla} \cdot \underline{\boldsymbol{F}}(\tilde{\mathbf{u}}, \tilde{\nabla}\tilde{\mathbf{u}}) - \mathbf{S}(\tilde{\mathbf{u}}, \tilde{\nabla}\tilde{\mathbf{u}}) = \mathbf{0}$$

$$\int_\Omega \mathcal{R}[\mathbf{u}] \; \mathbf{w}_n \, \mathrm{d}\mathbf{x} = \mathbf{0} \quad \text{for } n = 1, \ldots N_n \; \hookleftarrow$$

- **DG discerization leads to a system of ODEs to be integrated in time**

$$\underbrace{\sum_{m \in \mathrm{T}} \int_{\mathrm{T}_m} \boldsymbol{\phi}_{m,-} \boldsymbol{\phi}_{m,-}^T \, \mathrm{d}\mathbf{x}}_{\underline{\boldsymbol{M}}} \frac{\mathrm{d}\underline{\boldsymbol{U}}_{-,-,-}}{\mathrm{d}t} + \mathcal{N}^{\mathrm{SP}}(\underline{\boldsymbol{U}}_{-,-,-}) = 0$$

$$\begin{aligned}\hat{\mathcal{N}}^{\mathrm{SP}}(\mathbf{u}, \mathbf{w}) \equiv & \sum_{m \in \mathrm{T}} \mathcal{V}_m(\mathbf{u}_m, \mathbf{w}_m) \\ & + \sum_{e \in \mathrm{E}} \hat{\mathcal{E}}_e(\mathbf{u}^+_{m(e)}, \mathbf{u}^-_{m(e)}, \mathbf{w}^+_{m(e)}, \mathbf{w}^-_{m(e)}) \\ & + \sum_{b \in \mathrm{B}} \hat{\mathcal{B}}_b(\mathbf{u}^+_{m(b)}, \mathbf{w}^+_{m(b)}) \, .\end{aligned}$$

Application of DG spatial discretization to Navier-Stokes fluid equations

$$\underbrace{\sum_{m \in \mathrm{T}} \int_{\mathrm{T}_m} \boldsymbol{\phi}_{m,-} \boldsymbol{\phi}_{m,-}^{T} \, \mathrm{dx}}_{\underline{\boldsymbol{M}}} \frac{\mathrm{d}\underline{\boldsymbol{U}}_{-,-,-}}{\mathrm{d}t} + \mathcal{N}^{\mathrm{sp}}(\underline{\boldsymbol{U}}_{-,-,-}) = 0$$

Unsteady Explicit

$$\mathcal{N}^{\mathrm{tp}}(\mathbf{U}(t_{n+1})) + \mathcal{N}^{\mathrm{sp}}(\mathbf{U}(t_n)) = \mathbf{0}$$

- Linear temporal term -> solution at next time step directly available

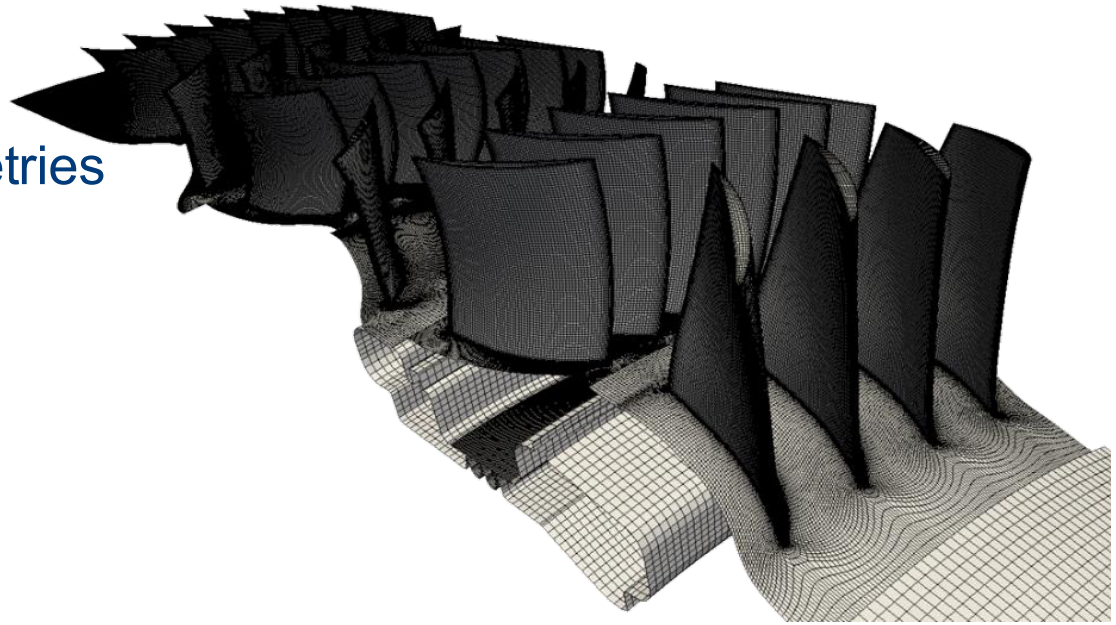
Time-marching steady or unsteady Implicit

