Accurate and Efficient Simulation and Design Using High-Order CFD Methods

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July 9, 2014

Modern Techniques for Aerodynamic Analysis and Design
2014 CFD Summer School, Beijing, China, July 7-11, 2014

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Background

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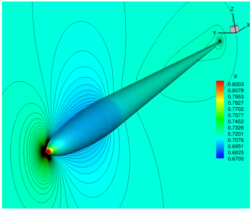
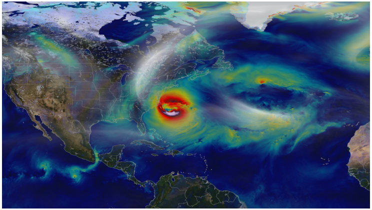
Fluid Flows of Practical Interest

- Responsible to most of transport and mixing phenomena
- Interaction of objects with surrounding air or water
- Meteorological phenomena such as wind, rain and hurricanes
- Combustion in aircraft or automobile engines
- Heating, ventilation and air conditioning



Pressure field for air flow over a 3D analytical body



Hurricane Sandy simulated by a NASA computer model

Fuel combustion of rocket engine in action

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Approaches to Fluid Dynamics Problems

- Analytical methods through simplifications of the governing equations
- Experimental methods on scaled models
- Computational fluid dynamics (CFD) methods
  - Predict fluid flows, heat and mass transfer, chemical reactions and etc.

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Approaches to Fluid Dynamics Problems

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Need for CFD

- Most real world problems do not have analytical solution.
- Reduction of the total effort and expenses required in experiments
- Conceptual studies of new designs
- Visualization of complex fluid-flow problems in both space and time
- Require code validation and error quantification

A Brief Overview

1. High-Order Discontinuous Galerkin Discretizations and Implicit Schemes
2. Multigrid Solution Acceleration Strategies
3. Adjoint-Based Mesh Adaptation and Shape Optimization
4. Simulation of Turbulence Using High-Order Discontinuous Galerkin Methods

A Brief Overview

1. High-Order Discontinuous Galerkin Discretizations and Implicit Schemes
2. Multigrid Solution Acceleration Strategies
3. Adjoint-Based Mesh Adaptation and Shape Optimization
4. Simulation of Turbulence Using High-Order Discontinuous Galerkin Methods

Outline (Lecture 1)

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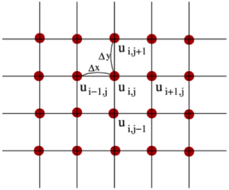
1. Motivation
2. DG Formulation for A Hyperbolic Equation
3. Interior Penalty Formulation for Elliptic Equations
4. Explicit and Implicit Time Integration
5. Numerical Examples
6. Conclusions

Motivation

- Popular CFD approaches

Finite Difference Methods

- Field variables are stored at each node
- Replace partial derivatives with FD approximations
  $\left(\frac{\partial u}{\partial x}\right)_{i,j} \approx \frac{u_{i+1,j} - u_{i,j}}{\Delta x}$ and $\left(\frac{\partial u}{\partial y}\right)_{i,j} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta y}$
- Limited to structured grids and good for simple geometries
- Require expanded stencil for higher-order accuracy



Motivation

- Popular CFD approaches

Finite Difference Methods

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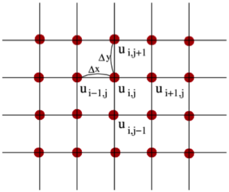


Finite Volume Methods

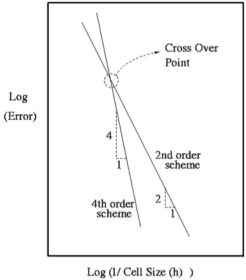
- Applied to unstructured grids
- Variables are stored at centroid of control volume
- Take integral form of the governing equations
- Difficulty on extending to higher-order accuracy

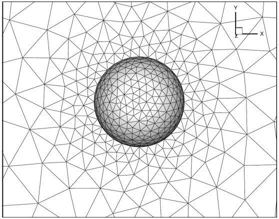
Motivation

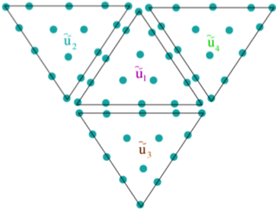
- Popular CFD approaches (Cont'd)

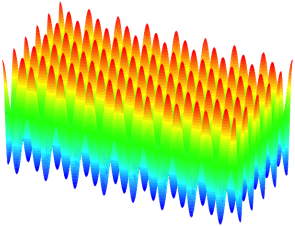
Finite Element Methods

- Easy handling of complicated geometries
- Compact stencil independent of order of scheme
- High order precision by increasing solution order
- Reduce mesh density
- Easy parallelization & $h-p$ adaptivity









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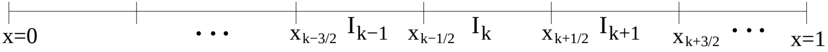
DG Formulation for A Hyperbolic Equation

- Consider a hyperbolic conservation law:

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

  - u: a scalar, which is the variable solved for
  - x: spatial Cartesian coordinate ($0 < x < 1$)
  - t: time ($t > 0$)
  - Initial condition: $u(x, 0) = u_0$
  - Boundary condition: periodic b.c. at $x = 0$ and $x = 1$

- Partition the domain into N intervals, $I_k = (x_{k-1/2}, x_{k+1/2})$ $(k = 1, \cdots, N)$



- Find u_h in space of piecewise polynomials of maximum degree p, $\mathcal{V}_h^p$

- Use a weak statement

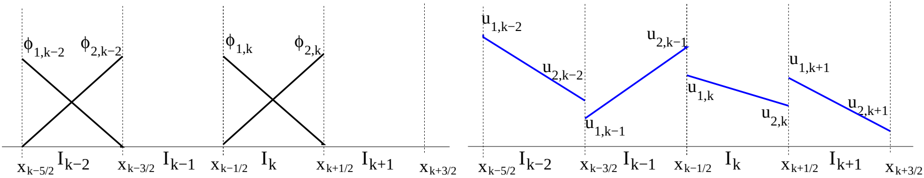
$$\int_0^1 \phi_j \frac{\partial u_h}{\partial t} dx + \int_0^1 \phi_j \frac{\partial f(u_h)}{\partial x} dx = 0$$

