High-order methods for the next generation of computational engineering software

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Overview

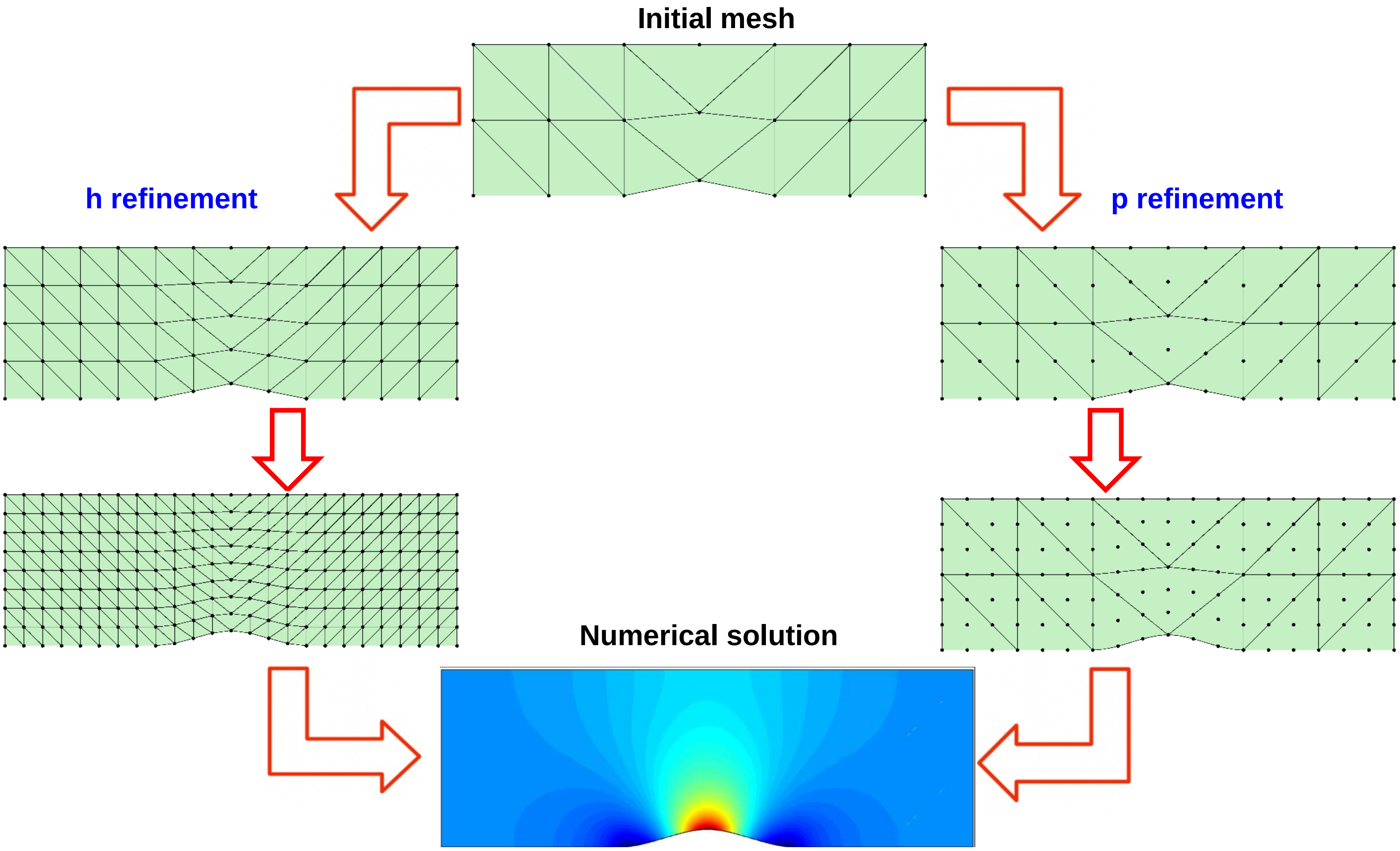
1. High-order finite element methods
2. Applications
   - Computational electromagnetics
   - Computational fluid dynamics
3. Challenges
   - High-order curved mesh generation
   - Geometry representation
4. Concluding remarks

1.

HIGH-ORDER FINITE ELEMENT METHODS

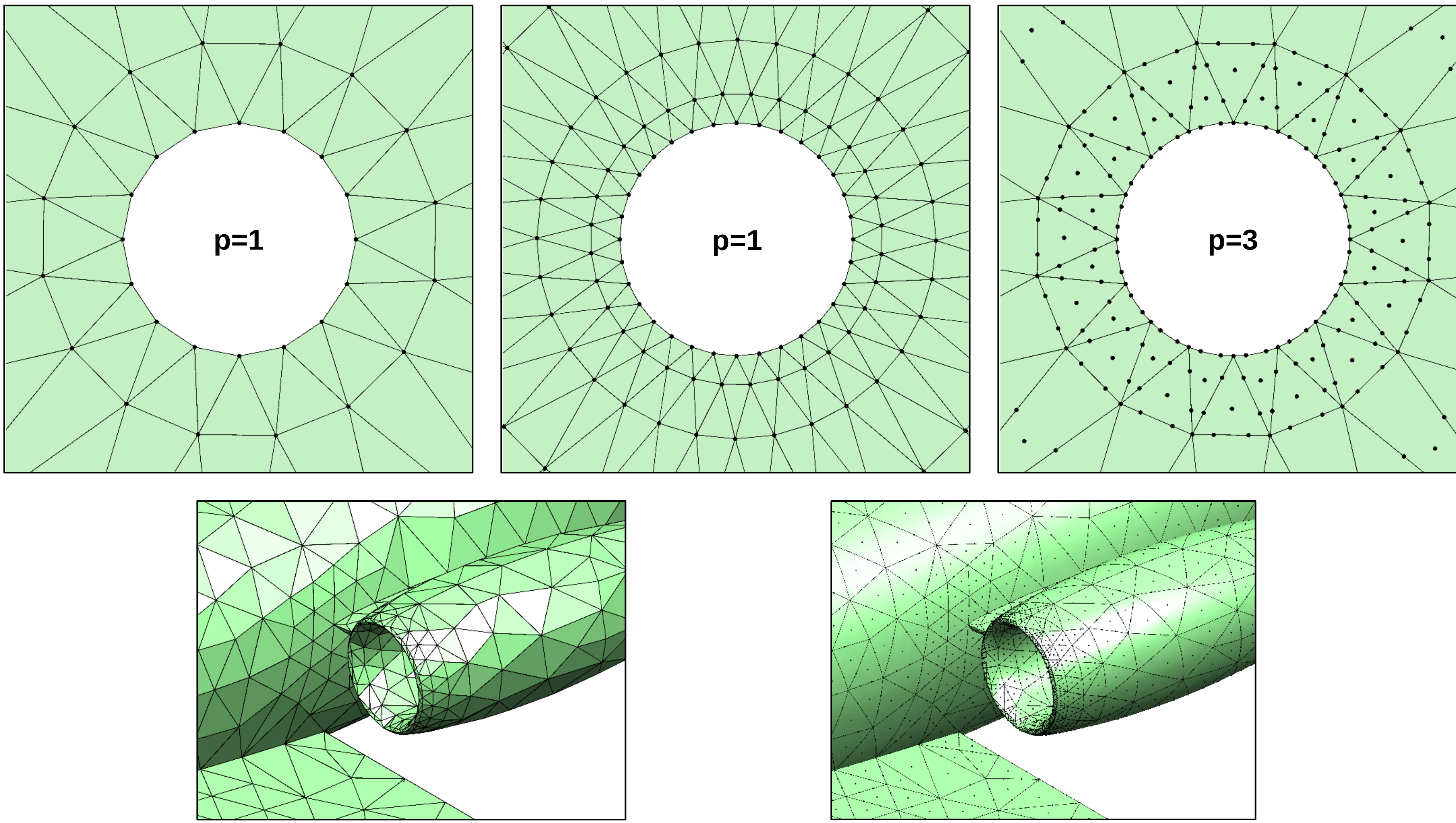
High-order finite element methods

- In the last decade there has been a great interest in evaluating the performance of high-order methods



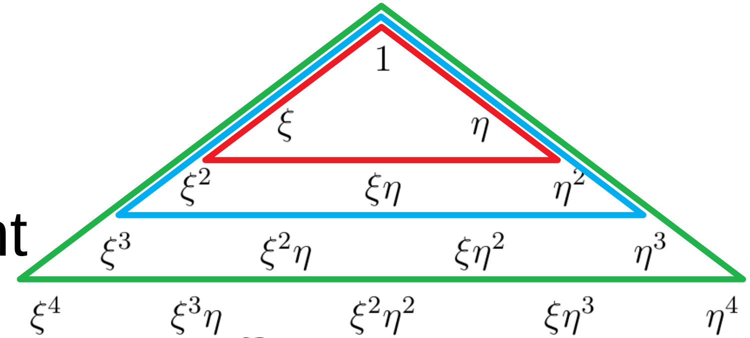
High-order finite element methods

- High-order elements provide
  - A better representation of the geometry with curved elements

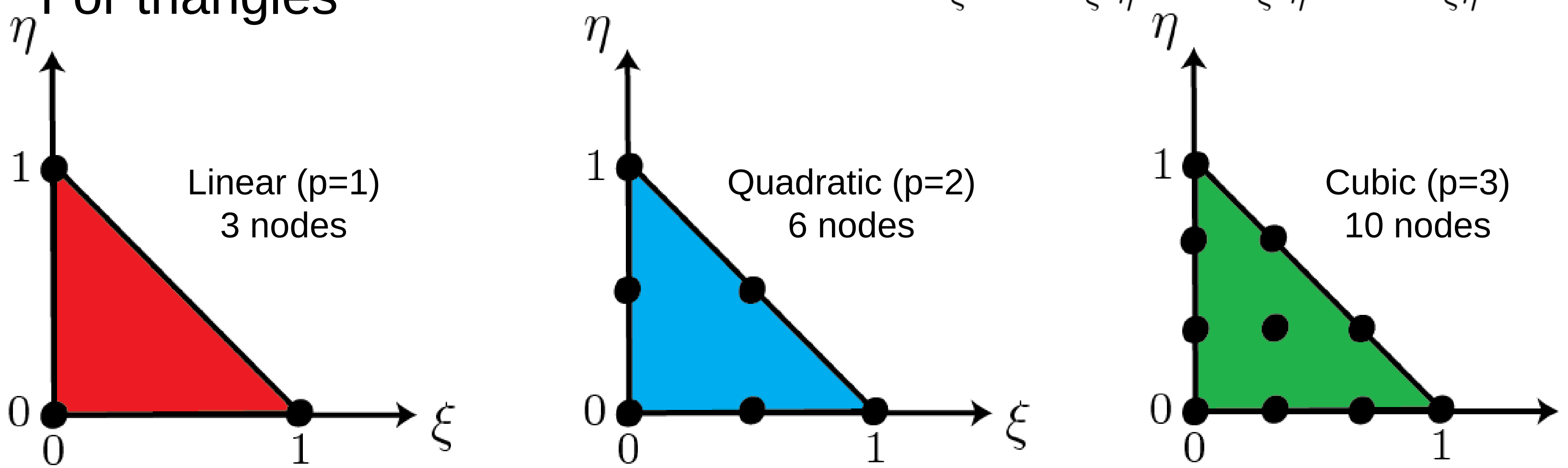


High-order finite element methods

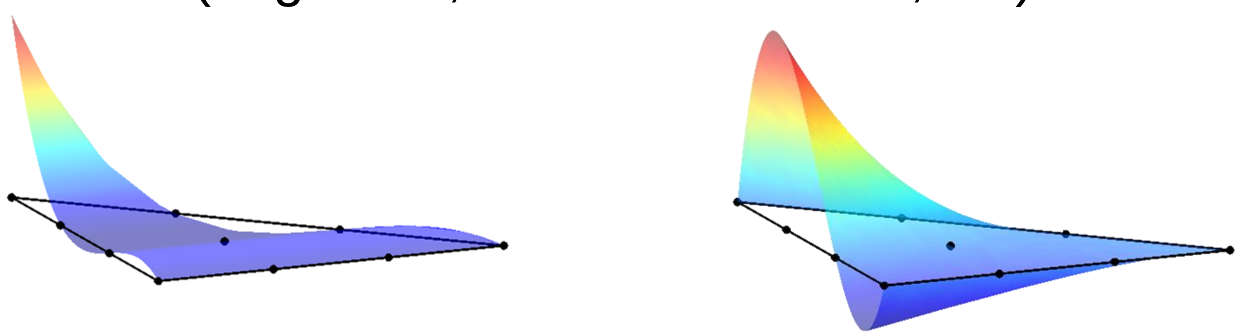
- A high-order polynomial basis are defined within the reference element



  - For triangles



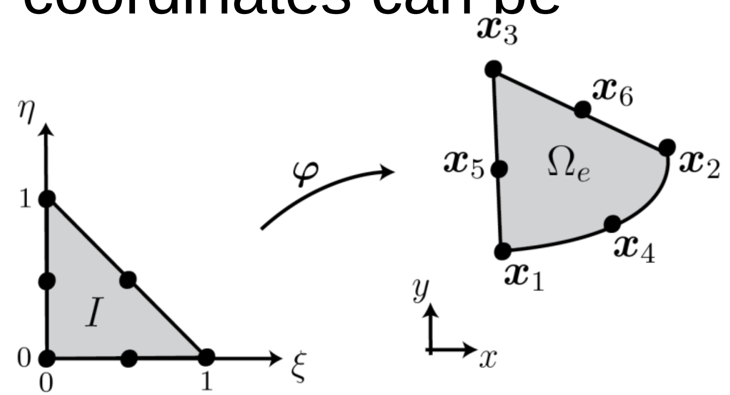
  - A polynomial basis of order p is build with (p+1)(p+2)/2 nodes
  - Lagrange polynomials are usually considered although other basis are common (Legendre, hierarchical basis, etc)



High-order finite element methods

- The mapping between the reference element and the physical element becomes nonlinear
- For a generic element with nodes $\boldsymbol{x}_i = \{(x_i, y_i)\}_{i=1,\dots,\mathtt{n_{en}}}$, the mapping between local and global coordinates can be expressed in terms of the shape functions (isoparametric)

$$\varphi(\boldsymbol{\xi}) = \sum_{i=1}^{\mathtt{n_{en}}} \boldsymbol{x}_i N_i(\boldsymbol{\xi})$$