$$\mathcal{N}^{\mathrm{tp}}(\mathbf{U}(t_{n+1})) + \mathcal{N}^{\mathrm{sp}}(\mathbf{U}(t_{n+1})) = \mathbf{0}$$

- Non-linear system to solve at each time step
- Linear system to solve at each iteration

Take-home messages about discontinuous Galerkin method

- Advantages
  - Ability to handle complex geometries



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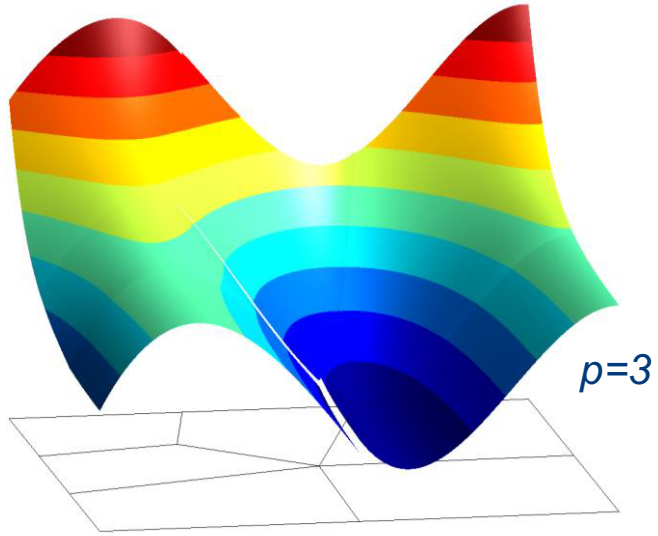
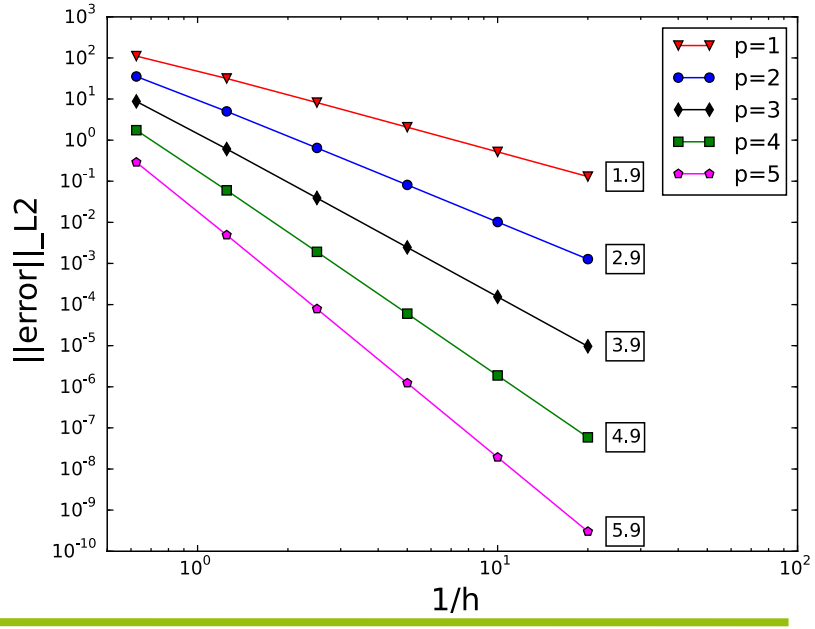
  - Guaranteed order of convergence p+1 on unstructured meshes
  - No degradation near size jumps/walls





