Introduction to high-order discontinuous spectral element methods for CFD

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CFD lecture 04/19/2017
I. Context and overview
   • Numerical method properties for current CFD
   • Discontinuous Spectral Element Methods
   • Review of literature

II. The Discontinuous Galerkin method
   • Description of the scheme for Euler equations
   • Bibliography for more complex problems
   • Some properties of DG schemes

III. Applications of the DG scheme
   • Turbulent flows
   • Shock capturing

IV. Other type of DSEM
   • Spectral Difference method
   • Flux Reconstruction method
Current challenges for CFD

- Complex geometries for industrial applications
- Large scale problems (require billions of degrees of freedom)
- Complex physics (turbulence, shocks, combustion, multiphase, …)

Requirements for numerical methods

- High precision/high-orders of accuracy
- Must handle complex geometries/unstructured meshes
- Efficient for parallelism/compact stencils
Order of accuracy

• Order of accuracy governs the convergence rate of the numerical error

![Graph showing the convergence rate of numerical error for different orders of accuracy.](image)

- 2nd order
- 3rd order
- 4th order
- 5th order

• High-order methods: order of accuracy strictly greater than 2
Meshes: Structured vs. Unstructured

- **Structured**: allows for using simple and accurate numerical methods, but restricted to mildly complex geometries
- **Unstructured**: different type of elements (hexahedra, tetrahedra,…) allow for the treatment of very complex geometries, numerical methods generally more difficult to implement and low order

Source: NASA
Stencil

• Stencil is defined by the number of neighbouring elements required to compute the solution in a cell of the discretization

Compact stencil 😊

Large stencil 😞

• Stencil is defined by the number of neighbouring elements required to compute the solution in a cell of the discretization

• Compact stencils limit the exchange of information between subdomains when implementing MPI parallel strategy, leading to good parallel efficiency

• Implementing high-order methods usually requires large stencils
Finite difference methods

**Properties**

- High-orders easy to implement
- Structured meshes only
- Good accuracy
- Restricted to relatively simple geometries

**Pointwise computation of derivatives**

\[
\frac{\partial u}{\partial x}_{i,j} = \sum_{k=-n}^{n} a_k u_{i+k,j}
\]
Finite volume methods

Constant values of the solution in mesh elements

Budget of fluxes at elements interfaces using Green theorem:

\[ \nabla \cdot F \rightarrow \int_{S} F \cdot n \, dS \]

Properties

- Unstructured meshes
- Can handle complex geometries
- Compact stencil
- Good parallel efficiency
- Low order (usually 2nd)
- Limited accuracy
Discontinuous Spectral Element methods

Polynomial representation of the solution in the mesh elements

Good overall properties

- Arbitrary high-order of accuracy
- Compact stencil
- Unstructured and curved meshes

→ High-precision attainable, adaption
→ Good parallel efficiency
→ Can handle complex geometries

BUT: still ongoing research (esp. for shock capturing, turbulence modeling, improvement of efficiency and robustness,...)
A brief review of the Literature

Past research on Discontinuous Galerkin (DG) schemes:
• Extension to viscous case by Bassi et al. [1997, 2005]

Recent attempts to reduce complexity and avoid quadrature:
• Spectral Difference (SD) scheme by Kopriva & Kolias [1996], Liu, Vinokur & Wang [2006]
• Nodal Discontinuous Galerkin (NDG) scheme by Atkins & Shu [1998], Hesthaven & Warburton [2007]
• Flux Reconstruction (FR) scheme by Huynh [2007, 2009]
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The Discontinuous Galerkin method

DG discretization of conservation laws (1)

• General formulation for systems of conservation laws

\[
\frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{w}) = 0
\]

• Euler equations (describes compressible fluid dynamics):

\[
\mathbf{w} = (\rho, \rho \mathbf{U}, \rho E)^T
\]

\[
\mathbf{F} = \begin{pmatrix}
\rho \mathbf{U}^T \\
\rho \mathbf{U} \otimes \mathbf{U} + \rho \mathbf{I} \\
(\rho E + \rho) \mathbf{U}^T
\end{pmatrix}
\]

\[
p = (\gamma - 1) \left( \rho E - \frac{1}{2} \rho \mathbf{U} \cdot \mathbf{U} \right)
\]
• Spatial discretization of the computational domain:

\[ \Omega = \bigcup_{j=1}^{N} \Omega_j \]

\( \Omega_j \): elements

\( \partial \Omega_j \): elt. boundaries

\( n \): external normal
DG discretization of conservation laws (3)