DG Formulation for A Hyperbolic Equation

- Expansion of the Galerkin approximation at element k, $u_{h\,k}$

$$u_{h\,k}(x) = \sum_{i=1}^{M} \tilde{u}_{i\,k}\phi_i(x)$$

- Example of piecewise linear functions ($p = 1$)



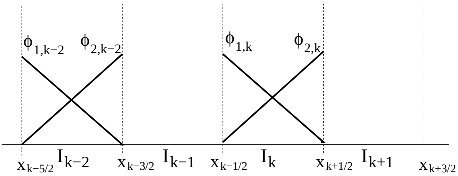
  - $\phi_i(x) = \begin{cases} a_0 + a_1 x & x \in [x_{k-1/2}, x_{k+1/2}] \\ 0 & \text{otherwise} \end{cases}$
  - u_h can be discontinuous at elemental interfaces.

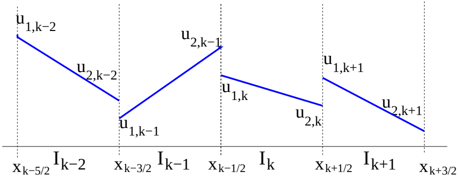
DG Formulation for A Hyperbolic Equation

- Expansion of the Galerkin approximation at element k, u_{hk}

$$u_{hk}(x) = \sum_{i=1}^{M} \tilde{u}_{ik}\phi_i(x)$$

- Example of piecewise linear functions ($p = 1$)





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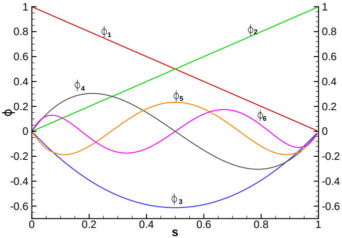
  - u_h can be discontinuous at elemental interfaces.



DG Formulation for A Hyperbolic Equation

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- Rewrite the weak statement for an interval k

$$\int_{x_{k-1/2}}^{x_{k+1/2}} \phi_j \frac{\partial u_h}{\partial t} dx + \int_{x_{k-1/2}}^{x_{k+1/2}} \phi_j \frac{\partial f(u_h)}{\partial x} dx = 0$$

- Integrate by parts

$$\int_{x_{k-1/2}}^{x_{k+1/2}} \phi_j \frac{\partial u_h}{\partial t} - \frac{d\phi_j}{dx} f(u_h) dx + f(u_h)_{x_{k+1/2}} \phi_j(x_{k+1/2}) - f(u_h)_{x_{k-1/2}} \phi_j(x_{k-1/2}) = 0$$

- Note that u_h at elemental boundaries, $x_{k+1/2}$ and $x_{k-1/2}$, are not well defined due to the discontinuities.

- Use a numerical flux function $F(u_L, u_R)$ to resolve the discontinuities

$$\int_{x_{k-1/2}}^{x_{k+1/2}} \phi_j \frac{\partial u_h}{\partial t} - \frac{d\phi_j}{dx} f(u_h) dx + F(u_{h\,k}, u_{h\,k+1}) \phi_j(x_{k+1/2}) - F(u_{h\,k-1}, u_{h\,k}) \phi_j(x_{k-1/2}) = 0$$

- Boundary conditions are enforced weakly through $F(u_L, u_b)$ and u_b is determined by desired boundary conditions (e.g. inflow/outflow, wall).

DG Formulation for A Hyperbolic Equation

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- Choose an upwinding scheme due to stability, for example $f(u) = au$

$$F(u_L, u_R) = \frac{1}{2}\left(f(u_L) + f(u_R) + |a|(u_L - u_R)\right)$$

- Replace the Galerkin approximation with the solution expansion (assuming $a > 0$)

$$\int_{x_{k-1/2}}^{x_{k+1/2}} \frac{\partial}{\partial t}\left(\sum_{i=1}^{M} \tilde{u}_{i\,k}\phi_i(x)\right)\phi_j - a\left(\sum_{i=1}^{M} \tilde{u}_{i\,k}\phi_i(x)\right)\frac{d\phi_j}{dx}dx$$

$$+ \mathrm{a}u_{h\,k}\phi_j(x_{k+1/2}) - au_{h\,k-1}\phi_j(x_{k-1/2}) = 0$$

- The discretized equation can thus be expressed as

$$M_k\frac{\partial \tilde{u}_k}{\partial t} - S_k\tilde{u}_k + a\begin{pmatrix} -u_{h\,k-1} \\ u_{h\,k} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = 0$$

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- The element matrices are given by

$$M_{ij\,k} = \int_{x_{k-1/2}}^{x_{k+1/2}} \phi_i \phi_j dx \quad S_{ij\,k} = \int_{x_{k-1/2}}^{x_{k+1/2}} a\frac{d\phi_j}{dx}\phi_i dx$$

- Compute the elementary matrices by Gaussian quadrature rule.
- The DG scheme of $p = 0$ is equivalent to a first-order cell-centered finite volume scheme.

$$\int_{x_{k-1/2}}^{x_{k+1/2}} \frac{\partial}{\partial t}\left(\sum_{i=1}^{M} \tilde{u}_{i\,k}\phi_i(x)\right)\phi_j - a\left(\sum_{i=1}^{M} \tilde{u}_{i\,k}\phi_i(x)\right)\frac{d\phi_j}{dx}dx$$
$$+ \mathrm{a}u_{h\,k}\phi_j(x_{k+1/2}) - au_{h\,k-1}\phi_j(x_{k-1/2}) = 0$$

- Rewrite the system of equations as

$$M\frac{d\tilde{u}}{dt} + R(\tilde{u}) = 0$$

- Solve this semi-discrete system with explicit or implicit temporal schemes

Outline (Lecture 1)