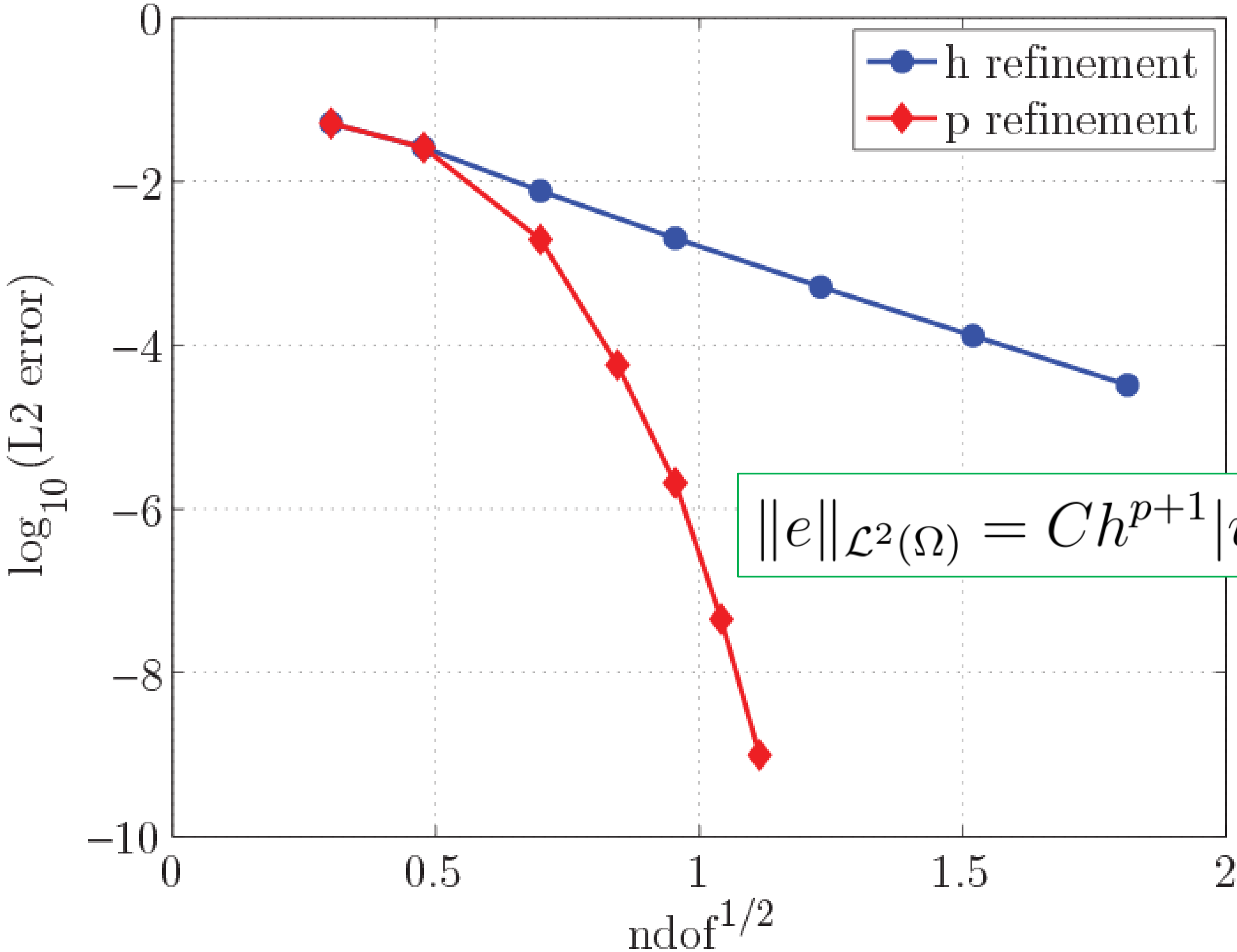


- The Jacobian $\boldsymbol{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix}$ is not constant
- Numerical integration is required to compute the integrals of the weak form

$$K_{ij}^e = \int_{\Omega_e} \boldsymbol{\nabla}_{\boldsymbol{x}} N_i(\boldsymbol{x}) \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} N_j(\boldsymbol{x}) \, d\Omega = \int_I \Big(\boldsymbol{J}^{-1} \boldsymbol{\nabla}_{\boldsymbol{\xi}} N_i(\boldsymbol{\xi})\Big) \cdot \Big(\boldsymbol{J}^{-1} \boldsymbol{\nabla}_{\boldsymbol{\xi}} N_j(\boldsymbol{\xi})\Big) |\boldsymbol{J}| \, d\boldsymbol{\xi}$$

High-order finite element methods

- High-order elements provide
  - Exponential convergence for smooth solutions



$$\|e\|_{\mathcal{L}^2(\Omega)} = Ch^{p+1}|u|_{\mathcal{H}^{p+1}(\Omega)}$$

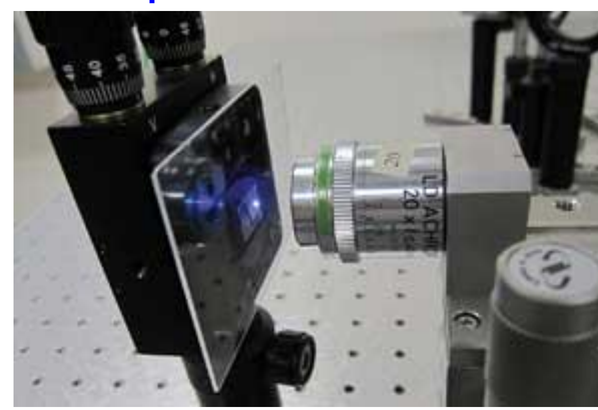
2.

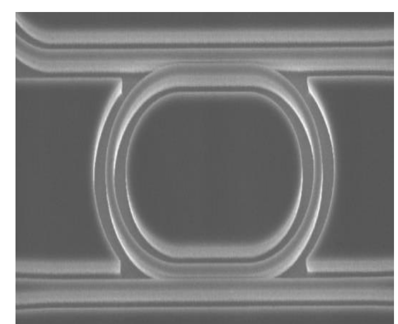
APPLICATIONS

Computational electromagnetics

Motivation

- Finite differences are still the predominant technique in research and industry.
- There is a need to improve numerical capabilities in order to
  - Simulate the interaction of electromagnetic waves with thin wires (multi-scale phenomena)
  - Study the effect of lighting strike in an aircraft
  - Reduce the design cycles of several optical and photonic devices





High-order discontinuous Galerkin (DG) formulation

- **Maxwell's equations**
- In dimensionless conservative form

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \mathbf{F}_k(\boldsymbol{U})}{\partial x_k} = \mathbf{S}(\boldsymbol{U})$$

where

$$\boldsymbol{U} = \begin{pmatrix} \varepsilon \mathbf{E} \\ \mu \mathbf{H} \end{pmatrix} \qquad \mathbf{F}_1 = \begin{pmatrix} 0 \\ H_3 \\ -H_2 \\ 0 \\ -E_3 \\ E_2 \end{pmatrix} \qquad \mathbf{F}_2 = \begin{pmatrix} -H_3 \\ 0 \\ H_1 \\ E_3 \\ 0 \\ -E_1 \end{pmatrix} \qquad \mathbf{F}_3 = \begin{pmatrix} H_2 \\ -H_1 \\ 0 \\ -E_2 \\ E_1 \\ 0 \end{pmatrix} \qquad \mathbf{S} = \begin{pmatrix} -\sigma \mathbf{E} \\ \mathbf{0} \end{pmatrix}$$

- Linear system of hyperbolic equations

$$\frac{\partial \boldsymbol{U}}{\partial t} + \mathbf{A}_k \frac{\partial \mathbf{U}}{\partial x_k} = \mathbf{S}(\boldsymbol{U})$$

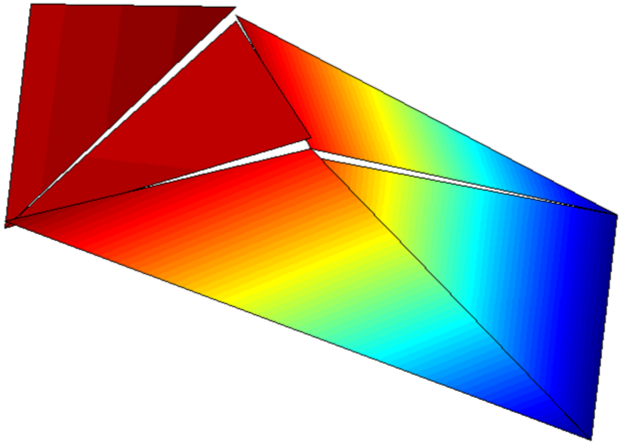
with $\mathbf{A}_k = \dfrac{\partial \mathbf{F}_k}{\partial x_k}$

High-order discontinuous Galerkin (DG) formulation

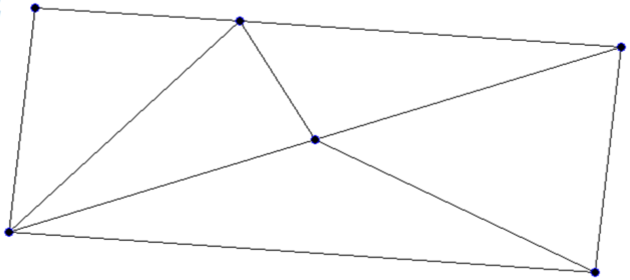
- **Weak formulation**
- The solution is sought in a broken space (i.e., discontinuous across elements). The weak form in an element is

$$\int_{\Omega_e} \boldsymbol{W} \cdot \frac{\partial \boldsymbol{U}_e}{\partial t}\, d\Omega - \int_{\Omega_e} \frac{\partial \boldsymbol{W}}{\partial x_k} \cdot \boldsymbol{F}_k(\boldsymbol{U}_e)\, d\Omega + \int_{\partial\Omega_e} \boldsymbol{W} \cdot \boldsymbol{F}_{\boldsymbol{n}}(\boldsymbol{U}_e)\, d\Gamma = \int_{\Omega_e} \boldsymbol{W} \cdot \boldsymbol{S}(\boldsymbol{U}_e)\, d\Omega$$

- The continuity of the fluxes across the element boundaries is weakly imposed by introducing a numerical flux



$$\int_{\Omega_e} \boldsymbol{W} \cdot \frac{\partial \boldsymbol{U}_e}{\partial t}\, d\Omega - \int_{\Omega_e} \frac{\partial \boldsymbol{W}}{\partial x_k} \cdot \boldsymbol{F}_k(\boldsymbol{U}_e)\, d\Omega + \int_{\partial\Omega_e} \boldsymbol{W} \cdot \boxed{\widetilde{\boldsymbol{F}}_n(\boldsymbol{U}_e, \boldsymbol{U}_e^{\text{out}})}\, d\Gamma = \int_{\Omega_e} \boldsymbol{W} \cdot \boldsymbol{S}(\boldsymbol{U}_e)\, d\Omega$$

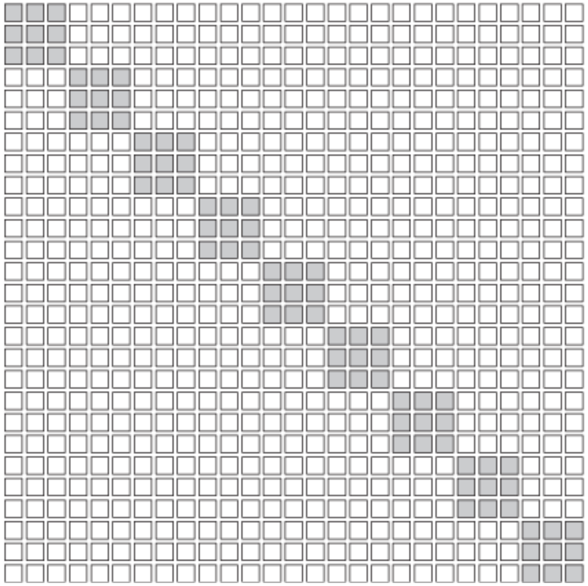


- The numerical flux in an exact or approximate Riemman solver

High-order discontinuous Galerkin (DG) formulation

- **System of ODEs**
- The semi-discrete system reads

$$\mathbf{M}\frac{d\mathbf{U}}{dt} + \mathbf{R}(\mathbf{U}) = \mathbf{0}$$



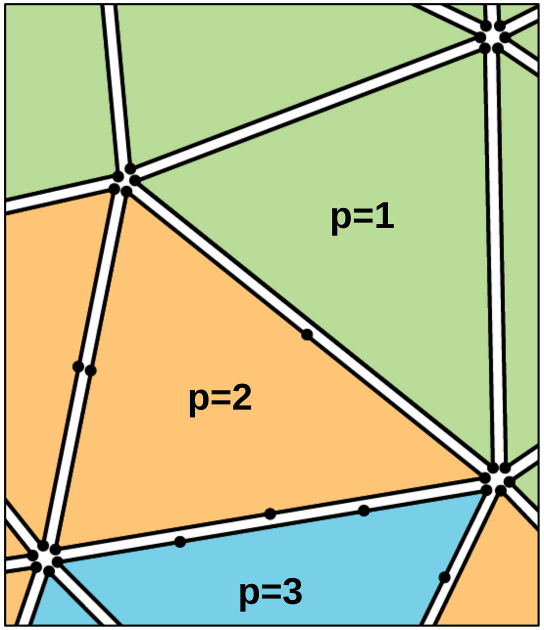
where the mass matrix is block-diagonal

Each block has dimension equal to the number of nodes per element

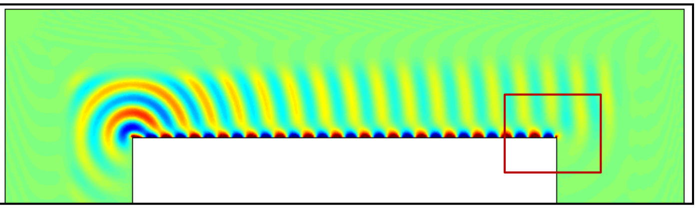
  - The global matrix is never stored

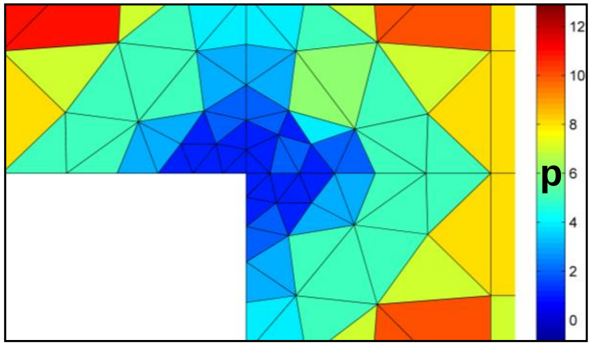
- A high-order Runge-Kutta explicit time marching algorithm is suitable for
  - Explicit time marching because in many CEM applications a uniform mesh spacing is required (dictated by the frequency of the waves)

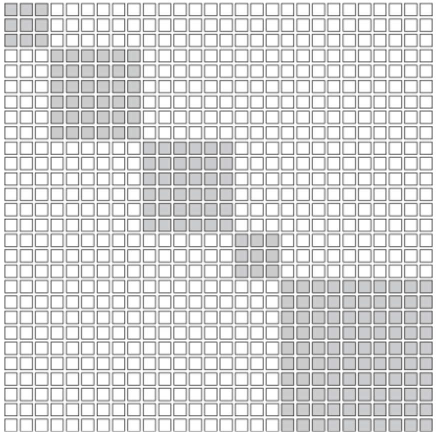
High-order discontinuous Galerkin (DG) formulation



- **Advantages of a DG formulation**
  - Easy to parallelise when explicit time marching is used (block diagonal matrix)
  - Ability to use non-uniform degree of approximation (p-adaptivity and singularities)
  - Efficient for very high-order approximations



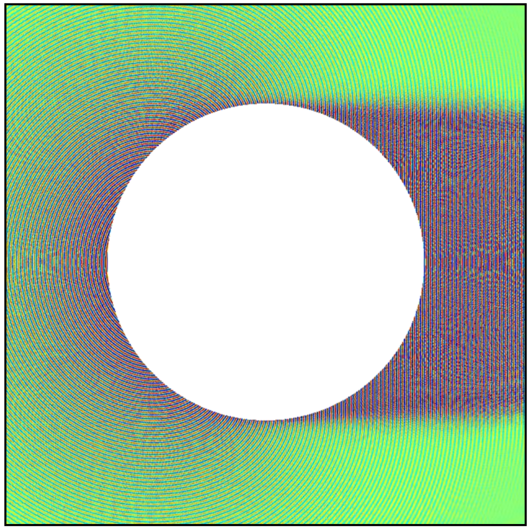


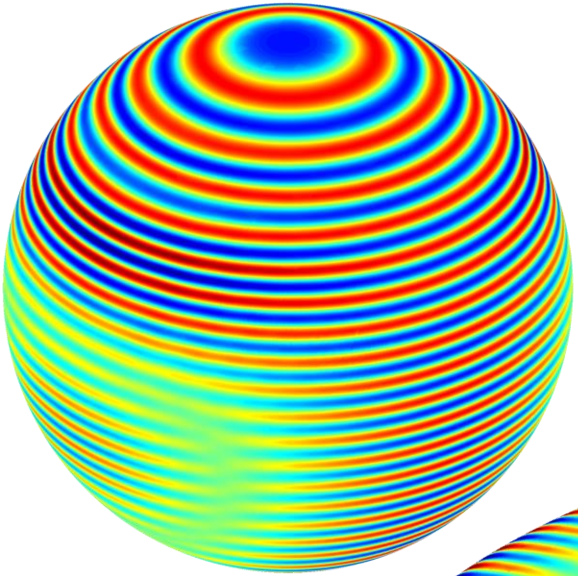


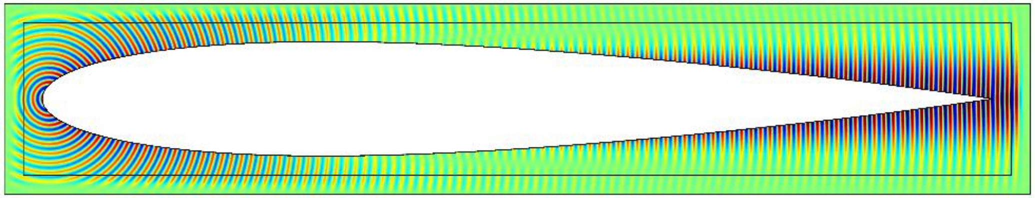
- **Disadvantages of a DG formulation**
  - For the same spatial resolution it uses more degrees of freedom than the standard continuous Galerkin formulation