- Objective: find the polynomial weights of the solution in the elements

\[ w(\mathbf{x}, t) = \sum_{k=1}^{Np} W_k(t) \phi_k(\mathbf{x}) \]

\( Np: \) number of DoF/modes per element

\[ Np = (p+1)^d \]

\( d: \) dimension of the problem

\( p: \) polynomial degree of the solution

\( \phi \) is the basis vector including all polynomial functions

1D illustration:

\[ p = 1 \quad W_1\phi_1 + W_2\phi_2 \]

\[ p = 2 \quad W_1\phi_1 + W_2\phi_2 + W_3\phi_3 \]
The Discontinuous Galerkin method

DG discretization of conservation laws (4)

• Let’s consider generic polynomial functions $\varphi$

  $$
  \varphi_1(x) = a, \varphi_2(x) = b+cx, \varphi_3(x) = d+ex+fx^2, \ldots
  $$

• For $d=2$ and $d=3$, a product of polynomial functions is considered:

  $$
  \phi^{1D}(x) = (\varphi_1(x), \ldots, \varphi_{p+1}(x))
  $$

  $$
  \phi^{2D}(x, y) = (\varphi_i(x)\varphi_j(y)) \quad , \quad i, j = 1, p+1
  $$

  $$
  \phi^{3D}(x, y, z) = (\varphi_i(x) \varphi_j(y) \varphi_k(z)) \quad , \quad i, j, k = 1, p+1
  $$

• Number of degrees of freedom per element:

<table>
<thead>
<tr>
<th></th>
<th>1D</th>
<th>2D</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p=0$ (FV)</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$p=1$</td>
<td>2</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>$p=2$</td>
<td>3</td>
<td>9</td>
<td>27</td>
</tr>
<tr>
<td>$p=3$</td>
<td>4</td>
<td>16</td>
<td>64</td>
</tr>
</tbody>
</table>
We want to compute the weights $W_k$ that satisfy the equations

\[ \int_{\Omega_j} \phi_i \frac{\partial w}{\partial t} \, dx + \int_{\Omega_j} \phi_i \nabla \cdot F(w) \, dx = 0 \quad i=1,\ldots, N_p \]

$N_p$ equations

- Variational formulation of equations in each cell:

\[ \int_{\Omega_j} \phi_i \frac{\partial w}{\partial t} \, dx - \int_{\Omega_j} \nabla \phi_i F \, dx + \int_{\partial \Omega_j} \phi_i F \cdot n \, dS = 0 \]

- Integration by parts yields:

\[ w(x, t) = \sum_{k=1}^{N_p} W_k(t) \phi_k(x) \]
DG discretization of conservation laws (6)

• Equations determining the polynomial weights of the solution:

\[
\frac{dW_k}{dt} \int_{\Omega_j} \phi_i \phi_k \, dx - \int_{\Omega_j} \nabla \phi_i F \, dx + \int_{\partial\Omega_j} \phi_i F \cdot n \, dS = 0
\]

- Mass matrix
- Volumic flux integral
- Surface flux integral + neighbour connection

• Need to solve a linear system for each cell of the discretization

• However, we can obtain a diagonal mass matrix with a wise choice of the polynomial basis and skip the costly matrix inversion
The Discontinuous Galerkin method

DG discretization of conservation laws (7)

- We seek an orthogonal basis that verifies
  \[ \int_{\kappa} \phi_i \phi_k \, d\xi = C_k \delta_{ik} \]

- Mass matrix in the reference element:
  \[ \int_{\Omega_j} \phi_i \phi_k \, dx = \int_{\kappa} \phi_i \phi_k \left| \frac{dx}{d\xi} \right| \, d\xi \]

- Linear mapping from physical to reference element:
  \[ \kappa = [-1, +1]^d \]

- For elements with parallel opposite edges, \( |d\mathbf{x}/d\xi| \) constant
  \[ \int_{\kappa} \mathbf{P}_i \mathbf{P}_k \, d\xi = C_k^{L} \delta_{i\mathbf{k}} \]

  \( \mathbf{P}_i \) : Legendre polynomials
The Discontinuous Galerkin method

DG discretization of conservation laws (8)

• Basis of Legendre polynomials:

\[ P_0(x) = 1, \quad P_1(x) = x, \quad (n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x). \]

\[ \frac{x^2 - 1}{n} \frac{d}{dx} P_n(x) = xP_n(x) - P_{n-1}(x) \]

Orthogonality

\[ \int_{-1}^{1} P_m(x)P_n(x) \, dx = \frac{2}{2n + 1} \delta_{mn} \]