Interior Penalty Formulation for Elliptic Equations

- Consider a classic linear elliptic problem governed by a Poisson equation

$$-\Delta u = g \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

  - Δ is the second-order Laplace operator, $\Delta u = \nabla^2 u = \nabla \cdot \nabla u$
  - Ω denotes an open bounded polygonal domain.
  - Homogeneous Dirichlet boundary conditions

- DG weak form for the Poisson problem through multiplying the equation with a test function ϕ and integrating over Ω

$$-\int_\Omega \phi \nabla \cdot \nabla u d\Omega = \int_\Omega g\phi d\Omega$$

- Split the integration into a set of non-overlapping elements T_h^p

$$-\sum_{k \in T_h^p} \int_{\Omega_k} \phi \nabla \cdot \nabla u_h dx = \sum_{k \in T_h^p} \int_{\Omega_k} g\phi dx$$

Interior Penalty Formulation for Elliptic Equations

- To approximate the diffusion operation $\nabla^2 u_h$, we define an auxiliary variable $\vec{q}_h$

$$\vec{q}_h = \nabla u_h$$

- The elliptic equation can then be written into two advection equations.

$$-\sum_{k\in T_h^p} \int_{\Omega_k} \phi \nabla \cdot \vec{q}_h dx = \sum_{k\in T_h^p} \int_{\Omega_k} g \phi dx \quad (1)$$

$$\sum_{k\in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \vec{q}_h dx = \sum_{k\in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \nabla u_h dx \quad (2)$$

- Note that the right hand side of (2) can be written as

$$\sum_{k\in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \nabla u_h dx = \sum_{k\in T_h^p} \int_{\Omega_k} \left(\nabla \cdot (\vec{\tau}_h u_h) - u_h \nabla \cdot \vec{\tau}_h \right) dx \quad (3)$$

- The weak form of the auxiliary equation becomes

$$\sum_{k\in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \vec{q}_h dx = \sum_{k\in T_h^p} \int_{\Omega_k} \left(\nabla \cdot (\vec{\tau}_h u_h) - u_h \nabla \cdot \vec{\tau}_h \right) dx \quad (4)$$

Interior Penalty Formulation for Elliptic Equations

- Integrate by parts and take the divergence theorem

$$\sum_{k\in T_h^p}\left(\int_{\Omega_k}\nabla\phi\cdot\vec{q}_h dx-\int_{\partial\Omega_k}\phi\hat{\vec{q}}_h\cdot\vec{n}ds\right)=\sum_{k\in T_h^p}\int_{\Omega_k}g\phi dx \quad (5)$$

$$\sum_{k\in T_h^p}\int_{\Omega_k}\vec{\tau}_h\cdot\vec{q}_h dx=\sum_{k\in T_h^p}\left(-\int_{\Omega_k}\nabla\cdot\vec{\tau}_h u_h dx+\int_{\partial\Omega_k}\hat{u}_h\vec{\tau}_h\cdot\vec{n}ds\right) \quad (6)$$

  - $\vec{n}$ denotes the unit normal vector pointing outward the elemental interface.
  - $\hat{u}_h$ and $\hat{\vec{q}}_h$ denote numerical flux for solution and solution gradients, respectively.

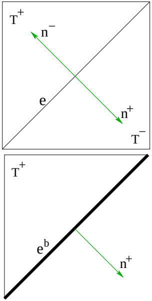
- Introduce notations for average and jump operators

$$T^{\pm}: \quad \{\varphi\}=\frac{\varphi^+ +\varphi^-}{2} \quad [\![\varphi]\!]=\varphi^+\vec{n}^+-\varphi^-\vec{n}^+$$

$$\{\vec{\beta}\}=\frac{\vec{\beta}^+ +\vec{\beta}^-}{2} \quad [\![\vec{\beta}]\!]=\vec{\beta}^+\vec{n}^+-\vec{\beta}^-\vec{n}^+$$

$$T^b: \quad \{\varphi\}=\varphi_b \quad [\![\varphi]\!]=\varphi_b\vec{n}^+$$

$$\{\vec{\beta}\}=\vec{\beta}_b \quad [\![\vec{\beta}]\!]=\vec{\beta}_b\vec{n}^+$$



Interior Penalty Formulation for Elliptic Equations

- Define the numerical flux $\hat{u}_h = \{u_h\}$ and use the average and jump operators

$$\sum_{k\in T_h^p}\int_{\Omega_k}\nabla\phi\cdot\vec{q}_h dx - \int_{\Gamma_I}[\![\phi]\!]\cdot\hat{\vec{q}}_h ds - \int_{\Gamma_b}\phi^+\vec{q}_b\cdot n ds = \sum_{k\in T_h^p}\int_{\Omega_k} g\phi dx \tag{7}$$

$$\sum_{k\in T_h^p}\int_{\Omega_k}\vec{\tau}_h\cdot\vec{q}_h dx = -\sum_{k\in T_h^p}\int_{\Omega_k}\nabla\cdot\vec{\tau}_h u_h dx + \int_{\Gamma_I}\{u_h\}[\![\vec{\tau}_h]\!] ds + \int_{\Gamma_b} u_b\vec{\tau}_h\cdot\vec{n} ds \tag{8}$$

- Similarly, we rewrite

$$\begin{aligned} -\sum_{k\in T_h^p}\int_{\Omega_k}\nabla\cdot\vec{\tau}_h u_h dx &= -\sum_{k\in T_h^p}\int_{\Omega_k}\left(\nabla\cdot(\vec{\tau}_h u_h) - \vec{\tau}_h\cdot\nabla u_h\right) dx \\ &= -\sum_{k\in T_h^p}\int_{\partial\Omega_k}\vec{\tau}_h u_h\cdot\vec{n} ds + \sum_{k\in T_h^p}\int_{\Omega_k}\vec{\tau}_h\cdot\nabla u_h dx \\ &= -\int_{\Gamma_I}(\vec{\tau}_h u_h\cdot\vec{n})^+ + (\vec{\tau}_h u_h\cdot\vec{n})^- ds - \int_{\Gamma_b}\vec{\tau}_h u_h\cdot\vec{n} ds \\ &\quad + \sum_{k\in T_h^p}\int_{\Omega_k}\vec{\tau}_h\cdot\nabla u_h dx \end{aligned} \tag{9}$$