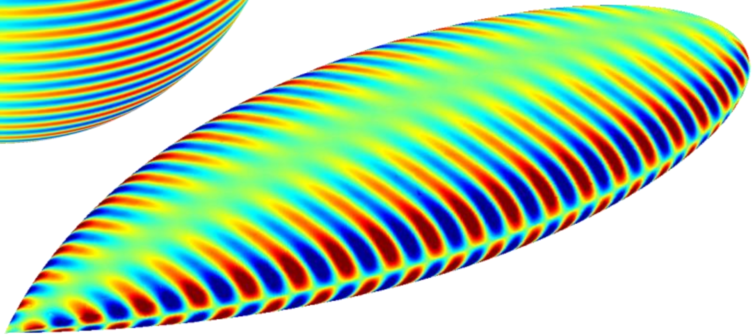
Electromagnetic scattering

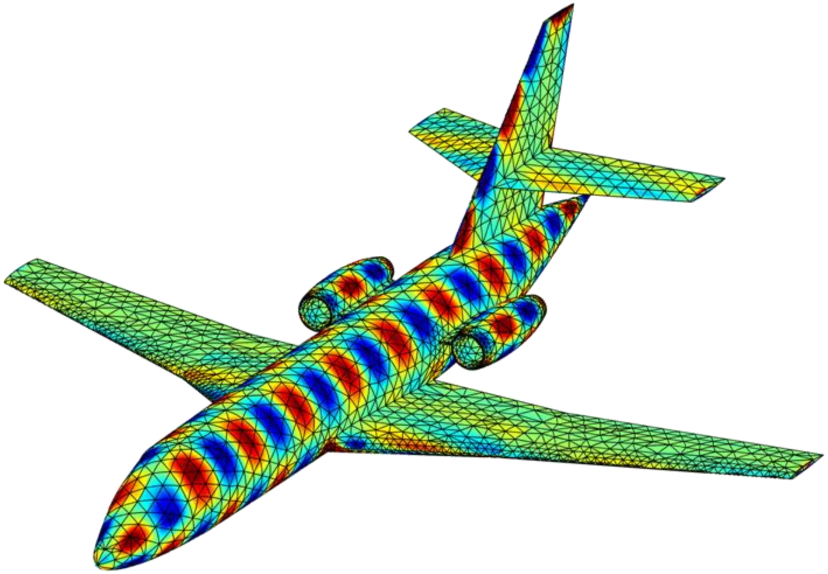
- With high-order approximations simulations can be performed with 4-6 nodes per wavelength opening the door to the simulation of higher frequency problems and more complex geometries







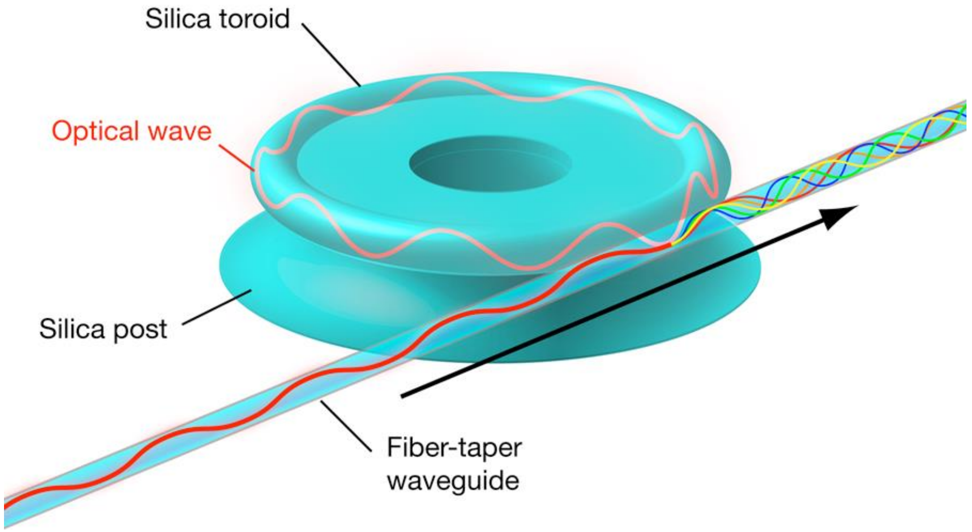




Photonics and optics

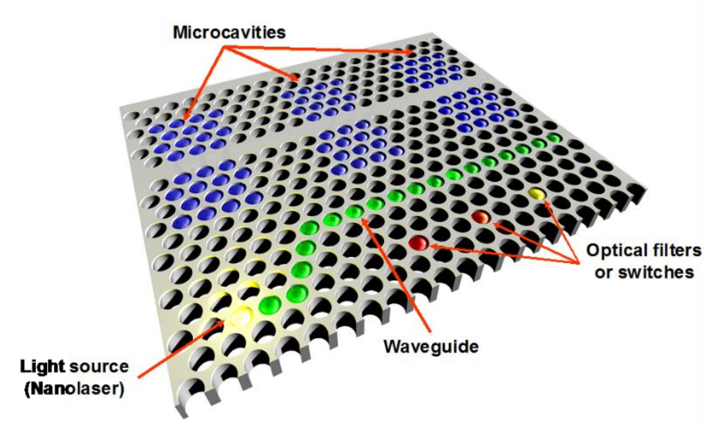
Physical problem

- Nano-lasers, resonators and photonic crystals



Y.K. Chembo and N. Yu, 2010

- Applications
  - Communications
    - Filtering, energy transfer,…
  - Medical
    - Surgical treatment, eye treatment,…
  - Nano-photonic devices

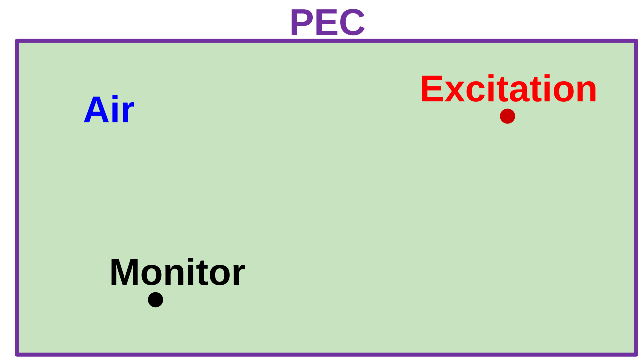


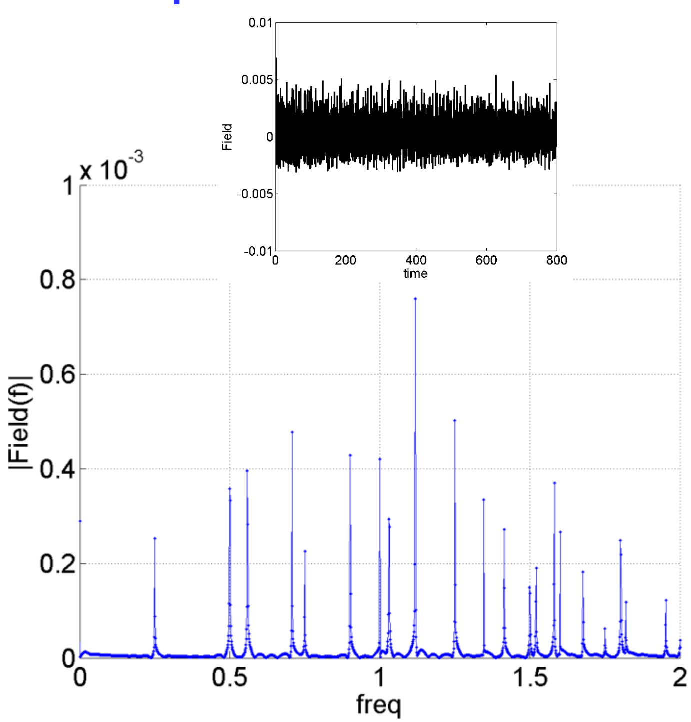
Photonics and optics

Wave Propataion 1
Tomorrow morning

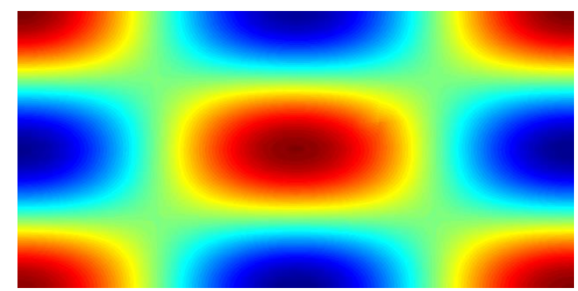
Resonances in cavities

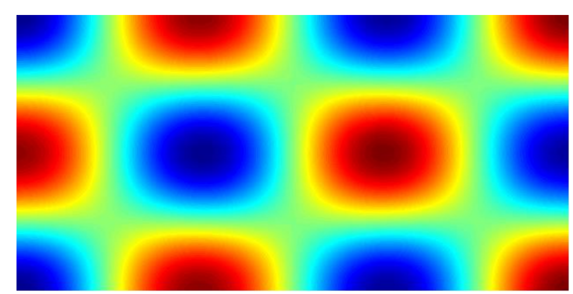
- Excite the fields using an initial condition or source
- Monitor the fields at certain point/s
- Transform the fields to the frequency domain to obtain the resonant frequencies





Approx	Exact
0.2497	0.2500
0.4994	0.5000
0.5585	0.5590
0.7069	0.7071
0.7503	0.7500
0.9011	0.9014
1.0000	1.0000
1.0302	1.0308
1.1183	1.1180
1.2497	1.2500
1.3462	1.3463
1.4138	1.4142





2.

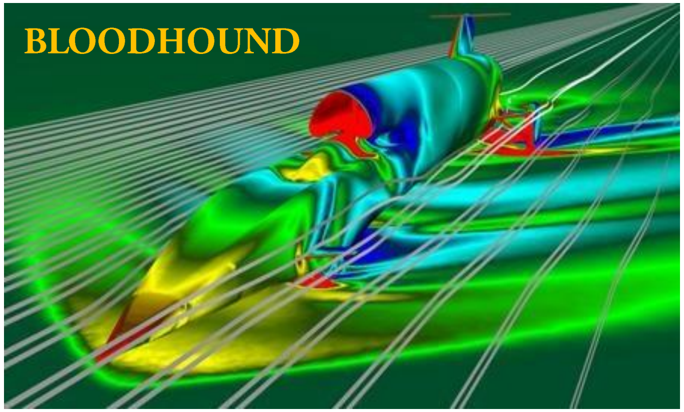
APPLICATIONS

Computational fluid dynamics

Motivation

- Europe needs to advance in the numerical simulation capabilities of aeronautical flows. This is partially motivated by the FlightPath 2050 vision

- Finite volumes are still today the predominant tool in industrial aerodynamic applications
    - TAU (DLR), FUN3D (NASA), FLITE (SU)



- Huge investment in developing high-order methods for the simulation of high Reynolds number flows in industry but… we are not quite there yet!

High-order stabilised FE formulation

- **Compressible Navier-Stokes equations**
- In dimensionless conservative form

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} - \frac{\partial \mathbf{G}_i}{\partial x_i} = \mathbf{0}$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho v_1 \\ \rho v_2 \\ \rho E \end{pmatrix} \qquad \mathbf{F}_i = \begin{pmatrix} \rho v_i \\ \rho v_1 v_i + P\delta_{1i} \\ \rho v_2 v_i + P\delta_{2i} \\ (\rho E + P) v_i \end{pmatrix} \qquad \mathbf{G}_i = \begin{pmatrix} 0 \\ \tau_{i1} \\ \tau_{i2} \\ v_k \tau_{ki} + q_i \end{pmatrix}$$

- **SUPG formulation**
- The standard Galerkin formulation introduces negative diffusion that needs to be balanced

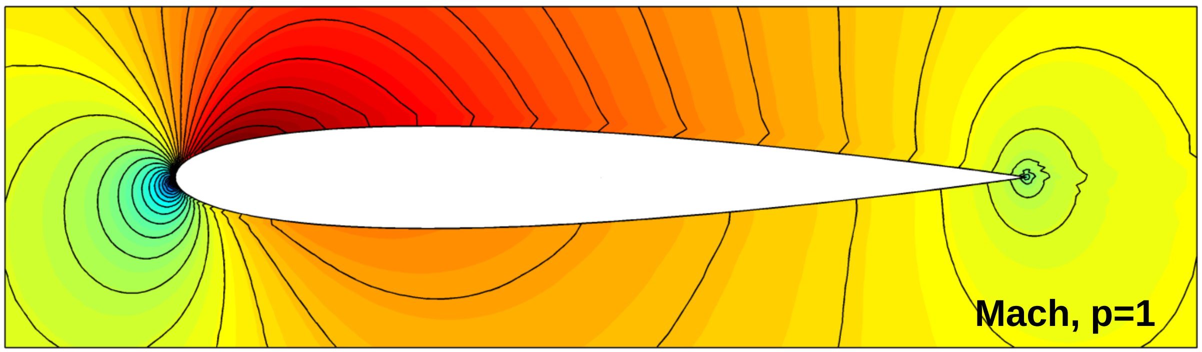
$$\int_\Omega \left(\mathbf{W} \cdot \frac{\partial \mathbf{U}}{\partial t} - \frac{\partial \mathbf{W}}{\partial x_k} \cdot \mathbf{F}_k(\mathbf{U}) + \frac{\partial \mathbf{W}}{\partial x_i} \cdot \left(\mathbf{K}_{ij} \frac{\partial \mathbf{U}}{\partial x_j} \right) \right) d\Omega$$

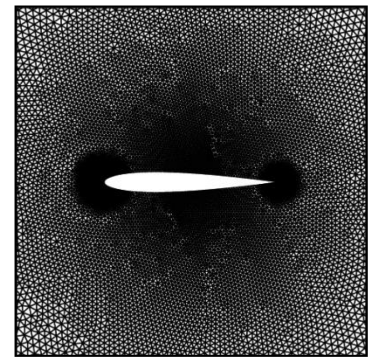
$$= \int_{\partial\Omega} \mathbf{W} \cdot \Big(- \mathbf{F}_k(\mathbf{U}) + \mathbf{G}_k(\mathbf{U}) \Big) n_k d\Gamma$$

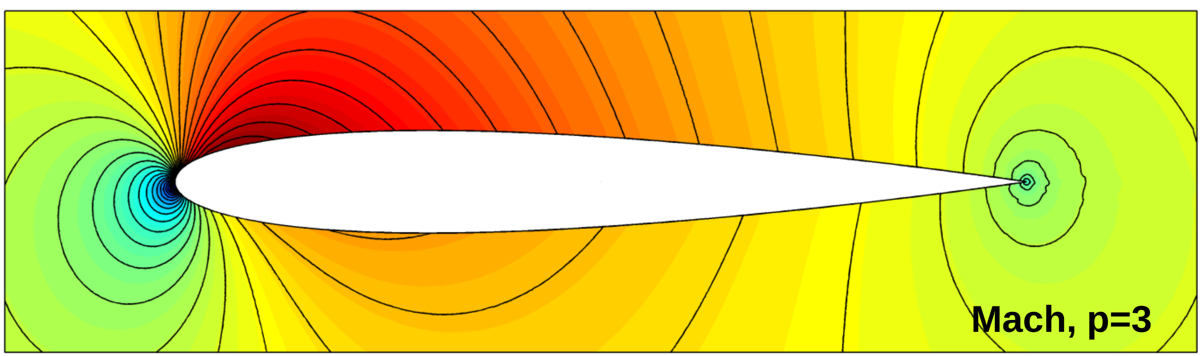
SUPG – CFD - Examples

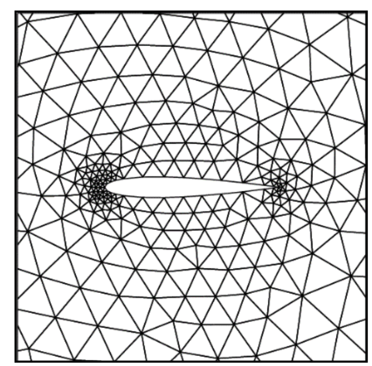
NACA0012, Mach 0.63, angle=2º

- Spurious entropy production substantially reduced by using high-order elements in coarse meshes