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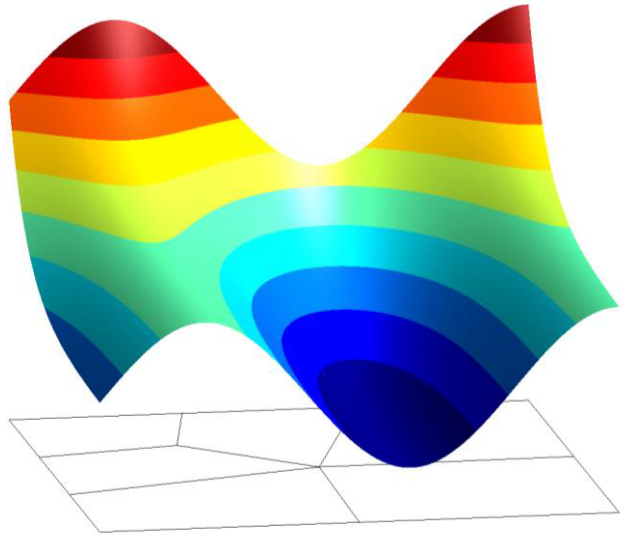

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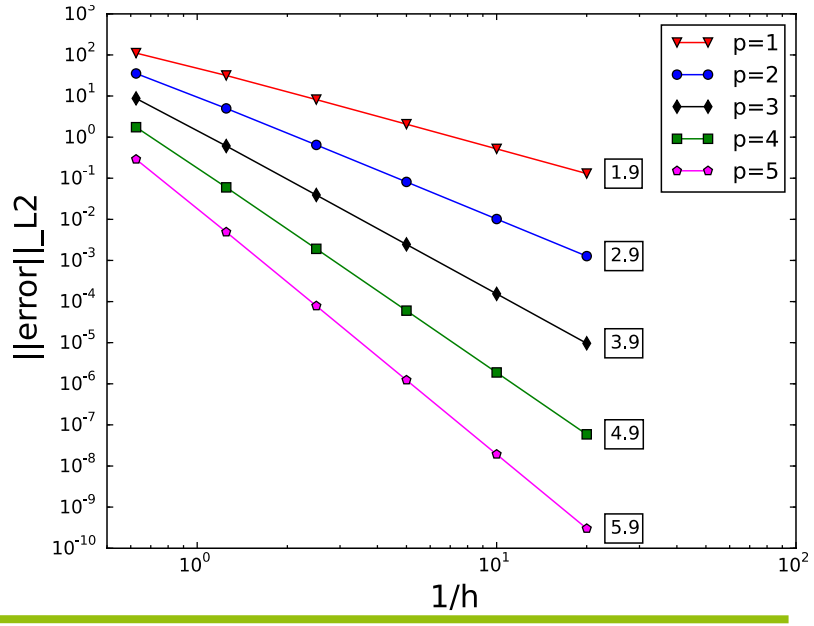

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  - Ability to handle complex geometries
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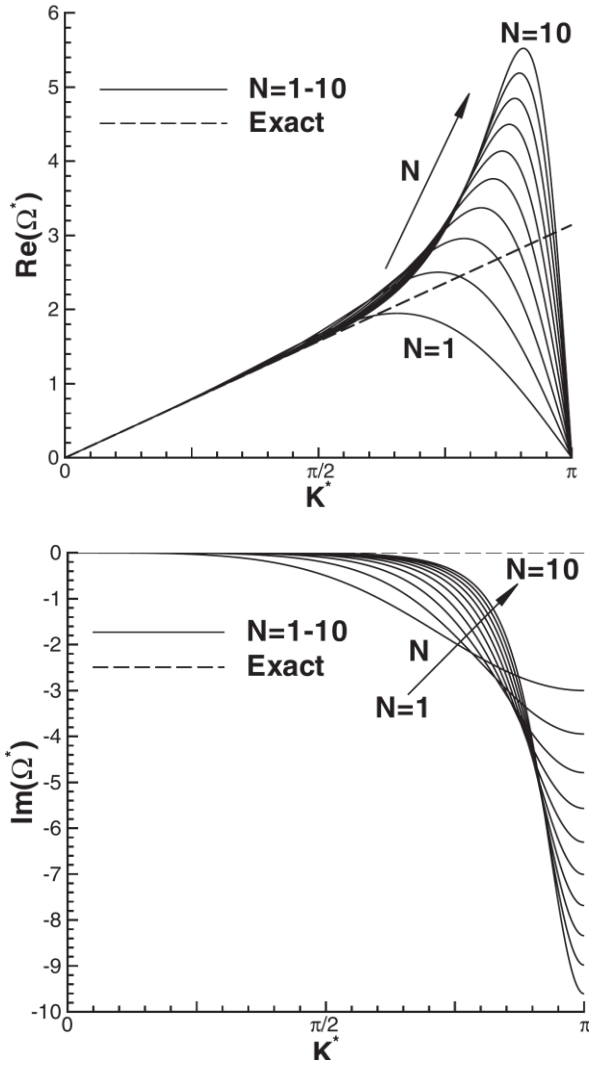
  - Good dispersion-dissipation properties