Interior Penalty Formulation for Elliptic Equations

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- Inspired by the following relation

$$a^+b^+ + a^-b^- = \frac{1}{2}(a^+ + a^-)(b^+ - b^-) + \frac{1}{2}(b^+ + b^-)(a^+ - a^-)$$

- We express the formulation as

$$\int_{\Gamma_I} (\vec{\tau}_h u_h \cdot \vec{n})^+ + (\vec{\tau}_h u_h \cdot \vec{n})^- ds = \int_{\Gamma_I} \{u_h\}[\![\vec{\tau}_h]\!] + \{\vec{\tau}_h\}[\![u_h]\!] ds$$

- Recall the previous derivation

$$-\sum_{k\in T_h^p}\int_{\Omega_k} \nabla\cdot\vec{\tau}_h u_h dx = -\int_{\Gamma_I} (\vec{\tau} u_h \cdot \vec{n})^+ + (\vec{\tau} u_h \cdot \vec{n})^- ds - \int_{\Gamma_b} \vec{\tau}_h u_h \cdot \vec{n} ds + \sum_{k\in T_h^p}\int_{\Omega_k} \vec{\tau}_h \cdot \nabla u_h dx$$

- Use this desired relation and then we have

$$-\sum_{k\in T_h^p}\int_{\Omega_k} \nabla\cdot\vec{\tau}_h u_h dx = -\int_{\Gamma_I} \{u_h\}[\![\vec{\tau}_h]\!] + \{\vec{\tau}_h\}[\![u_h]\!] ds - \int_{\Gamma_b} \vec{\tau}_h u_h \cdot \vec{n} ds + \sum_{k\in T_h^p}\int_{\Omega_k} \vec{\tau}_h \cdot \nabla u_h dx$$

- Substitute the above expression into the weak form of the auxiliary equation (8) and rearrange $\cdots$

Interior Penalty Formulation for Elliptic Equations

- The system of equations (primary and auxiliary) is expressed as

$$\sum_{k \in T_h^p} \int_{\Omega_k} \nabla \phi \cdot \vec{q}_h dx - \int_{\Gamma_I} [\![\phi]\!] \cdot \hat{\vec{q}}_h ds - \int_{\Gamma_b} \phi^+ \vec{q}_b \cdot n ds = \sum_{k \in T_h^p} \int_{\Omega_k} g \phi dx \quad (10)$$

$$\sum_{k \in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \vec{q}_h dx = \sum_{k \in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \nabla u_h dx - \int_{\Gamma_I} \{\vec{\tau}_h\} [\![u_h]\!] ds - \int_{\Gamma_b} (u_h - u_b) \vec{\tau}_h \cdot \vec{n} ds \quad (11)$$

- In symmetric interior penalty method, $\hat{\vec{q}}_h$, $\vec{q}_b$ and $\vec{\tau}_h$ are defined to ideally eliminate the auxiliary equation

$$\begin{aligned} \hat{\vec{q}}_h &= \{\nabla u_h\} - \eta [\![u_h]\!] \\ \vec{q}_b &= \nabla u_h^+ - \eta (u_h - u_b) \cdot \vec{n} \\ \vec{\tau}_h &= \nabla \phi \end{aligned}$$

- Using the above definitions yields the following formulation for the auxiliary equation (11)

$$\sum_{k \in T_h^p} \int_{\Omega_k} \nabla \phi \cdot \vec{q}_h dx = \sum_{k \in T_h^p} \int_{\Omega_k} \nabla \phi \cdot \nabla u_h dx - \int_{\Gamma_I} \{\nabla \phi\} [\![u_h]\!] ds - \int_{\Gamma_b} (u_h - u_b) \nabla \phi \cdot \vec{n} ds \quad (12)$$

Interior Penalty Formulation for Elliptic Equations

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$$\sum_{k \in T_h^p} \int_{\Omega_k} \nabla\phi \cdot \vec{q}_h dx - \int_{\Gamma_I} [\![\phi]\!] \cdot \hat{\vec{q}}_h ds - \int_{\Gamma_b} \phi^+ \vec{q}_b \cdot n ds = \sum_{k \in T_h^p} \int_{\Omega_k} g\phi dx \quad (10)$$

$$\sum_{k \in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \vec{q}_h dx = \sum_{k \in T_h^p} \int_{\Omega_k} \vec{\tau}_h \cdot \nabla u_h dx - \int_{\Gamma_I} \{\vec{\tau}_h\} [\![u_h]\!] ds - \int_{\Gamma_b} (u_h - u_b) \vec{\tau}_h \cdot \vec{n} ds \quad (11)$$

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- Now we can combine the weak forms of the primary and auxiliary equations into 1!

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- The final discretized system of the elliptic equation for the symmetric interior penalty method is written as

$$\sum_{k\in T_h^p}\int_{\Omega_k}\nabla\phi\cdot\nabla u_h dx-\int_{\Gamma_I}\{\nabla u_h\}[\![\phi]\!]+\{\nabla\phi\}[\![u_h]\!]-\eta[\![\phi]\!]\cdot[\![u_h]\!]\ ds$$
$$-\int_{\Gamma_b}\phi^+\nabla u_h^+\cdot\vec{n}+\nabla\phi^+\cdot(u_h-u_b)\cdot\vec{n}-\eta\phi^+(u_h-u_b)\vec{n}\cdot\vec{n}\ ds$$
$$=\sum_{k\in T_h^p}\int_{\Omega_k}g\phi dx$$