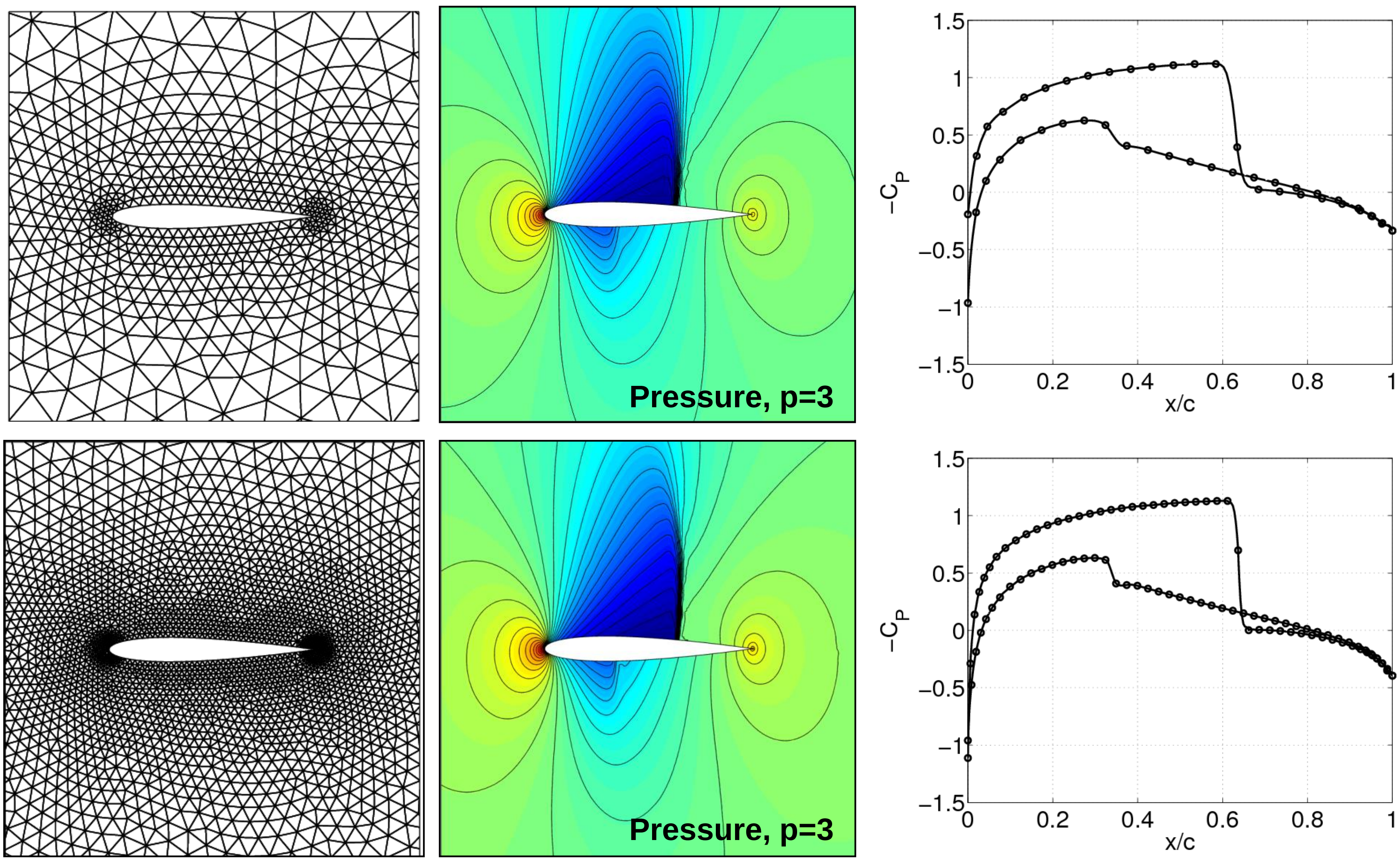




SUPG – CFD - Examples

NACA0012, Mach 0.8, angle=1.25º

- Good performance of high-order elements in coarse meshes with the shock-capturing term

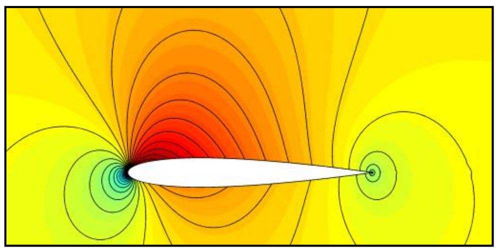


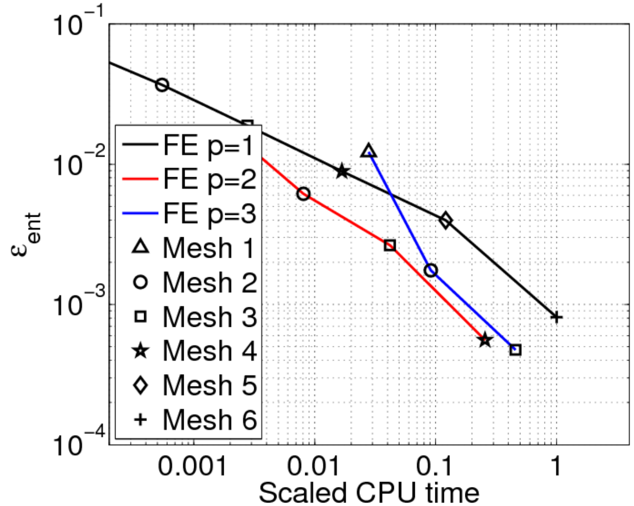
SUPG – CFD - Examples

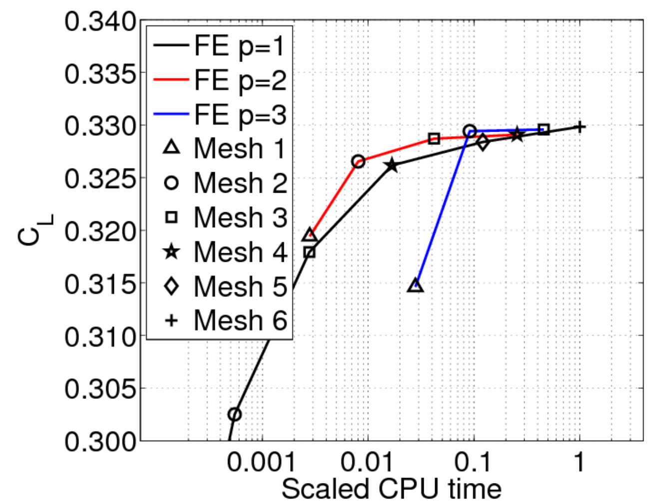
Performance

- For a given accuracy, an important reduction of CPU time and number of dofs by using high-order approximations

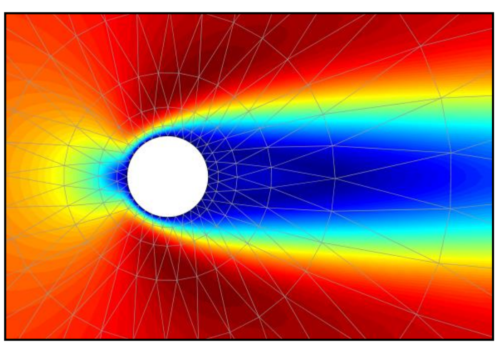
NACA0012, Mach 0.63, AoA=2º

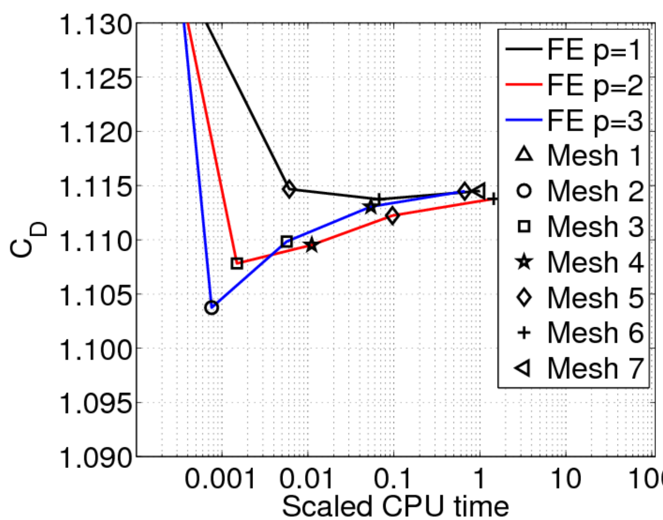


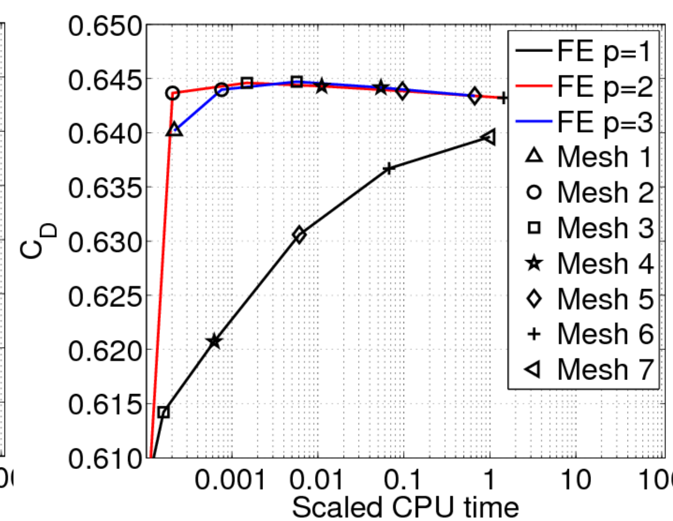




Circular cylinder, Mach 0.1, Re=30



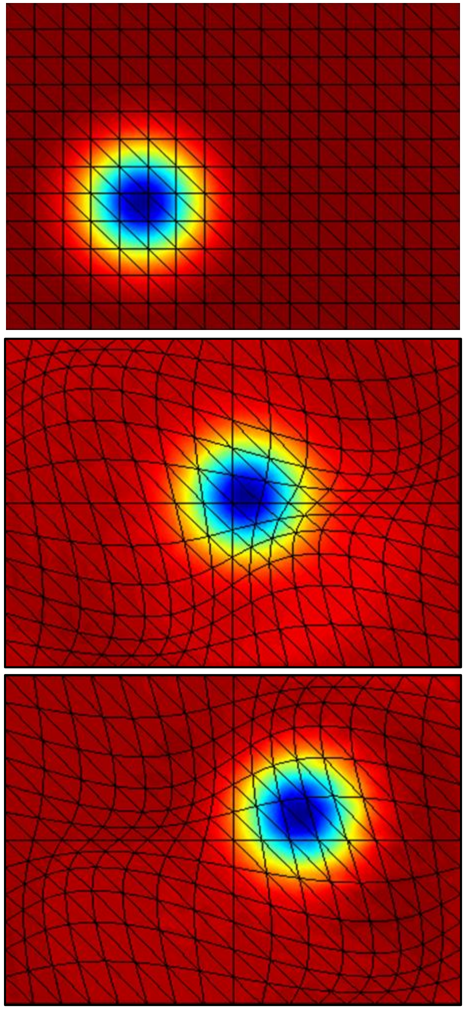


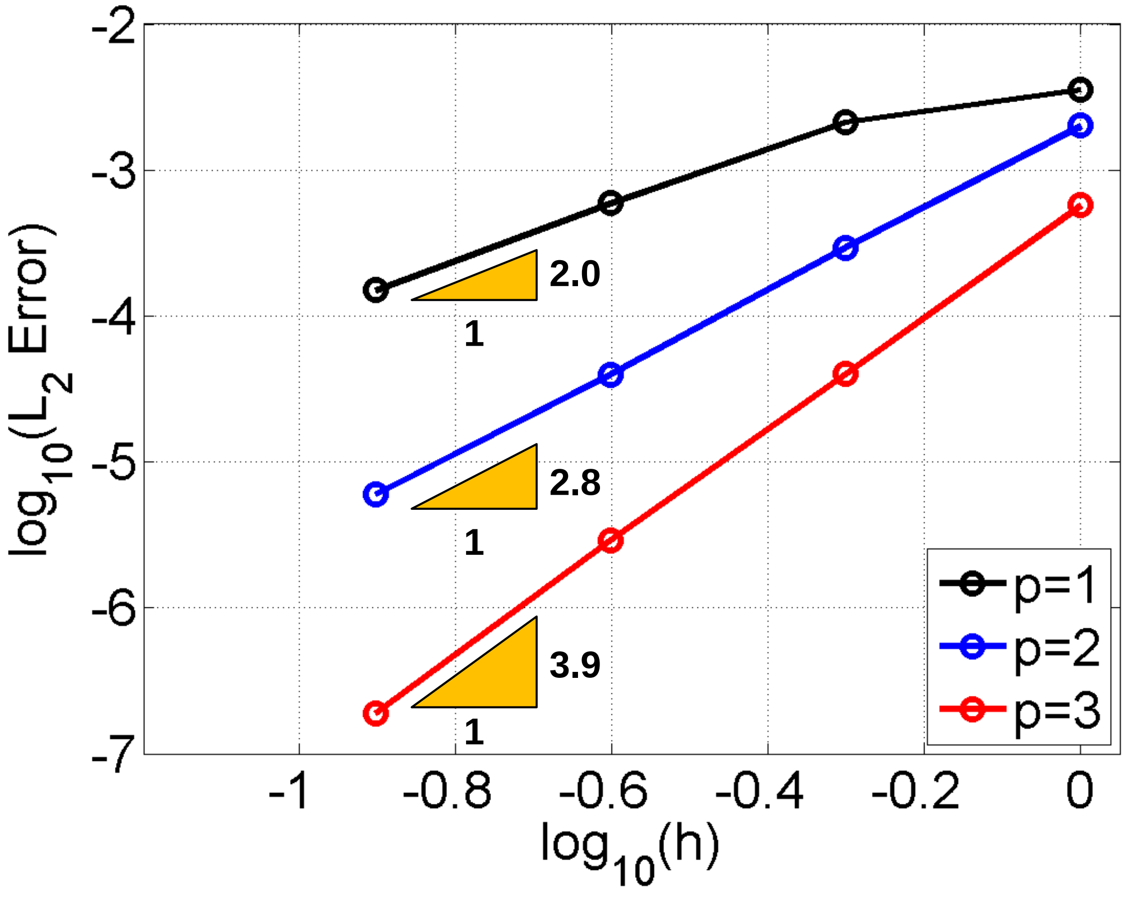


Moving domains

Validation

- Euler vortex – Given mapping
  - Optimal convergence for different orders of approximation





3.