![Plot of Legendre polynomials](image-url)
The Discontinuous Galerkin method

DG discretization of conservation laws (9)

• Second term: integral of the flux over the element

\[ \int_{\Omega_j} \nabla \phi_i F \, dx = \int_{\kappa} \nabla \phi_i F \left| \frac{dx}{d\xi} \right| \, d\xi \]

• Can be computed with a quadrature rule set in the reference element

\[ \int_{\kappa} \nabla \phi_i F \left| \frac{dx}{d\xi} \right| \, d\xi = \sum_{l=1}^{Nq} \nabla \phi_i(y_l) F(y_l) \left| \frac{dx}{d\xi} \right| \omega_l \]

• The fluxes, derivatives of basis functions and jacobian determinant must be computed on quadrature points

• Usual practice is to select \( Nq \geq Np \) so that the integral is sufficiently well resolved, esp. for nonlinear fluxes
DG discretization of conservation laws (10)

- Third term: integral of the flux over the surface of the element:

\[
\frac{dW_k}{dt} \int_{\Omega_j} \phi_i \phi_k \, d\mathbf{x} - \int_{\Omega_j} \nabla \phi_i \mathbf{F} \, d\mathbf{x} + \int_{\partial\Omega_j} \phi_i \mathbf{F} \cdot \mathbf{n} \, dS = 0
\]

- Solution is **discontinuous** at the interface

- We introduce a numerical flux \( h \) that depends on both values

\[
\int_{\partial\Omega_j} \phi_i \mathbf{F} \cdot \mathbf{n} \, dS \rightarrow \int_{\partial\Omega_j} \phi_i h(\mathbf{w}^+, \mathbf{w}^-, \mathbf{n}) \, dS
\]
DG discretization of conservation laws (11)

- The numerical flux for convection must be **consistent and conservative**.

- **Conservative**: guarantees the mass, momentum, energy conservation

  \[ h(w^+, w^-, n) = -h(w^-, w^+, -n) \]

- **Consistent**: recover the exact flux when no discontinuities

  \[ h(w, w, n) = F(w) \cdot n \]

- **Example**: the Lax-Friedrichs flux

  \[ h(w^+, w^-, n) = \frac{1}{2}(F(w^+) + F(w^-)) \cdot n + \frac{1}{2} \max \left( |U^\pm \cdot n + c^\pm| \right) (w^+ - w^-) \]

  - **Centered part**
  - **Upwind part**

- **Upwinding is necessary to yield stable computations**
The Discontinuous Galerkin method

DG discretization of conservation laws (12)

• Recap: equations in the mesh elements $\Omega_j$

\[
\frac{dW_k}{dt} = \frac{1}{JC_k^L} \left( \int_{\Omega_j} \nabla \phi_k F \, dx - \int_{\partial \Omega_j} \phi_k h \, ds \right)
\]

J = \left| \frac{d\vec{x}}{d\xi} \right|

Residual

• Once the residual is computed, we can find $W_k$ using an explicit time-stepping algorithm (e.g. Runge-Kutta)

• This strategy does not involve any inversion of linear systems
The Discontinuous Galerkin method

DG discretization of conservation laws (13)

• Boundary conditions: set using the surface flux integral

\[ \int_{\partial \Omega_j} \phi_i F(w) \cdot n \, dS \rightarrow \int_{\partial \Omega_j} \phi_i F(w_b) \cdot n \, dS \]

• Weak imposition of BCs: boundary information is considered in the computation of weights through fluxes integrals

• Initial conditions: need to compute corresponding polynomial weights

\[ W_k(t = 0) \int_{\Omega_j} \phi_i \phi_k J \, d\xi = \int_{\Omega_j} \phi_i w_{ini}(x) J \, d\xi \]

Computed using quadrature rule
Biblio for more complex problems

- **Extension to viscous flows:**

  - BR1, BR2, Interior Penalty, LDG, …

- **Polynomial basis orthogonal for complex mesh elements:**

  - Basis for general shaped elements (tetra, hexa, prisms, …):
  - Basis for curved elements (Gram-Schmidt orthogonalization procedure):
    - « On the flexibility of agglomeration based physical space DG discretization », Bassi et al. 2012

- **Other numerical fluxes for hyperbolic systems:**

  - « Riemann solvers and numerical methods for fluid dynamics: a practical introduction »
  - E.F. Toro, published by Springer
Some properties of DG schemes

Convergence of DG numerical error

- Test case: compressible laminar channel flow (full Navier-Stokes)

\[ p=1, p=2, p=3, p=4, p=5, \ldots \quad O(p+1) \]

