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

Rubén Sevilla

Zienkiewicz Centre for Computational Engineering
College of Engineering
Swansea University
Swansea
Wales, UK

4th ACME School
Swansea, 8 April, 2015
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

![Diagram of different mesh densities with p=1 and p=3 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 built with $(p+1)(p+2)/2$ nodes
    - Lagrange polynomials are usually considered although other bases are common (Legendre, hierarchical basis, etc)

![Diagram of high-order finite element methods]
High-order finite element methods

- The mapping between the reference element and the physical element becomes **nonlinear**
- For a generic element with nodes \( \mathbf{x}_i = \{(x_i, y_i)\}_{i=1,...,n_{en}} \), the mapping between local and global coordinates can be expressed in terms of the shape functions (**isoparametric**)
  \[
  \varphi(\xi) = \sum_{i=1}^{n_{en}} \mathbf{x}_i \mathbf{N}_i(\xi)
  \]
- The **Jacobian** \( \mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} \) is not constant
- Numerical integration is required to compute the integrals of the weak form

\[
K_{ij}^e = \int_{\Omega_e} \nabla_x \mathbf{N}_i(\mathbf{x}) \cdot \nabla_x \mathbf{N}_j(\mathbf{x}) \, d\Omega = \int_{I} \left( \mathbf{J}^{-1} \nabla_\xi \mathbf{N}_i(\xi) \right) \cdot \left( \mathbf{J}^{-1} \nabla_\xi \mathbf{N}_j(\xi) \right) |\mathbf{J}| \, d\xi
\]
High-order finite element methods

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

\[
\|e\|_{L^2(\Omega)} = C h^{p+1} |u|_{H^{p+1}(\Omega)}
\]
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

\[
\frac{\partial U}{\partial t} + \frac{\partial F_k(U)}{\partial x_k} = S(U)
\]

where

\[
U = \left( \begin{array}{c}
\varepsilon E \\
\mu H
\end{array} \right)
\]

\[
F_1 = \left( \begin{array}{c}
0 \\
H_3 \\
-H_2 \\
0 \\
-E_3 \\
E_2
\end{array} \right)
\]

\[
F_2 = \left( \begin{array}{c}
-H_3 \\
0 \\
H_1 \\
E_3 \\
0 \\
-E_1
\end{array} \right)
\]

\[
F_3 = \left( \begin{array}{c}
H_2 \\
-H_1 \\
0 \\
-E_2 \\
E_1 \\
0
\end{array} \right)
\]

\[
S = \left( \begin{array}{c}
-\sigma E \\
0
\end{array} \right)
\]

- Linear system of hyperbolic equations

\[
\frac{\partial U}{\partial t} + A_k \frac{\partial U}{\partial x_k} = S(U)
\]

with \[
A_k = \frac{\partial F_k}{\partial x_k}
\]
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

\[
\int_{\Omega_e} W \cdot \frac{\partial U_e}{\partial t} \, d\Omega - \int_{\Omega_e} \frac{\partial W}{\partial x_k} \cdot F_k(U_e) \, d\Omega + \int_{\partial\Omega_e} W \cdot F_n(U_e) \, d\Gamma = \int_{\Omega_e} W \cdot S(U_e) \, d\Omega
\]

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

\[
\int_{\Omega_e} W \cdot \frac{\partial U_e}{\partial t} \, d\Omega - \int_{\Omega_e} \frac{\partial W}{\partial x_k} \cdot F_k(U_e) \, d\Omega + \int_{\partial\Omega_e} W \cdot \tilde{F}_n(U_e, U_e^{\text{out}}) \, d\Gamma = \int_{\Omega_e} W \cdot S(U_e) \, d\Omega
\]

- The numerical flux in an exact or approximate **Riemman solver**
High-order discontinuous Galerkin (DG) formulation

- System of ODEs
- The semi-discrete system reads

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

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

Applications

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

Y.K. Chembo and N. Yu, 2010
Photonics and optics

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**

<table>
<thead>
<tr>
<th>Approx</th>
<th>Exact</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2497</td>
<td>0.2500</td>
</tr>
<tr>
<td>0.4994</td>
<td>0.5000</td>
</tr>
<tr>
<td>0.5585</td>
<td>0.5590</td>
</tr>
<tr>
<td>0.7069</td>
<td>0.7071</td>
</tr>
<tr>
<td>0.7503</td>
<td>0.7500</td>
</tr>
<tr>
<td>0.9011</td>
<td>0.9014</td>
</tr>
<tr>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>1.0302</td>
<td>1.0308</td>
</tr>
<tr>
<td>1.1183</td>
<td>1.1180</td>
</tr>
<tr>
<td>1.2497</td>
<td>1.2500</td>
</tr>
<tr>
<td>1.3462</td>
<td>1.3463</td>
</tr>
<tr>
<td>1.4138</td>
<td>1.4142</td>
</tr>
</tbody>
</table>

Excitation

Air

PEC

Monitor

Wave Propagation 1

Tomorrow morning
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
  \[
  \frac{\partial U}{\partial t} + \frac{\partial F_i}{\partial x_i} - \frac{\partial G_i}{\partial x_i} = 0
  \]

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

\[
U = \begin{pmatrix}
    \rho \\
    \rho v_1 \\
    \rho v_2 \\
    \rho E
\end{pmatrix},
F_i = \begin{pmatrix}
    \rho v_i \\
    \rho v_1 v_i + P \delta_{1i} \\
    \rho v_2 v_i + P \delta_{2i} \\
    (\rho E + P) v_i
\end{pmatrix},
G_i = \begin{pmatrix}
    0 \\
    \tau_{i1} \\
    \tau_{i2} \\
    v_k \tau_{ki} + q_i
\end{pmatrix}
\]

\[
\int_{\Omega} \left( W \cdot \frac{\partial U}{\partial t} - \frac{\partial W}{\partial x_k} \cdot F_k(U) + \frac{\partial W}{\partial x_i} \cdot \left( K_{ij} \frac{\partial U}{\partial x_j} \right) \right) d\Omega
\]

\[
= \int_{\partial \Omega} W \cdot \left( - F_k(U) + G_k(U) \right) n_k d\Gamma
\]
SUPG – CFD - Examples

NACA0012, Mach 0.63, angle=2°

- 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=2°

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
  - $p=3$
  - $Re = 3 \cdot 10^6$
  - $M = 0.4$
  - $AoA = 13.3^\circ$

Courtesy of Ralf Hartmann (DLR)
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

  \[
  \begin{align*}
  p=1; & \quad 8192 \text{ dof} \\
  p=2; & \quad 6144 \text{ dof} \\
  p=6 & \quad \text{FEM}
  \end{align*}
  \]

Bassi and Rebay (1997), Barth (1998)
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

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
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)

- h for 27 nodes p.w.l.
- h/10

- h for 22 nodes p.w.l.
- h/2

Reference, $p=2$

NEFEM, $p=10$

Tomorrow morning
Mesh generation
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)
Acknowledgements

Oubay Hassan
Kenneth Morgan

Antonio Huerta
Sonia Fernández-Méndez

Alan Shore

Ettore Barbieri

Juan J. Rodenas
Onofre Marco
Bibliography


2. R. Sevilla and E. Barbieri. NURBS distance fields for extremely curved cracks, Computational Mechanics, 54 (6); 1431-1446 , 2014


5. Z. Q. Xie, R. Sevilla, O. Hassan and K. Morgan, The generation of arbitrary order curved meshes for 3D finite element analysis, Computational Mechanics, 51 (3); 361-374, 2013