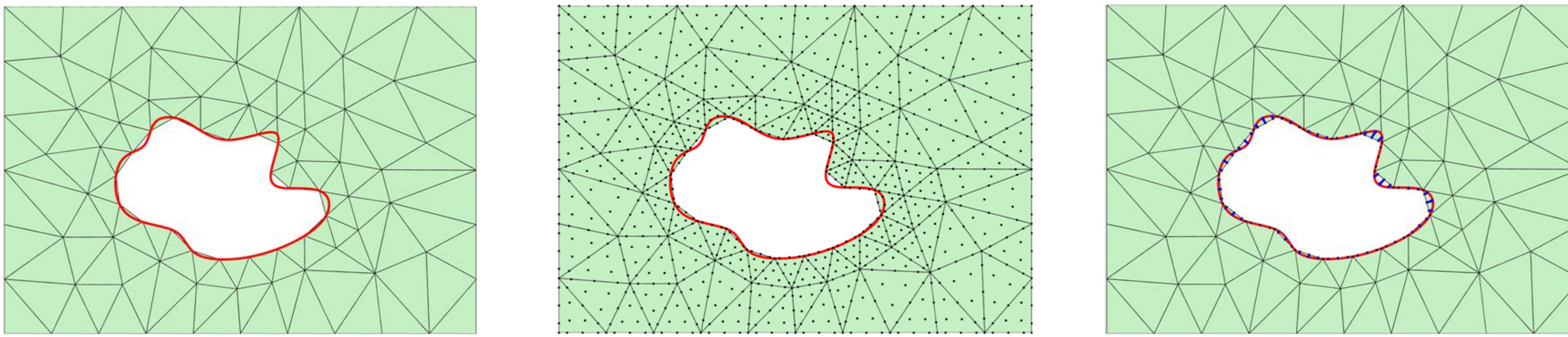
CHALLENGES

High-order mesh generation

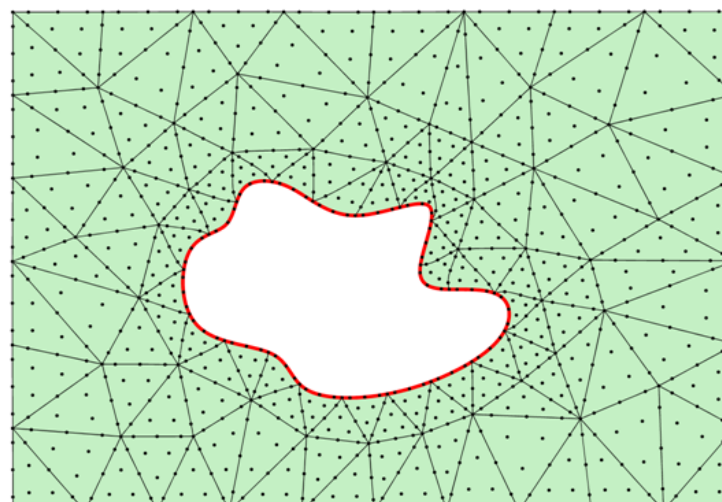
Elastic analogy

Rationale

- Starting from a standard linear mesh, build a high-order nodal distribution on each element with straight edges



- “Project” boundary nodes on the true (CAD) boundary
- Solve a linear elastic problem
  - Dirichlet boundary conditions are applied in curved boundaries corresponding to the displacement given by the projection

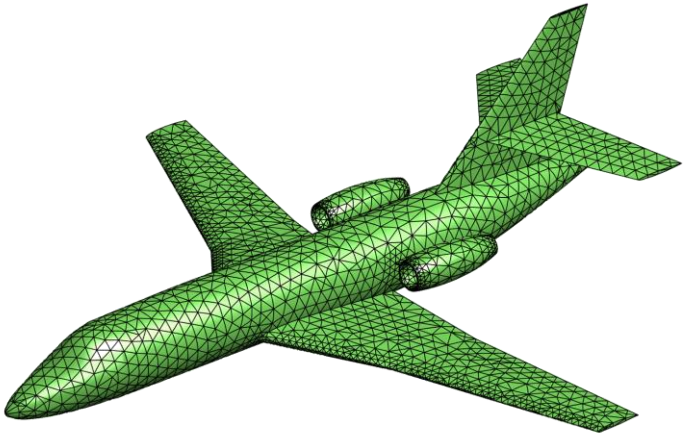


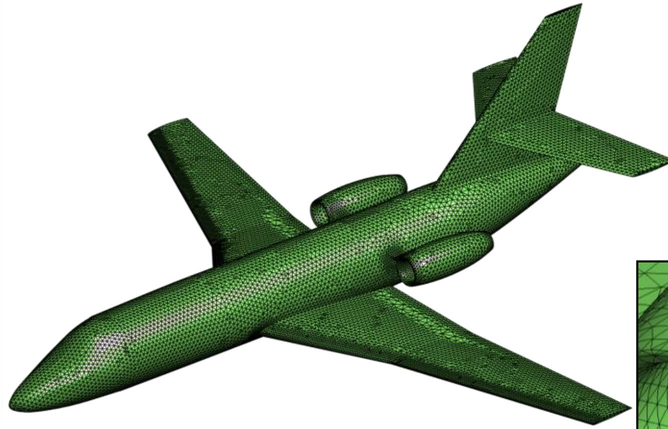
Persson & Peraire (2009)

3D examples

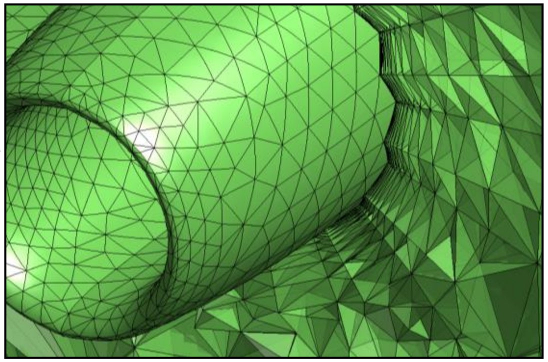
Falcon

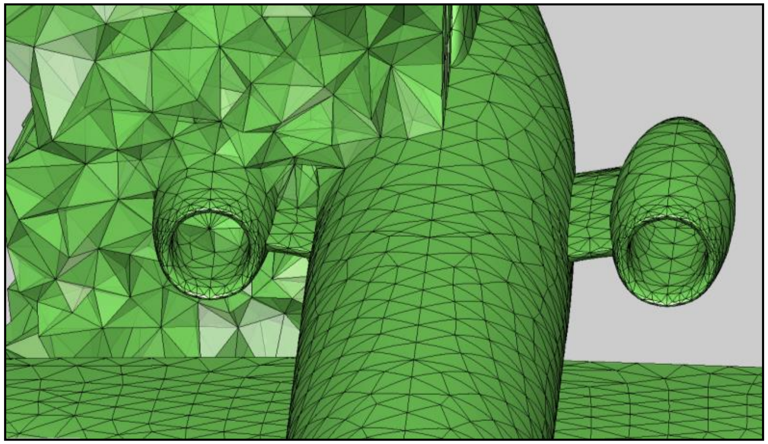
- Isotropic and boundary layer meshes of a complete aircraft

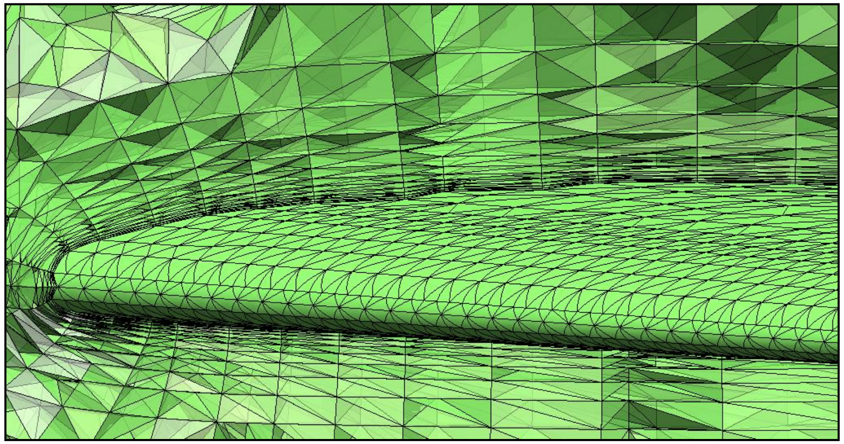




- Minimum element quality 0.2 (isotropic) and 0.1 (boundary layer)