  - The symmetry term ensures the system be positive definite.
  - Addition of the penalty term is for stability.
  - Penalty parameter: $\eta=\frac{(p+1)(p+D)}{(2D)}\max(\frac{S_k^+}{V_k^+},\frac{S_k^-}{V_k^-})$
  - Obtain $\nabla\phi$ analytically and $\nabla u_h=\sum_{i=1}^M\tilde{u}_i\nabla\phi_i$

Interior Penalty Formulation for Elliptic Equations

- The final discretized system of the elliptic equation for the symmetric interior penalty method is written as

$$\sum_{k\in T_h^p}\int_{\Omega_k}\nabla\phi\cdot\nabla u_h dx - \int_{\Gamma_I}\{\nabla u_h\}[\![\phi]\!] + \{\nabla\phi\}[\![u_h]\!] - \eta[\![\phi]\!]\cdot[\![u_h]\!]\ ds$$
$$-\int_{\Gamma_b}\phi^+\nabla u_h^+\cdot\vec{n} + \nabla\phi^+\cdot(u_h-u_b)\cdot\vec{n} - \eta\phi^+(u_h-u_b)\vec{n}\cdot\vec{n}\ ds$$
$$=\sum_{k\in T_h^p}\int_{\Omega_k} g\phi dx$$

  - The symmetry term ensures the system be positive definite.
  - Addition of the penalty term is for stability.
  - Penalty parameter: $\eta = \frac{(p+1)(p+D)}{(2D)}\max(\frac{S_k^+}{V_k^+},\frac{S_k^-}{V_k^-})$
  - Obtain $\nabla\phi$ analytically and $\nabla u_h = \sum_{i=1}^{M}\tilde{u}_i\nabla\phi_i$

Outline (Lecture 1)

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1. Motivation
2. DG Formulation for A Hyperbolic Equation
3. Interior Penalty Formulation for Elliptic Equations
4. Explicit and Implicit Time Integration
5. Numerical Examples
6. Conclusions

- Model problem: governed by the Euler or Navier-Stokes equations
  - Conservation of mass (continuity):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0$$

  - Conservation of momentum:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} + \frac{\partial \rho uv}{\partial y} + \frac{\partial \rho uw}{\partial z} - \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{xy}}{\partial y} - \frac{\partial \tau_{xz}}{\partial z} = 0$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \rho uv}{\partial x} + \frac{\partial (\rho v^2 + p)}{\partial y} + \frac{\partial \rho vw}{\partial z} - \frac{\partial \tau_{xy}}{\partial x} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial \tau_{yz}}{\partial z} = 0$$

$$\frac{\partial \rho w}{\partial t} + \frac{\partial \rho uw}{\partial x} + \frac{\partial \rho vw}{\partial y} + \frac{\partial (\rho w^2 + p)}{\partial z} - \frac{\partial \tau_{xz}}{\partial x} - \frac{\partial \tau_{yz}}{\partial y} - \frac{\partial \tau_{zz}}{\partial z} = 0$$

  - Conservation of energy:

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p)u}{\partial x} + \frac{\partial (\rho E + p)v}{\partial y} + \frac{\partial (\rho E + p)w}{\partial z} - \frac{\partial (u\tau_{xx} + v\tau_{xy} + w\tau_{xz} + \kappa \frac{\partial T}{\partial x})}{\partial x}$$
$$- \frac{\partial (u\tau_{xy} + v\tau_{yy} + w\tau_{yz} + \kappa \frac{\partial T}{\partial y})}{\partial y} - \frac{\partial (u\tau_{xz} + v\tau_{yz} + w\tau_{zz} + \kappa \frac{\partial T}{\partial z})}{\partial z} = 0$$

  - Additional transport equation may be added depending on complexity of the problem.

High-Order Discontinuous Galerkin Discretizations

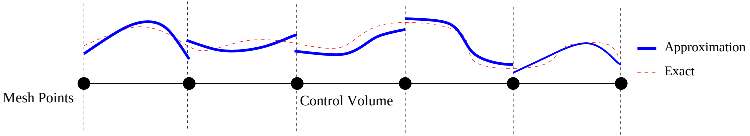
- Write the governing equations in the conservative form:

$$\frac{\partial \mathbf{U}(\mathbf{x},t)}{\partial t} + \nabla \cdot (\mathbf{F}_e(\mathbf{U}) - \mathbf{F}_v(\mathbf{U}, \nabla \mathbf{U})) = 0 \quad \text{in} \quad \Omega$$

  - $\mathbf{U} = \{\rho, \rho\mathbf{u}, \rho E\}^T$: Conservative variables of density, momentum and total energy
  - $\mathbf{F}_e$, $\mathbf{F}_v$: Cartesian inviscid and viscous flux vectors

- Divide the domain into non-overlapping elements

- Represent the solution using piecewise polynomial functions, $\mathbf{U}_h = \sum_{i=1}^{M} \tilde{\mathbf{U}}_{h_i} \; \phi_i(\mathbf{x})$



- Take the integral form and multiply by test functions, $\{\phi_j\}$

$$\sum_k \int_{\Omega_k} \phi_j \left[\frac{\partial \mathbf{U}_h(\mathbf{x},t)}{\partial t} + \nabla \cdot (\mathbf{F}_e(\mathbf{U}_h) - \mathbf{F}_v(\mathbf{U}_h, \nabla \mathbf{U}_h)) \right] d\Omega_k = 0$$

High-Order Discontinuous Galerkin Discretizations

- Weak statement

$$\sum_k \int_{\Omega_k} \phi_j \left[\frac{\partial \mathbf{U}_h(\mathbf{x},t)}{\partial t} + \nabla \cdot (\mathbf{F}_e(\mathbf{U}_h) - \mathbf{F}_v(\mathbf{U}_h, \nabla \mathbf{U}_h)) \right] d\Omega_k = 0$$