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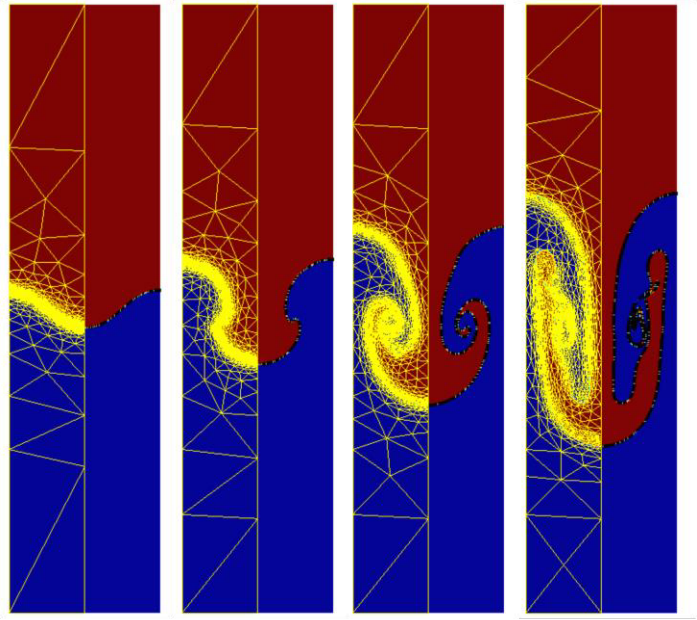

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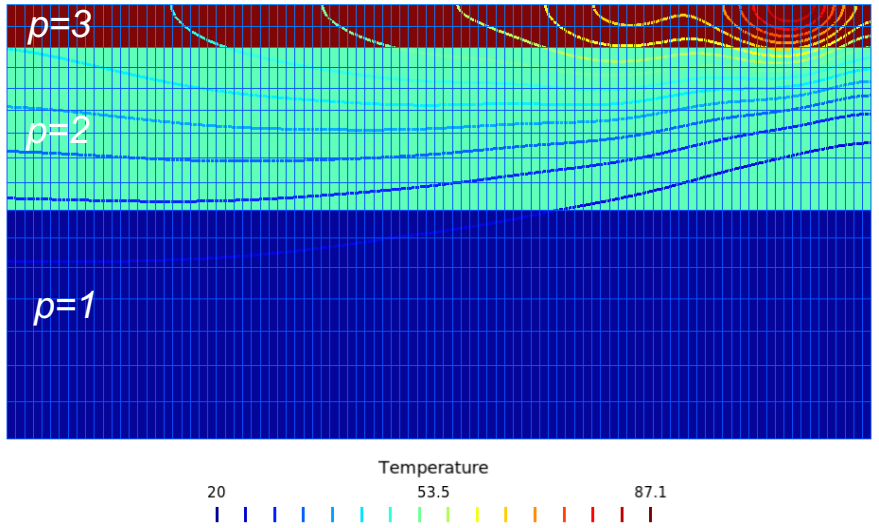