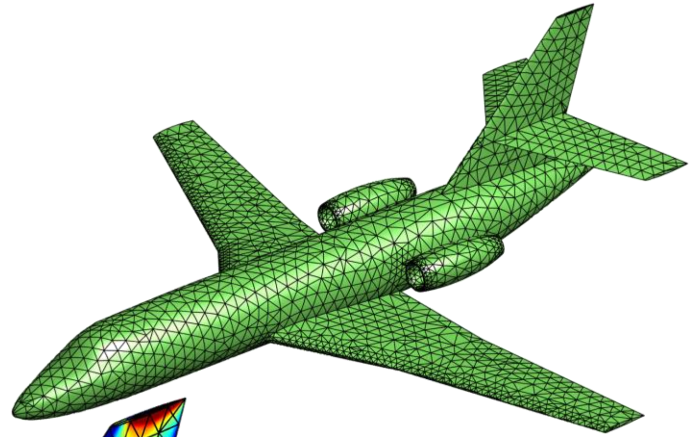


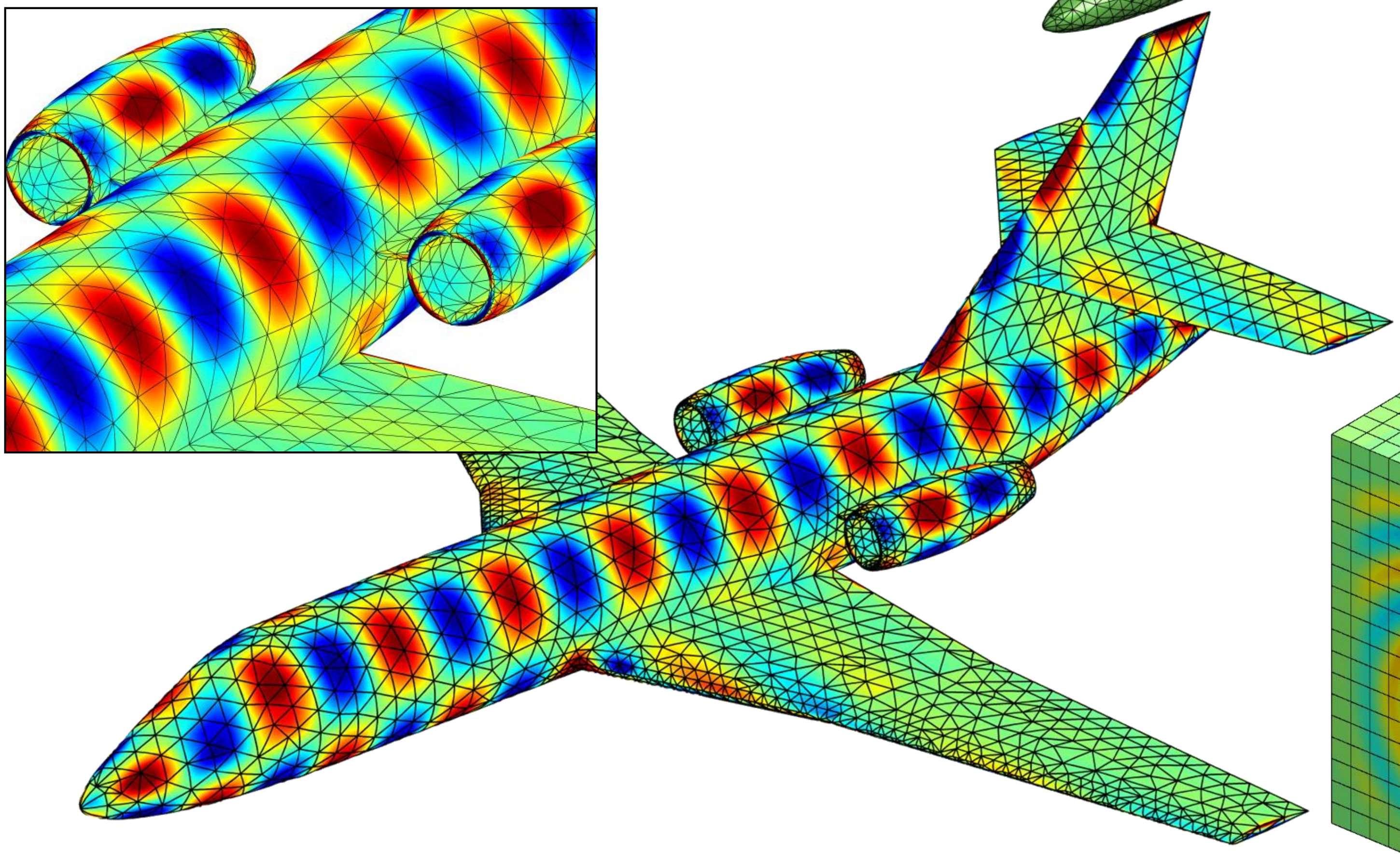


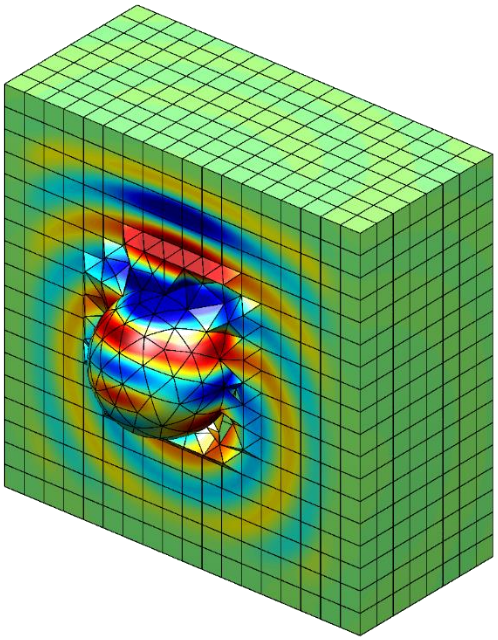
3D examples

Electromagnetic scattering

- High-order DG
- Hybrid meshes



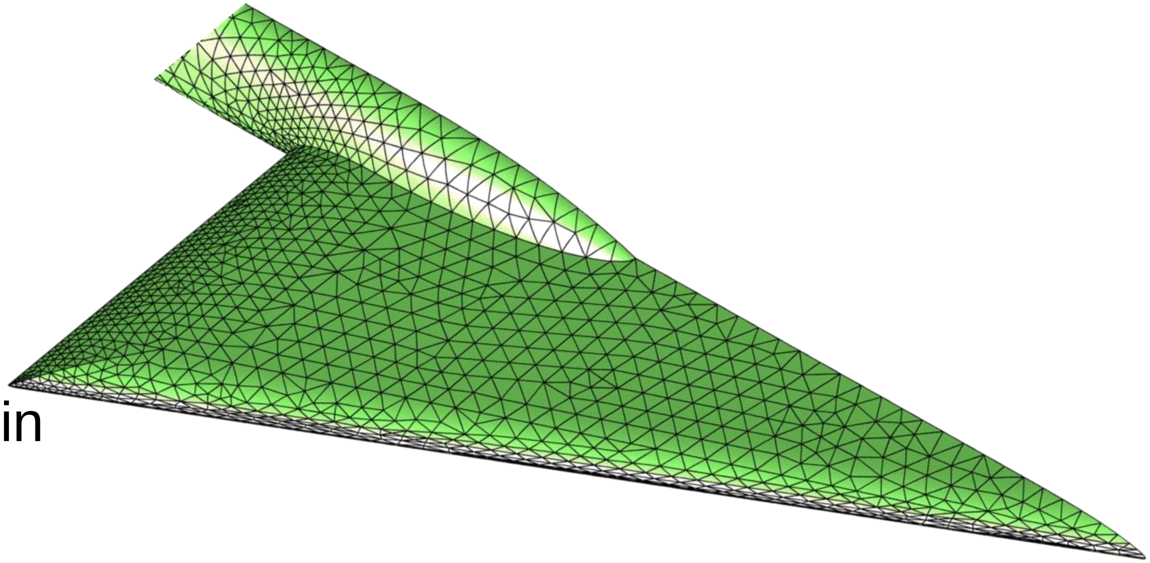


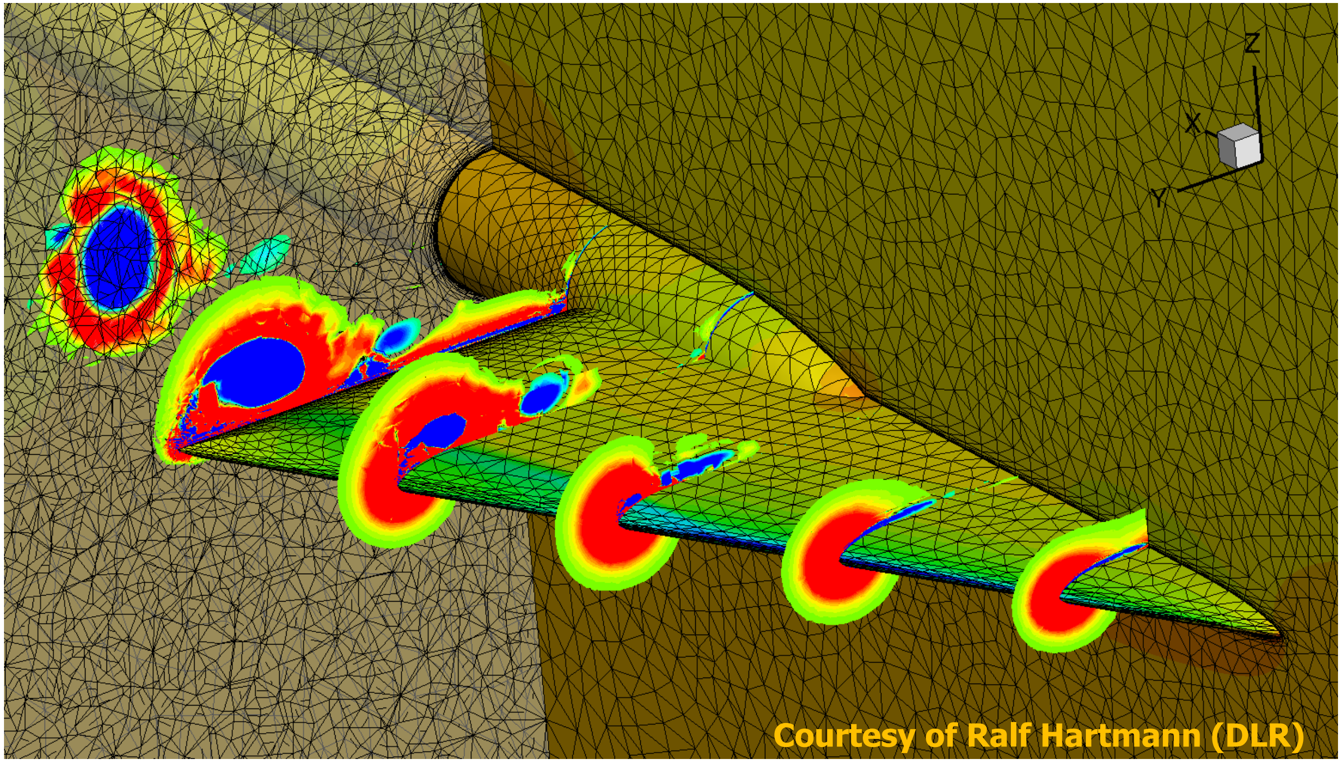


3D examples

Delta wing

- Subsonic turbulent flow simulation
  - discontinuous Galerkin
  - p=3
  - Re = $3 \cdot 10^6$
  - M = 0.4
  - AoA = 13.3º





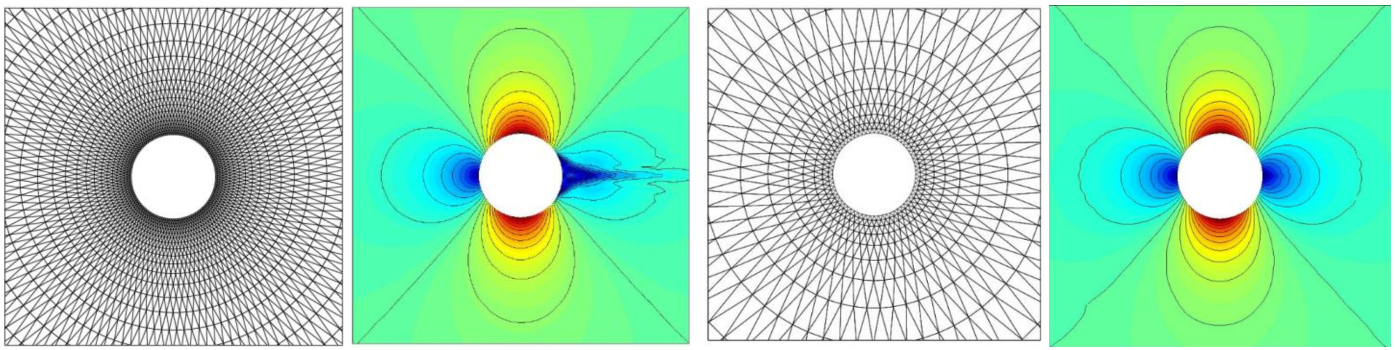
3.

CHALLENGES

Geometry representation

The importance of the geometrical model

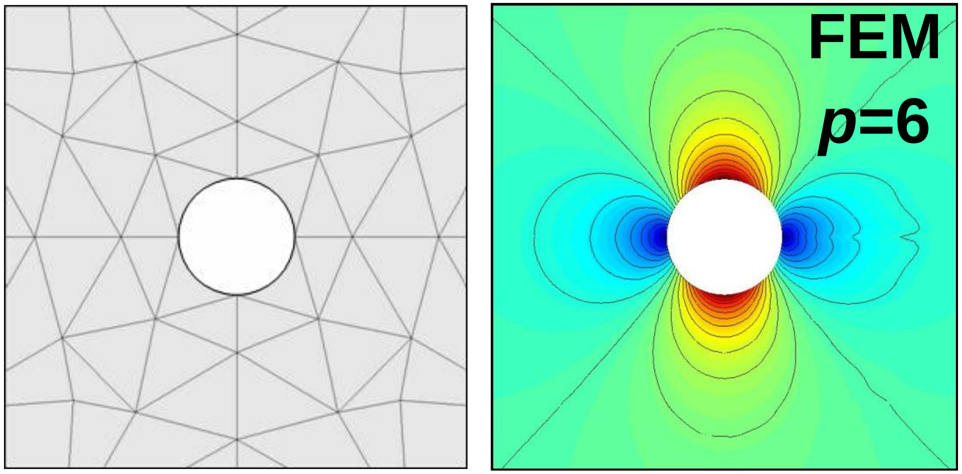
- The higher the order the better, but a poor geometric approximation can prevent to exploit the full potential of high-order methods
  - Inviscid subsonic flow around a circle at free-stream Mach 0.3



Bassi and Rebay (1997), Barth (1998)

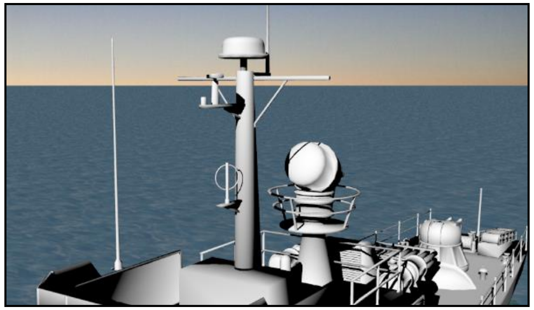
p=1; 8 192 dof

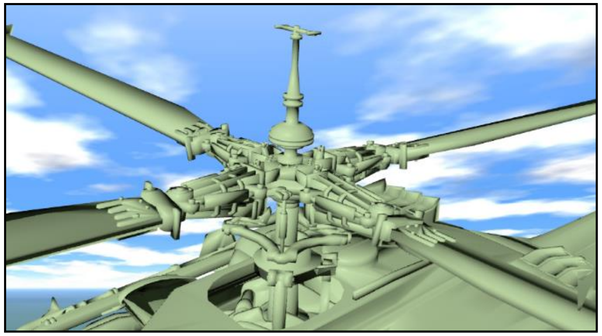
p=2; 6 144 dof

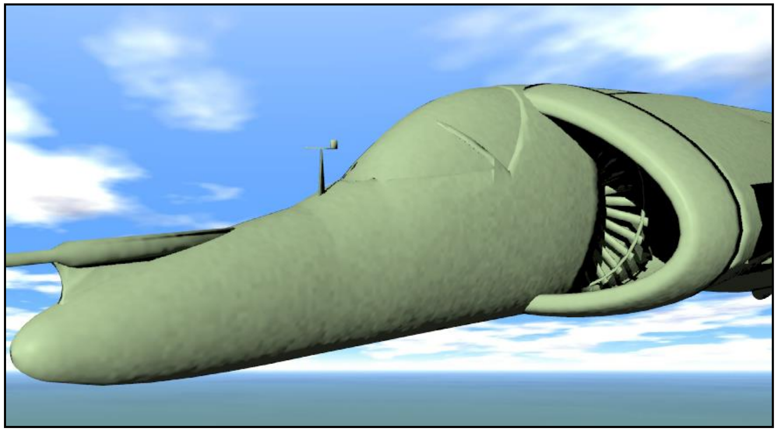


The importance of the geometrical model

- **Small geometric features**
- Drastically refined meshes and supercomputers are needed to simulate problems involving complex geometries. However, some *small* geometric features of the real model are neglected in the simulation (defeaturing)

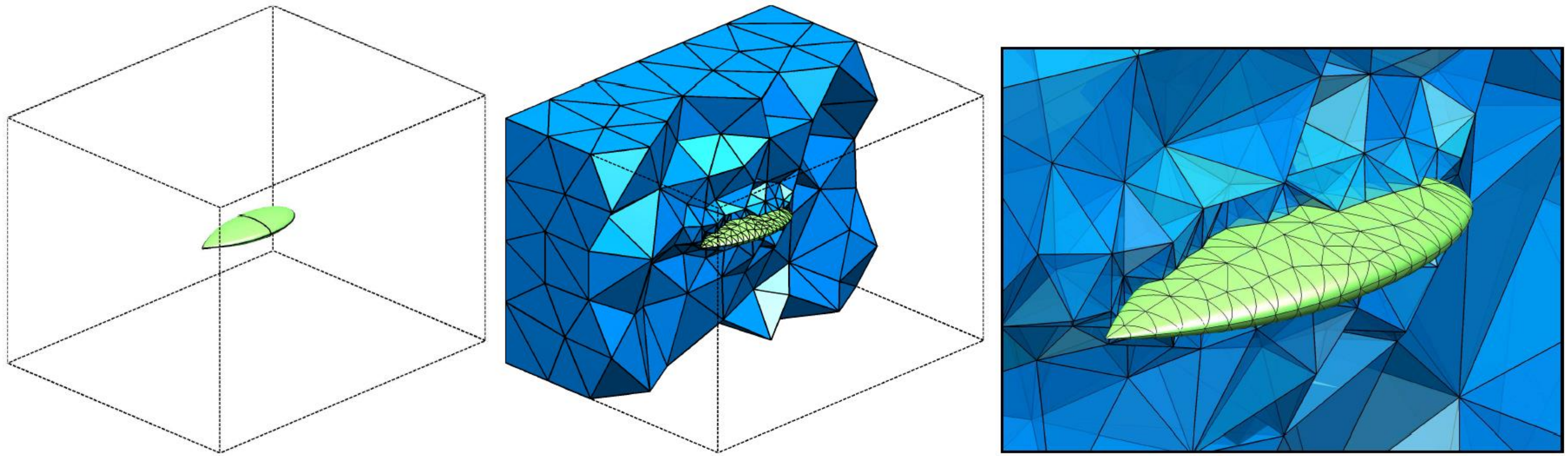






NEFEM – Rationale

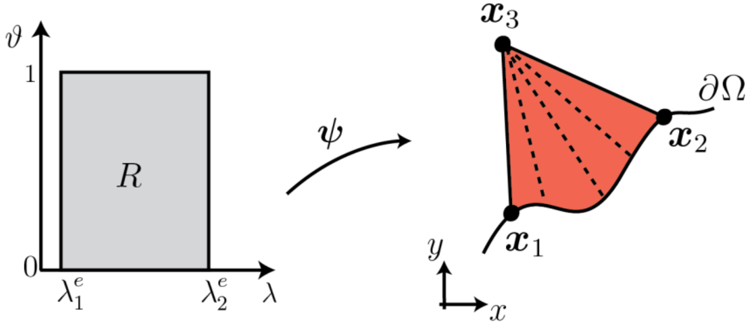
- A domain is considered, whose boundary (or a portion of its boundary) is described by NURBS



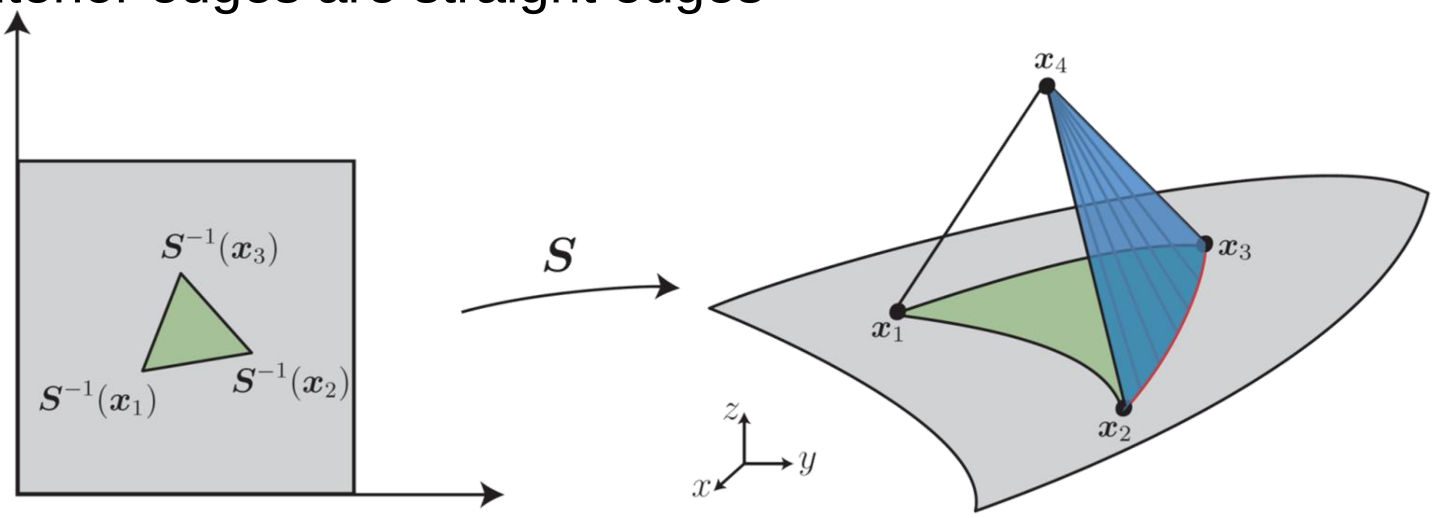
- Interior elements (straight edges/faces): treated as standard finite elements (FEs)
- Curved elements (NURBS edges/faces): interpolation and integration with exact geometry description (overhead reduced to boundary elements)

NEFEM – Rationale

- Curved elements are defined using the NURBS boundary
  - **2D**
    - **Curved element**:



  - **3D**
    - **Curved NURBS face**: image of a straight-sided triangle in the parametric space
    - **Curved face with a NURBS edge**: convex linear combination of the edge and the interior node
  - Interior edges are straight edges