- Integrate by parts and Implement an explicit symmetric interior penalty method

$$\int_{\Omega_k} \phi_j \frac{\partial \mathbf{U}_h}{\partial t} d\Omega_k - \int_{\Omega_k} \nabla \phi_j \cdot (\mathbf{F}_e(\mathbf{U}_h) - \mathbf{F}_v(\mathbf{U}_h, \nabla_h \mathbf{U}_h))\, d\Omega_k + \int_{\partial\Omega_k \setminus \partial\Omega} \underline{[[\phi_j]]} \mathbf{H}_c(\mathbf{U}_h^+, \mathbf{U}_h^-, \mathbf{n}) dS$$
$$- \int_{\partial\Omega_k \setminus \partial\Omega} \{\mathbf{F}_v(\mathbf{U}_h, \nabla_h \mathbf{U}_h)\} \cdot [[\phi_j]] dS - \int_{\partial\Omega_k \setminus \partial\Omega} \{(\mathbf{G}_{i1} \frac{\partial \phi_j}{\partial \mathbf{x}_i}, \mathbf{G}_{i2} \frac{\partial \phi_j}{\partial \mathbf{x}_i}, \mathbf{G}_{i3} \frac{\partial \phi_j}{\partial \mathbf{x}_i})\} \cdot [[\mathbf{U}_h]] dS + \int_{\partial\Omega_k \setminus \partial\Omega} \eta \{\mathbf{G}\} [[\mathbf{U}_h]] \cdot [[\phi_j]] dS$$
$$- \int_{\partial\Omega_k \cap \partial\Omega} \phi_j^+ \mathbf{F}_v^b(\mathbf{U}_b, \nabla_h \mathbf{U}_h^+) \cdot \mathbf{n} dS - \int_{\partial\Omega_k \cap \partial\Omega} (\mathbf{G}_{i1}(\mathbf{U}_b) \frac{\partial \phi_j^+}{\partial \mathbf{x}_i}, \mathbf{G}_{i2}(\mathbf{U}_b) \frac{\partial \phi_j^+}{\partial \mathbf{x}_i}, \mathbf{G}_{i3}(\mathbf{U}_b) \frac{\partial \phi_j^+}{\partial \mathbf{x}_i}) \cdot (\mathbf{U}_h^+ - \mathbf{U}_b) \mathbf{n} dS$$
$$+ \int_{\partial\Omega_k \cap \partial\Omega} \eta \mathbf{G}(\mathbf{U}_b)(\mathbf{U}_h^+ - \mathbf{U}_b)\mathbf{n} \cdot \phi_j^+ \mathbf{n} dS + \int_{\partial\Omega_k \cap \partial\Omega} \phi_j \mathbf{F}_e(\mathbf{U}_b) \cdot \mathbf{n} dS = 0$$

where $\mathbf{G}_{1j} = \partial \mathbf{F}_v^x / \partial(\partial \mathbf{U}/\partial \mathbf{x}_j)$, $\mathbf{G}_{2j} = \partial \mathbf{F}_v^y / \partial(\partial \mathbf{U}/\partial \mathbf{x}_j)$ and $\mathbf{G}_{3j} = \partial \mathbf{F}_v^z / \partial(\partial \mathbf{U}/\partial \mathbf{x}_j)$

- Solution expansion and geometric mapping

$$\mathbf{U}_h = \sum_{i=1}^{M} \tilde{\mathbf{U}}_{h_i}\ \phi_i(\xi, \eta, \zeta) \qquad \mathbf{x}_k = \sum_{i=1}^{M} \tilde{\mathbf{x}}_{k_i} \phi_i(\xi, \eta, \zeta)$$

Explicit Time Integration

- Rewrite the weak statement as an ordinary differential equation (ODE):

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

- First-order forward Euler method

$$\mathbf{M}\frac{\tilde{\mathbf{U}}_h^{n+1} - \tilde{\mathbf{U}}_h^{n}}{\Delta t} + \mathbf{R}(\tilde{\mathbf{U}}_h^n) = 0$$

$$\tilde{\mathbf{U}}_h^{n+1} = \tilde{\mathbf{U}}_h^{n} - \Delta t M^{-1}\mathbf{R}(\tilde{\mathbf{U}}_h^n)$$

- Second-order TVD Runge-Kutta method [Shu and Osher 1988]

$$\begin{aligned}
\tilde{\mathbf{U}}_h^{(1)} &= \tilde{\mathbf{U}}_h^{(n)} - \Delta t M^{-1}\mathbf{R}(\tilde{\mathbf{U}}_h^n) \\
\tilde{\mathbf{U}}_h^{n+1} &= \frac{1}{2}\tilde{\mathbf{U}}_h^{(n)} + \frac{1}{2}\left(\tilde{\mathbf{U}}_h^{(1)} - \Delta t M^{-1}\mathbf{R}(\tilde{\mathbf{U}}_h^{(1)})\right)
\end{aligned}$$

Explicit Time Integration

- Rewrite the weak statement as an ordinary differential equation (ODE):

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

- First-order forward Euler method

$$\mathbf{M}\frac{\tilde{\mathbf{U}}_h^{n+1} - \tilde{\mathbf{U}}_h^{n}}{\Delta t} + \mathbf{R}(\tilde{\mathbf{U}}_h^{n}) = 0$$

$$\tilde{\mathbf{U}}_h^{n+1} = \tilde{\mathbf{U}}_h^{n} - \Delta t M^{-1}\mathbf{R}(\tilde{\mathbf{U}}_h^{n})$$

- Second-order TVD Runge-Kutta method [Shu and Osher 1988]

$$\begin{aligned} \tilde{\mathbf{U}}_h^{(1)} &= \tilde{\mathbf{U}}_h^{(n)} - \Delta t M^{-1}\mathbf{R}(\tilde{\mathbf{U}}_h^{n}) \\ \tilde{\mathbf{U}}_h^{n+1} &= \frac{1}{2}\tilde{\mathbf{U}}_h^{(n)} + \frac{1}{2}\left(\tilde{\mathbf{U}}_h^{(1)} - \Delta t M^{-1}\mathbf{R}(\tilde{\mathbf{U}}_h^{(1)})\right) \end{aligned}$$

- Pros/Cons of explicit time integration
  - \+ Simple implementation and no linearization (to obtain Jacobian matrix) is required.
  - \+ Mass matrix M is block diagonal, which allows for fast local inversion.