Ref for test case: C. Brun et al., « Large-Eddy Simulation of compressible channel flow», 2008
Some properties of DG schemes

Spectral numerical errors (modified wavenumber)

- For high orders, low errors at low wavenumbers, strong dissipation and dispersion at high-wavenumbers

Some properties of DG schemes

Parallel efficiency

- Exchange of flux information at interfaces via MPI
- Strong scalability, Taylor-Green vortex problem
Some properties of DG schemes

Curved elements: flow around circular cylinder

Linear elements

Cubic elements

FIG. 7. Mach isolines around a circle with P1Q1 elements on the $64 \times 16$ grid.

FIG. 22. Mach isolines around a circle with P3Q3 elements on the $32 \times 8$ grid.

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Applications of the DG scheme

DG scheme applications: turbulent flows

Taylor-Green vortex (TGV)

- Freely decaying turbulence inside a periodic box $\Omega = [-\pi L, +\pi L]^3$
- $Re = V_0 L/\nu, M_0 = 0, 1$
- Flow evolution

---

$\omega$-surfaces, DNS using a Fourier pseudo-spectral code (R. Cant, Cambridge Univ.)
Applications of the DG scheme

DG scheme applications: turbulent flows

TGV : $Re=500$ Case

<table>
<thead>
<tr>
<th>DG computations</th>
<th>DG 48p1</th>
<th>DG 32p2</th>
<th>DG 24p3</th>
<th>DG 16p5</th>
<th>DG 12p7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Order $(p+1)$</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>#DOF</td>
<td>$96^3$</td>
<td>$96^3$</td>
<td>$96^3$</td>
<td>$96^3$</td>
<td>$96^3$</td>
</tr>
<tr>
<td>CPU time</td>
<td>$t_{ref}$</td>
<td>$2t_{ref}$</td>
<td>$4t_{ref}$</td>
<td>$14.5t_{ref}$</td>
<td>$52t_{ref}$</td>
</tr>
</tbody>
</table>

Evolution of energy

Evolution of enstrophy

Energy spectra at $t=9$

Reference computation: Fourier spectral code developed at Cambridge by R. Cant Chapelier et al., Comput. Fluids. 2014
Applications of the DG scheme

DG scheme applications: turbulent flows

Turbulent channel flow

- Turbulent flow between two parallel, infinite isothermal walls

- Streamwise and spanwise periodicity

- Forcing term to maintain the mass flow rate constant in the channel
Applications of the DG scheme

DG scheme applications: turbulent flows

Turbulent channel: Low Mach case ($M = 0.1$)

<table>
<thead>
<tr>
<th>Computation</th>
<th>Mach</th>
<th>$Re_{\ell}$</th>
<th>#DOF</th>
<th>#Integration points</th>
</tr>
</thead>
<tbody>
<tr>
<td>6th order DG</td>
<td>0.1</td>
<td>178</td>
<td>$2,1 \times 10^6$</td>
<td>$2,1 \times 10^6$</td>
</tr>
<tr>
<td>Moser et al. $^6$</td>
<td>-</td>
<td>178</td>
<td>$2,1 \times 10^6$</td>
<td>$7,1 \times 10^6$</td>
</tr>
</tbody>
</table>


Chapelier et al., Comput. Fluids. 2014
Applications of the DG scheme

DG scheme applications: turbulent flows

Turbulent channel: Compressible case ($M = 1.5$)

<table>
<thead>
<tr>
<th>Computation</th>
<th>Mach</th>
<th>$Re_t$</th>
<th>#DOF</th>
<th>#Integration points</th>
</tr>
</thead>
<tbody>
<tr>
<td>4th order DG</td>
<td>1.5</td>
<td>221</td>
<td>$6.1 \times 10^5$</td>
<td>$1.2 \times 10^6$</td>
</tr>
<tr>
<td>Coleman et al. $^7$</td>
<td>1.5</td>
<td>221</td>
<td>$6 \times 10^5$</td>
<td>$1.4 \times 10^6$</td>
</tr>
</tbody>
</table>