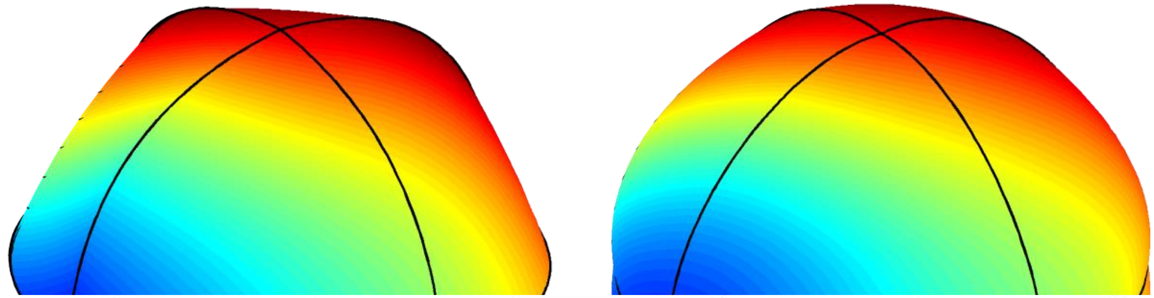


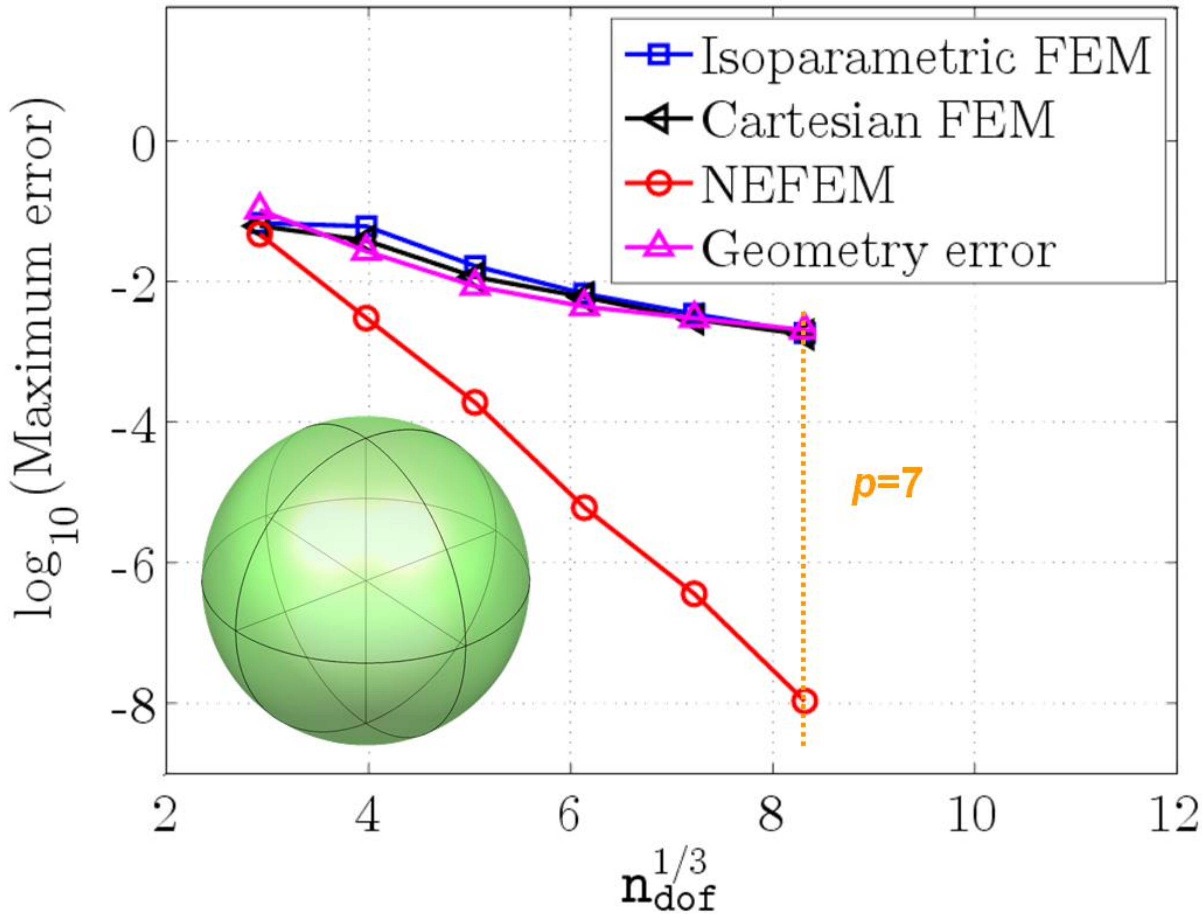
Heat transfer – Comparison

- 3D example

- Numerical solution with FEM and NEFEM on the sphere surface

- Geometry errors introduced by the isoparametric formulation are clearly observed for quadratic and cubic interpolation

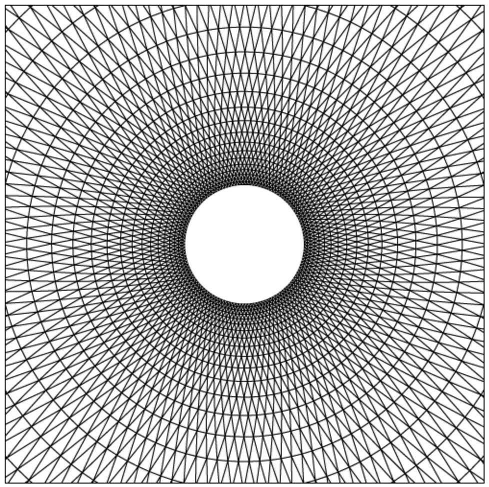


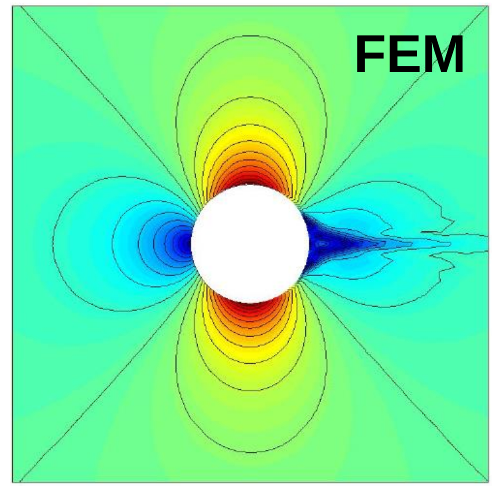


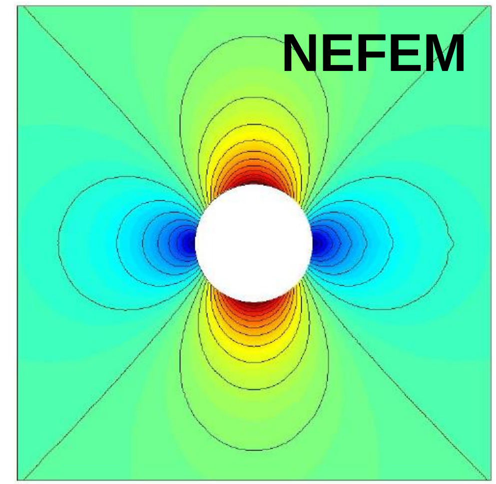
CFD – Comparison

- Low-order comparison

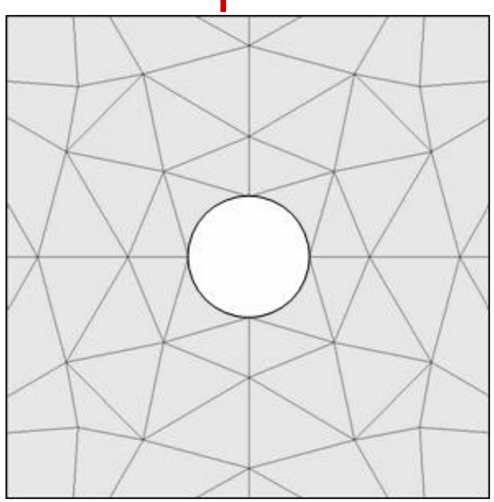
128
elements
describing
the circle

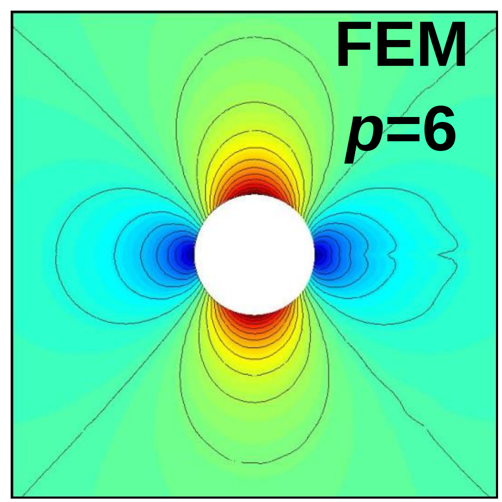


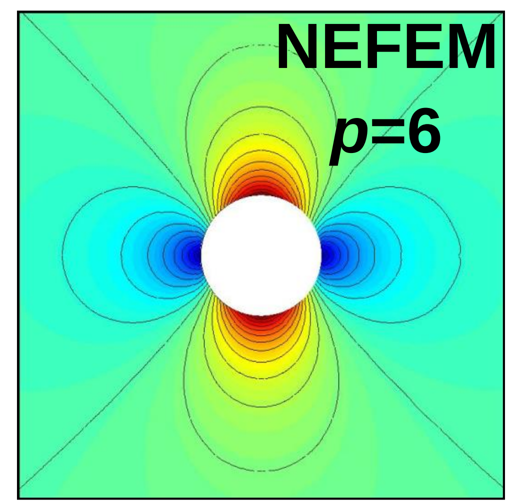




- High-order comparison



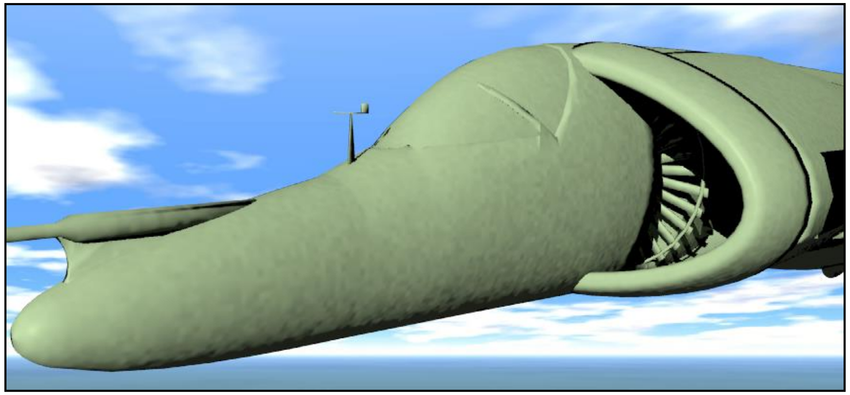


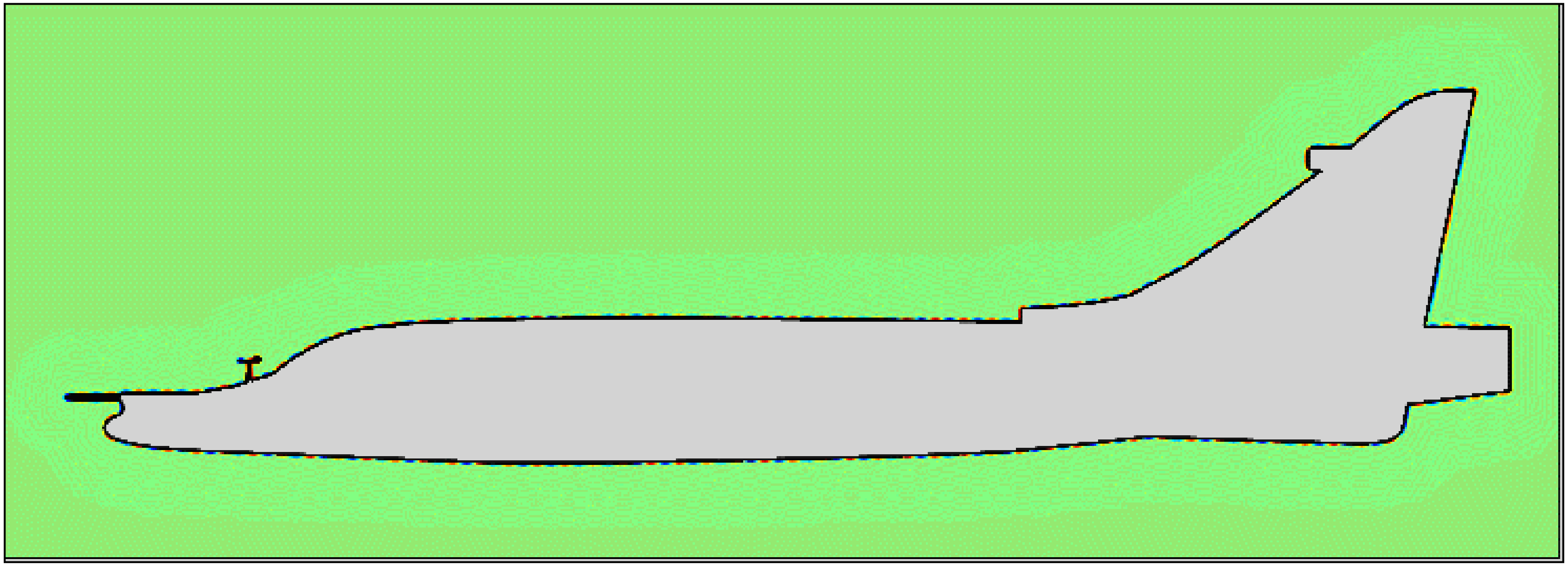


R. Sevilla, S. Fernandez-Mendez and A. Huerta, Arc. Comp. Met. Eng., 2011

Small geometric features

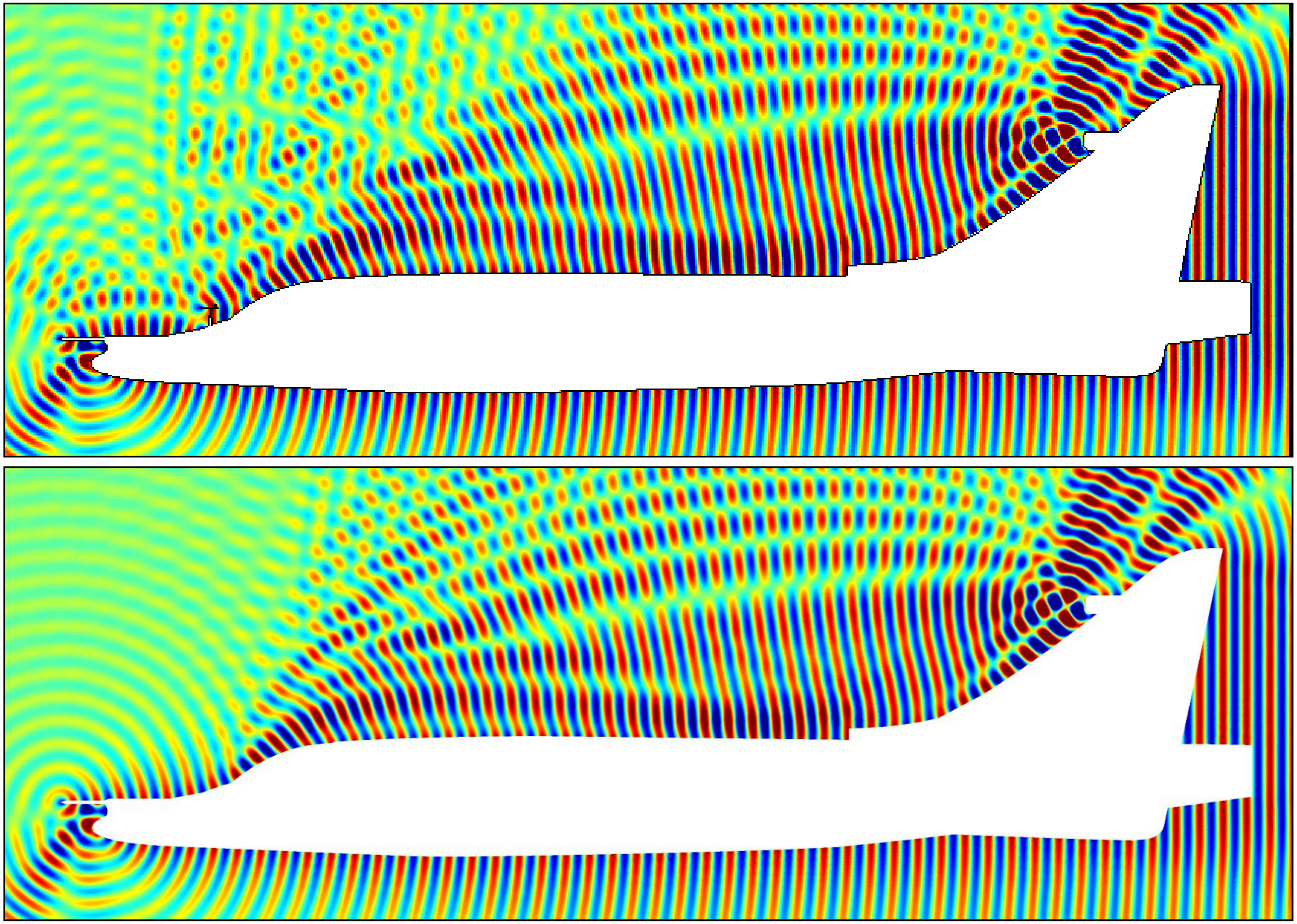
- Engineering quantities of interest on the boundary, or near it (scattering, aerodynamics,…)
- The size of the model is sometimes subsidiary to the geometrical complexity and not only on the solution itself
- **Electromagnetic scattering**