Explicit Time Integration

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- Rewrite the weak statement as an ordinary differential equation (ODE):

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

- First-order forward Euler method

$$\mathbf{M}\frac{\tilde{\mathbf{U}}_h^{n+1} - \tilde{\mathbf{U}}_h^{n}}{\Delta t} + \mathbf{R}(\tilde{\mathbf{U}}_h^n) = 0$$

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\end{aligned}$$

- Pros/Cons of explicit time integration
  - \+ Simple implementation and no linearization (to obtain Jacobian matrix) is required.
  - \+ Mass matrix M is block diagonal, which allows for fast local inversion.
  - – Selection of Δt is restricted by stability limit but not the temporal accuracy.
  - – Stability issue becomes more severe as the spatial order p is increased ($CFL \sim 1/p^2$).
  - – Not desired for problems with diverse length and time scales.

Implicit Time Discretization

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- Return to the semi-discrete form

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

- Advance in time using an implicit temporal scheme

First-order Backward Difference Formula (BDF1)

$$\mathbf{R}_e^{n+1}(\tilde{\mathbf{U}}_h^{n+1}) = \frac{\mathbf{M}}{\Delta t}(\tilde{\mathbf{U}}_h^{n+1}) + \mathbf{R}(\tilde{\mathbf{U}}_h^{n+1}) - \frac{\mathbf{M}}{\Delta t}\tilde{\mathbf{U}}_h^{n} = 0$$

Second-order Backward Difference Formula (BDF2)

$$\mathbf{R}_e^{n+1}(\tilde{\mathbf{U}}_h^{n+1}) = \frac{\mathbf{M}}{\Delta t}(\tfrac{3}{2}\tilde{\mathbf{U}}_h^{n+1}) + \mathbf{R}(\tilde{\mathbf{U}}_h^{n+1}) - \frac{\mathbf{M}}{\Delta t}(2\tilde{\mathbf{U}}_h^{n} - \tfrac{1}{2}\tilde{\mathbf{U}}_h^{n-1}) = 0$$

Second-order Crank-Nicolson (CN2) Scheme

$$\mathbf{R}_e^{n+1}(\tilde{\mathbf{U}}_h^{n+1}) = \frac{\mathbf{M}}{\Delta t}\tilde{\mathbf{U}}_h^{n+1} + \tfrac{1}{2}\mathbf{R}(\tilde{\mathbf{U}}_h^{n+1}) - \frac{\mathbf{M}}{\Delta t}(\tilde{\mathbf{U}}_h^{n} - \tfrac{1}{2}\mathbf{R}(\tilde{\mathbf{U}}_h^{n})) = 0$$

Implicit Time Discretization

- Fourth-order Six-stage Implicit Runge-Kutta (IRK4) Scheme

$$
\begin{array}{ll}
(i) & \tilde{\mathbf{U}}^{(0)_h} = \tilde{\mathbf{U}}_h^n \\
(ii) & For\ s = 1, \cdots, \mathcal{S} \\
 & \tilde{\mathbf{U}}^{(s)_h} = \tilde{\mathbf{U}}_h^n - \Delta t \sum_{j=1}^{s} a_{sj} M^{-1} \mathbf{R}(\tilde{\mathbf{U}}_h^{(j)}) \\
(iii) & \tilde{\mathbf{U}}_h^{n+1} = \tilde{\mathbf{U}}_h^n - \Delta t \sum_{j=1}^{\mathcal{S}} b_j M^{-1} \mathbf{R}(\tilde{\mathbf{U}}_h^{(j)})
\end{array}
$$

- Butcher table for the ESDIRK scheme

$c_1 = 0$	0	0	0	0	0	0
c_2	a_{21}	$a_{22} = a_{66}$	0	0	0	0
c_3	a_{31}	a_{32}	$a_{33} = a_{66}$	0	0	0
c_4	a_{41}	a_{42}	a_{43}	$a_{44} = a_{66}$	0	0
c_5	a_{51}	a_{52}	a_{53}	a_{54}	$a_{55} = a_{66}$	0
$c_6 = 1$	$a_{61} = b_1$	$a_{62} = b_2$	$a_{63} = b_3$	$a_{64} = b_4$	$a_{65} = b_5$	a_{66}
$\tilde{\mathbf{u}}^{n+1}$	b_1	b_2	b_3	b_4	b_5	b_6

Fourth-order Six-stage Implicit Runge-Kutta (IRK4) Scheme

$$\mathbf{R}_e^{n+1}(\tilde{\mathbf{U}}_h^{(s),n+1}) = \frac{\mathbf{M}}{\Delta t}\tilde{\mathbf{U}}_h^{(s),n+1} + a_{ss}\mathbf{R}(\tilde{\mathbf{U}}_h^{(s),n+1}) - \left[\frac{\mathbf{M}}{\Delta t}\tilde{\mathbf{U}}_h^n - \sum_{j=1}^{s-1} a_{sj}\mathbf{R}(\tilde{\mathbf{U}}_h^{(j),n+1})\right] = 0$$

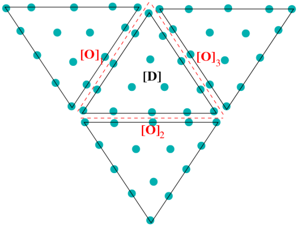
Solution Methods for Implicit Schemes

- Require extra computation to solve the matrix problem
- Use an approximate Newton method