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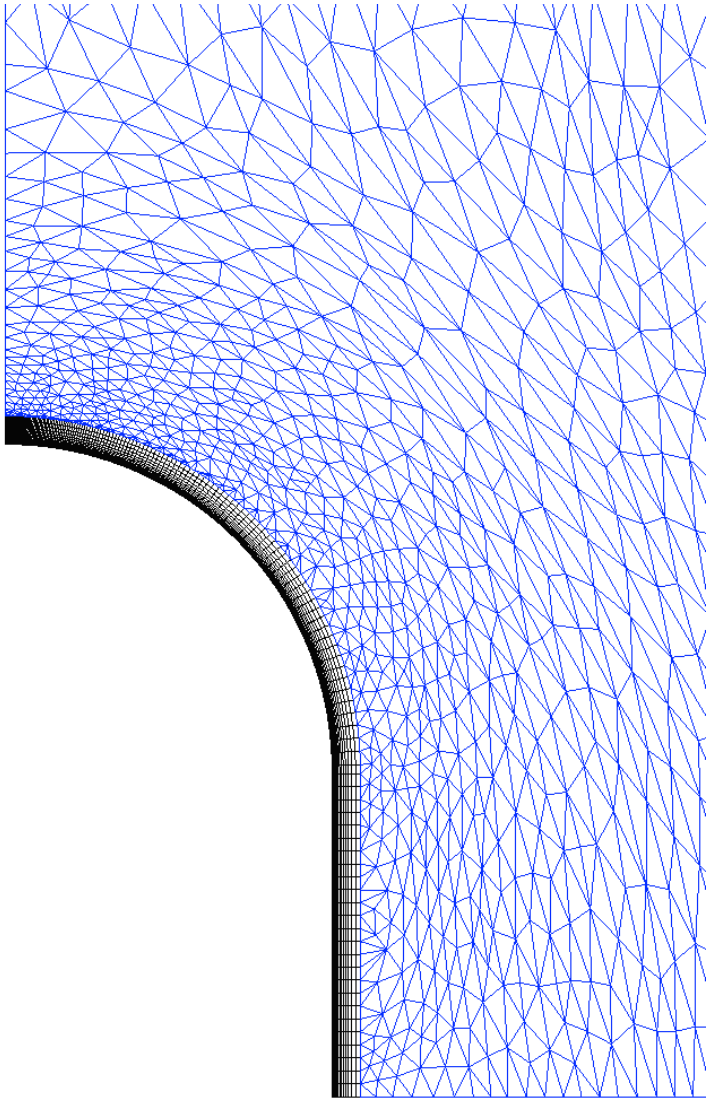

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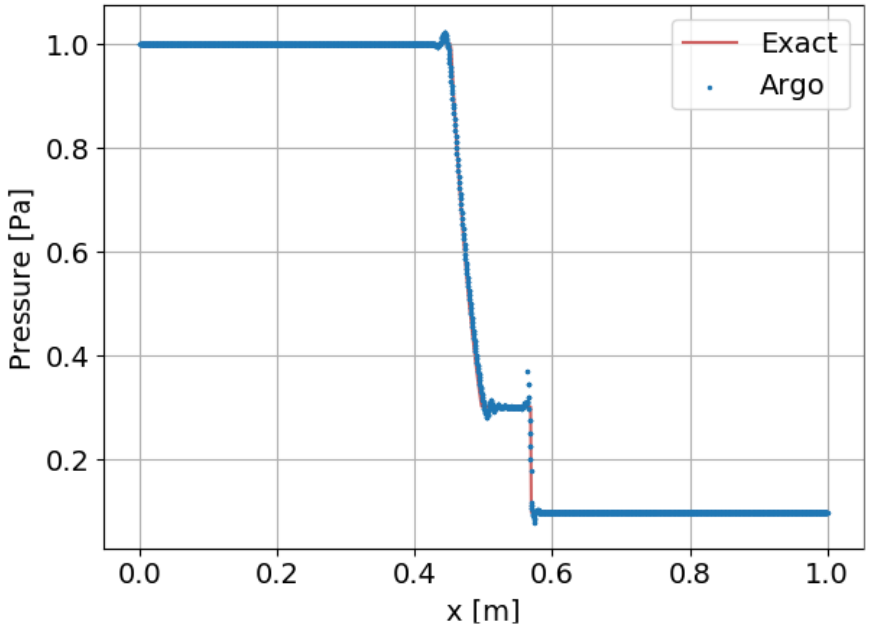
- Drawbacks
  - Duplication of the degrees of freedom on the element boundaries (costly)
  - Sensitive to under-resolved features



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Reference to go further into details

- Hartmann, Ralf. "Numerical analysis of higher order discontinuous Galerkin finite element methods." (2008)