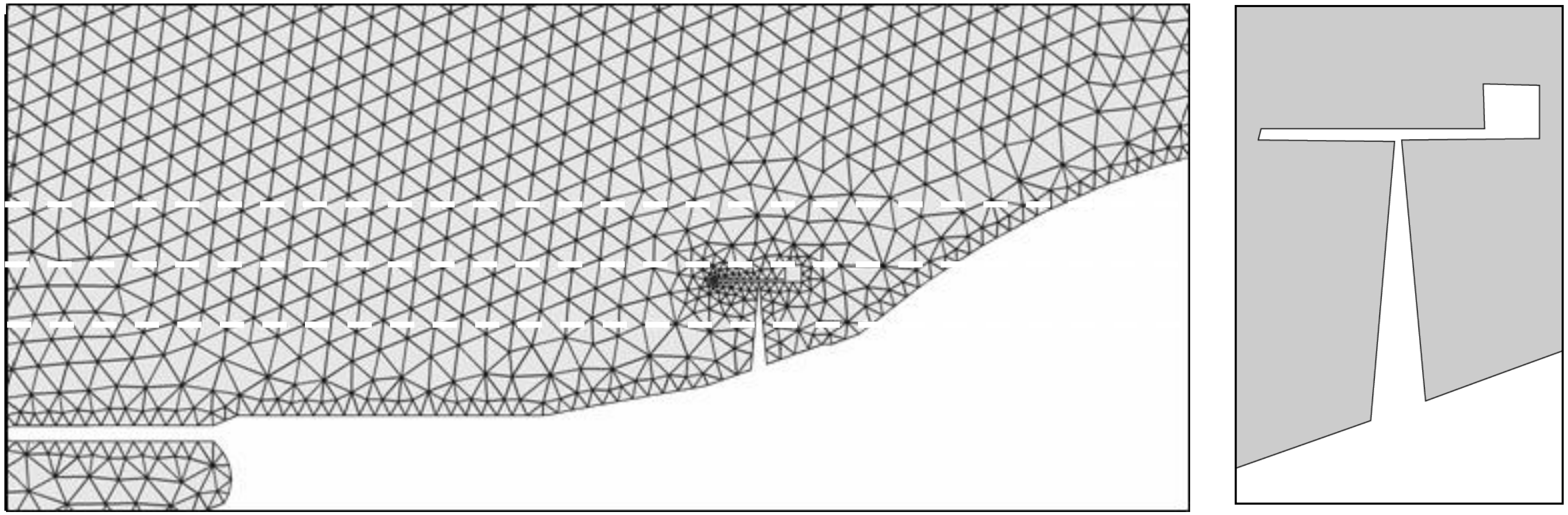


Small geometric features

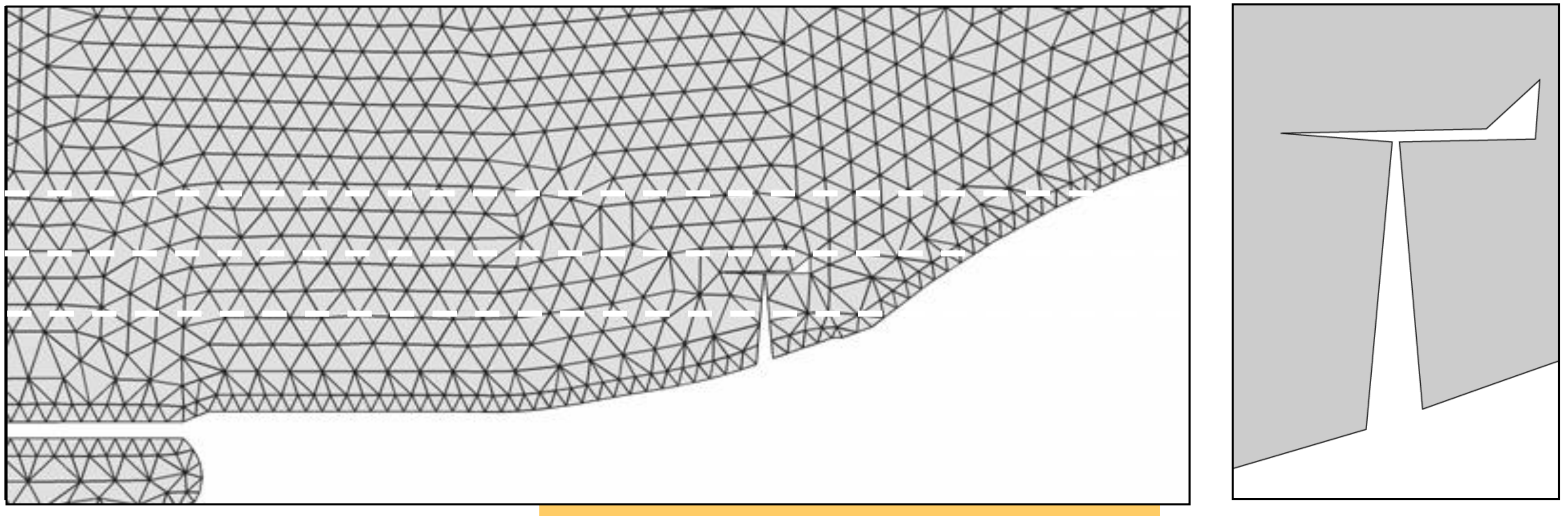
- Small geometric features cause global changes on the solution



Small geometric features

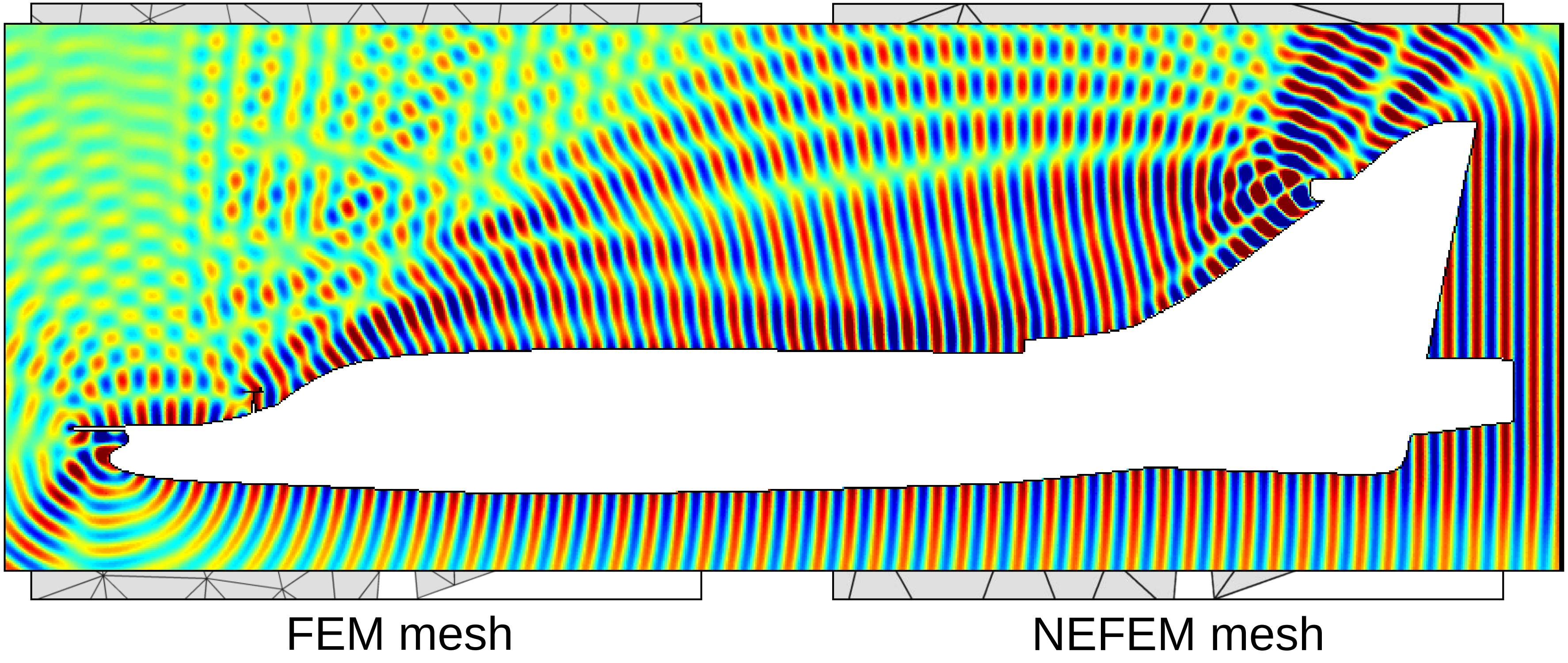


- Can we simplify the geometry to avoid *h*-refinement?



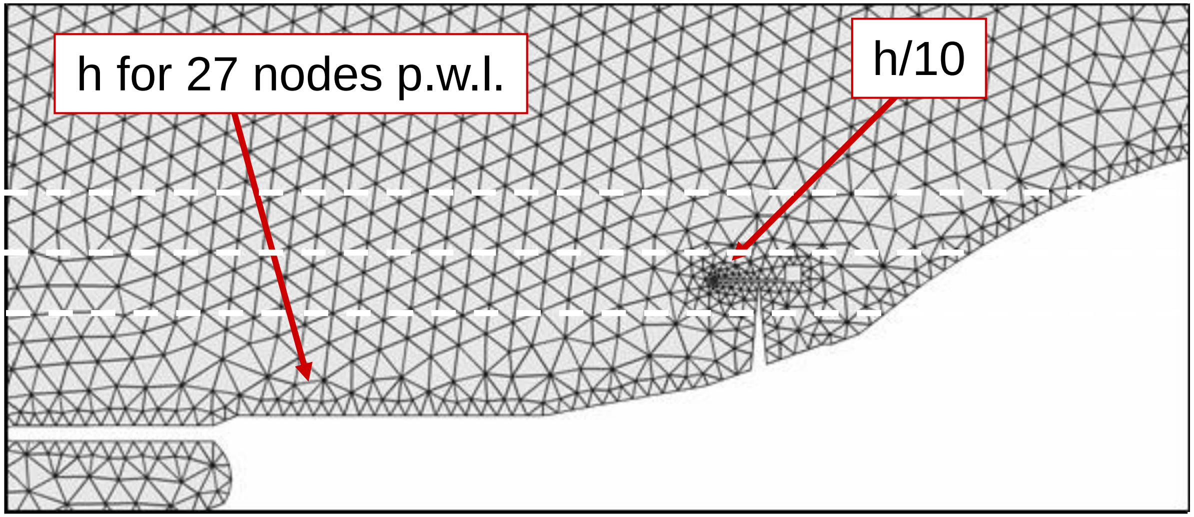
Small geometric features

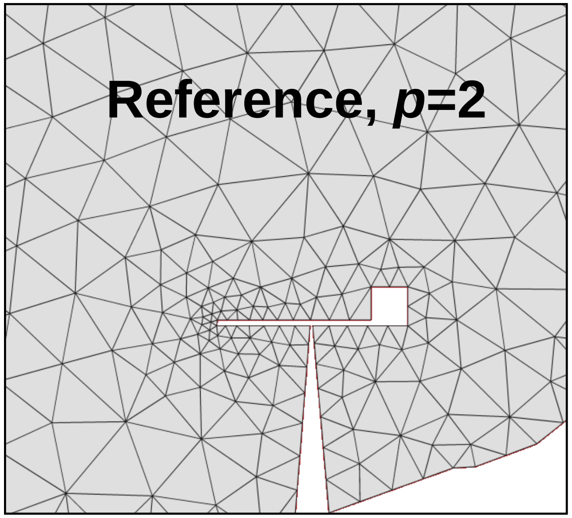
- Standard FEM meshes need *h*-refinement to capture small geometric features
- With NEFEM the mesh size is no longer subsidiary to the geometrical complexity

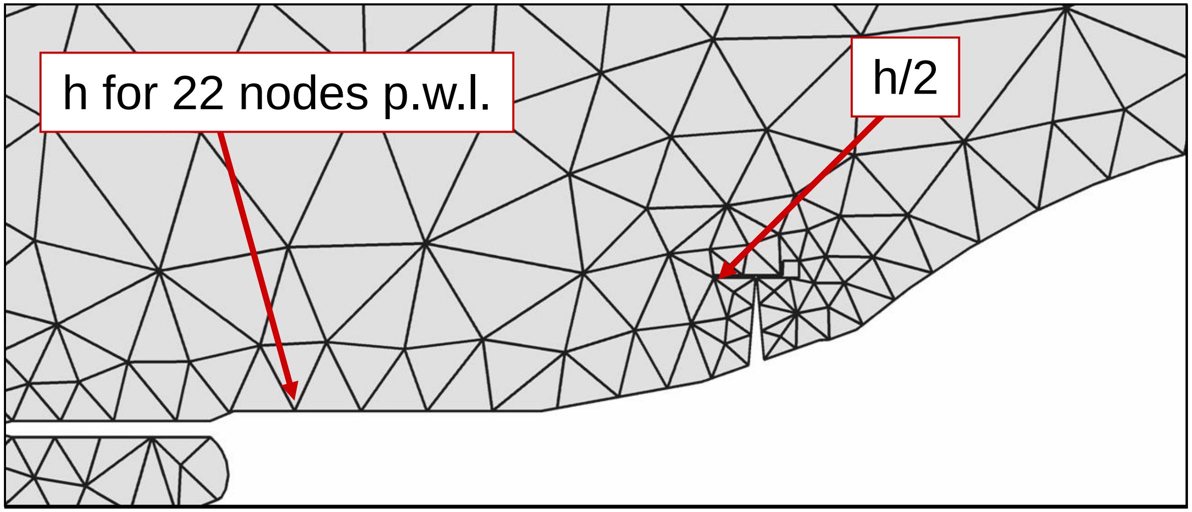


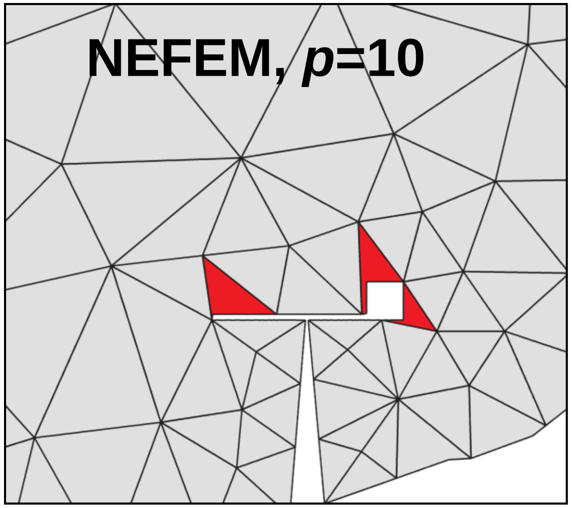
Small geometric features

- Scattering by a PEC aircraft profile (50 wavelengths)









4.

CONCLUDING REMARKS

Concluding remarks

- There is an industrial need to improve the numerical simulation capabilities in the fields of CEM and CFD
- High-order methods are a promising alternative but some issues have hampered the widespread application of these methods to problems of industrial relevance
- Ideas to solve or alleviate these problems
  - High-order curved mesh generation
    - Elasticity analogy
  - Geometry representation
    - NURBS-Enhanced Finite Element Method (NEFEM)

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