Chapelier et al., Comput. Fluids. 2014
Applications of the DG scheme

DG scheme applications: turbulent flows

Turbulent channel: Low Mach, variable $p$, $Re_\tau = 392$

<table>
<thead>
<tr>
<th>Computation</th>
<th>Mach</th>
<th>$u_\tau$</th>
<th>#DOF</th>
<th>#Integration points</th>
</tr>
</thead>
<tbody>
<tr>
<td>DG order 5-6-8</td>
<td>0.3</td>
<td>$5.8 \times 10^{-2}$</td>
<td>$7.02 \times 10^5$</td>
<td>$1.12 \times 10^6$</td>
</tr>
<tr>
<td>Moser et al.</td>
<td>-</td>
<td>$5.7 \times 10^{-2}$</td>
<td>$1.26 \times 10^7$</td>
<td>$4.27 \times 10^7$</td>
</tr>
</tbody>
</table>

DOF distribution

$p=4, p=5, p=7$

Chapelier et al., Comput. Fluids. 2014

Mean velocity

RMS velocity
Applications of the DG scheme

DG scheme applications: turbulent flows

More complex turbulent flow problems

Eighth order DG computation of a detached airfoil at $\text{Re}=60000$

Beck et al., IJNMF, 2014
Applications of the DG scheme

DG scheme applications: supersonic flows

How to capture shocks using DG schemes?

Supersonic flow around cylinder using a DG approach

Persson and Peraire, AIAA Paper, 2006
Applications of the DG scheme

DG scheme applications: supersonic flows

Shock detection using polynomial energy spectra

\[ \Omega_j \]

Smooth flow

\[ W_k^2 \]

Fast energetic decay in spectral space

\[ \Omega_j \]

Shocked flow

\[ W_k^2 \]

Important energy at high wavenumbers

Shockwave
Applications of the DG scheme

DG scheme applications: supersonic flows

Persson and Peraire, AIAA Paper, 2006: Shock detection using polynomial spectra then add artificial viscosity

Figure 4. Supersonic flow around a NACA0012 airfoil at Mach 1.5, with interpolation of degree $p = 4$. Again we see how the shocks are resolved within the elements, and the diffusion is only applied to elements around the shocks.
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Other type of DSEM

Spectral Difference method for 1D conservation law (1)

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \]

Spatial discretization and transformation towards reference element [-1,+1]

\[ x_0, x_0 + jh, x_0 + (j + 1)h \]

2 sets of points inside each element: \( \bullet \) N Solution points \( \square \) N+1 Flux points
Other type of DSEM

Spectral Difference method for 1D conservation law (2)

1. Lagrange interpolation of the solution on flux points
2. Computation of $\tilde{f}_L$, $\tilde{f}_R$ using numerical flux (same properties as DG)
3. Lagrange interpolation of fluxes derivatives on solution points

$\hat{f}_L$, $f_1$, $f_2$, $\hat{f}_R$

- $N$ Solution points: $u_h = \sum_{j=1}^{n} u_j l_j(x)$
- $N+1$ Flux points: $f^D_h = \sum_{j=2}^{n} f_j^D l_j(x)$

$\frac{\partial u_i}{\partial t} + \left[ \sum_{j=2}^{n} f_j^D \frac{dl_j}{dx} + \hat{f}_L \frac{dl_1}{dx} + \hat{f}_R \frac{dl_{n+1}}{dx} \right] = 0$

Spectral Difference (SD) vs. DG

• Equivalent properties
  • Arbitrary high-order of accuracy
  • Excellent parallel efficiency
  • Unstructured meshes and curved elements

• Disadvantages compared to DG
  • SD slightly less accurate than DG
  • High-order SD not yet stable on tetrahedral elements

• Advantages compared to DG
  • More efficient than DG (esp. for high-orders)
  • Simpler formulation
Flux Reconstruction method

1. Express the flux as a Lagrange polynomial $f_d$ (discontinuous across elements)
2. Define a correction function $f_c$ of the flux that leads to a continuous flux across interfaces

Huynh, AIAA P. 2007-4079; Huynh, AIAA P. 2009-403;
Properties of the Flux Reconstruction (FR) scheme

- Arbitrary high-order of accuracy
- Excellent parallel efficiency
- All type of mesh elements
- Can recover DG or SD schemes by tuning reconstruction functions
Some open source DSEM codes

Nektar++:
• Continuous and Discontinuous Galerkin for compressible or incompressible flows
• Comprehensive (various element types, equations, flow problems, …)
• Well documented
• http://www.nektar.info/

PyFR:
• Flux reconstruction Navier-Stokes solver developed at Imperial College, Prof. Vincent’s group
• Python based, parallel implementation with GPUs
• http://www.pyfr.org

HiFiLES:
• Flux reconstruction Navier-Stokes solver developed at Stanford, Prof. Jameson’s group
• 2D, 3D, various types of mesh elements, designed for Large-Eddy Simulation
• https://hifiles.stanford.edu/