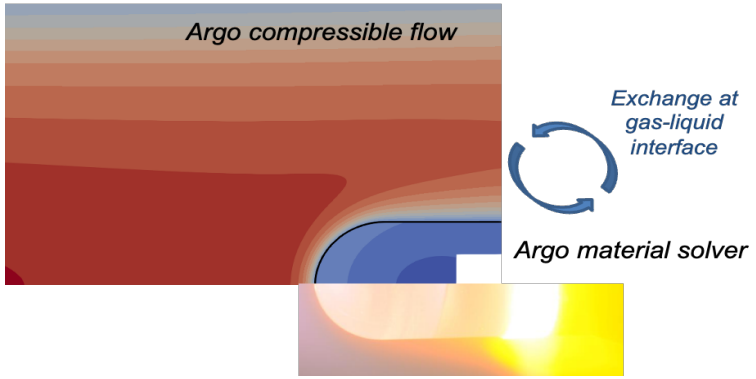
Applications - Detailed thermo-chemical degradation study of critical space debris materials

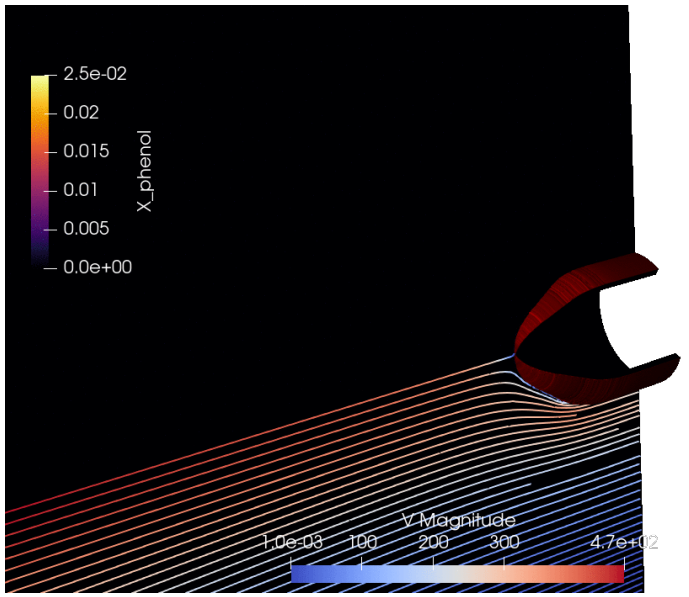
Argo flow solver (steady state) coupled with Argo Material solver (unsteady simulation with immersed method)

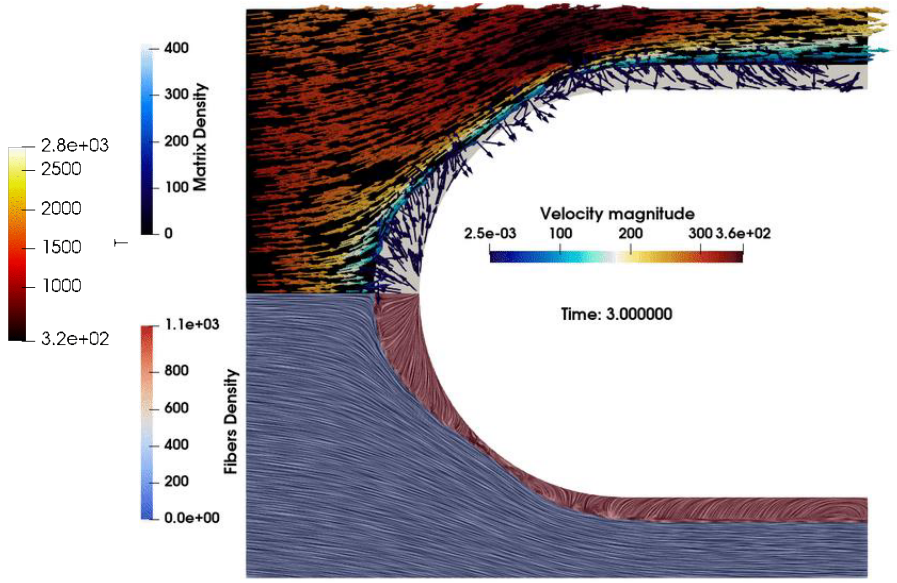
- Mostly used for melting materials (coupled with hydrodynamic conservation laws)
- Staggered approach exploits the difference in time scale for flow/material response

Argo flow solver accounting for the presence of reacting porous material (unified method)

- Use of volume averaging method to develop single set of equations valid for low/dense reactive porous materials







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