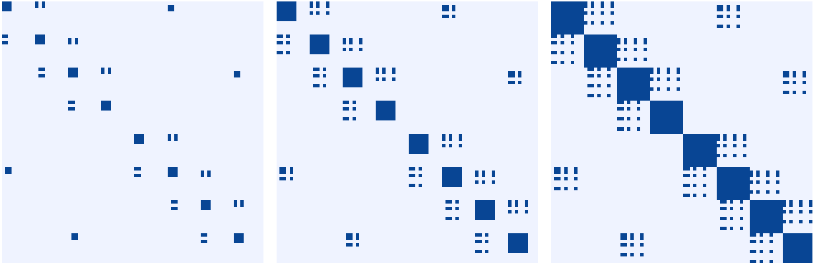
Find $\tilde{\mathbf{U}}$ such that $\mathbf{R}_e(\tilde{\mathbf{U}}) = 0$:

$$\tilde{\mathbf{U}}_{j+1} = \tilde{\mathbf{U}}_j - \alpha \left[\frac{\partial \mathbf{R}_e}{\partial \tilde{\mathbf{U}}} \right]_j^{-1} \mathbf{R}_e(\tilde{\mathbf{U}}_j)$$

  - α is an under-relaxation parameter ($0 < \alpha < 1$)



- Structure of the Jacobian matrix (block sparsity)



$p = 1$ $p = 2$ $p = 3$

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1. Motivation
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Numerical Examples

- Convection of an isentropic vortex
- Shedding flow over a triangular wedge
- Laminar flow over a circular cylinder

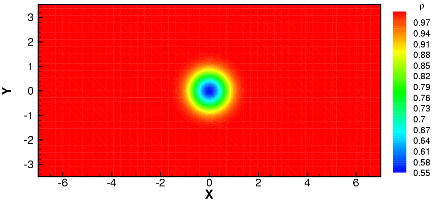
Convection of an Isentropic Vortex

- Examine the accuracy of various implicit time-integration schemes
- Initial condition: uniform flow $(\rho_\infty, u_\infty, v_\infty, p_\infty, T_\infty) = (1, 0.5, 0, 1, 1)$ perturbed by an isentropic vortex

$$\delta u = -\frac{\sigma}{2\pi}(y - y_0)e^{\vartheta(1-r^2)}$$

$$\delta v = \frac{\sigma}{2\pi}(x - x_0)e^{\vartheta(1-r^2)}$$

$$\delta T = -\frac{\sigma^2(\gamma - 1)}{16\vartheta\gamma\pi^2}e^{2\vartheta(1-r^2)}$$



- Determine conservative variables through the assumption of isentropic flow and a perfect gas (i.e. $\gamma p/\rho^\gamma = 1$ and $T = \gamma p/\rho$)

$$\rho = T^{1/(\gamma-1)} = (T_\infty + \delta T)^{1/(\gamma-1)} = \left[1 - \frac{\sigma^2(\gamma - 1)}{16\vartheta\gamma\pi^2}e^{2\vartheta(1-r^2)}\right]^{1/(\gamma-1)}$$

- A rectangular domain of $[-7, 7] \times [-3.5, 3.5]$ partitioned with 10,000 triangular elements
- Periodic boundary condition in the horizontal direction

Convection of an Isentropic Vortex

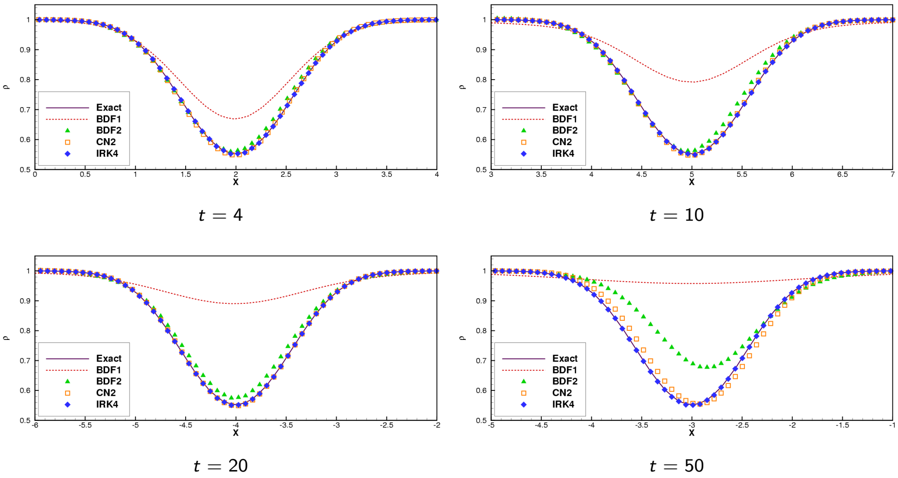
- Simulations from the BDF1 and IRK4 schemes (fixed $\Delta t = 0.2$ and DG $p = 3$)

BDF1 BDF1

IRK4 IRK4

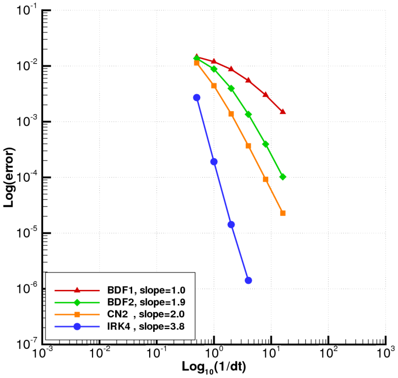
Convection of an Isentropic Vortex

- Comparison of various temporal schemes ($\Delta t = 0.2$) with the exact solution
- Density profiles

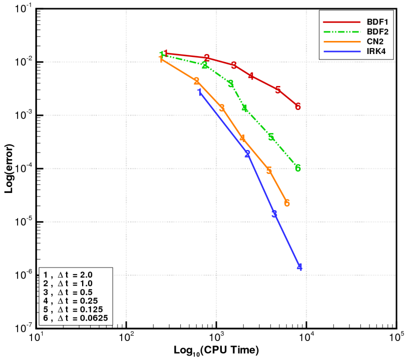


Convection of an Isentropic Vortex

- Examination of temporal accuracy and efficiency



Temporal accuracy



Temporal efficiency

- Desired order of temporal accuracy is achieved.
- Higher-order temporal scheme performs more efficiently than a lower-order counterpart.

Shedding Flow over a Triangular Wedge

- Free-stream Mach number $= 0.2$
- Unstructured mesh with 10,836 elements
- Various spatial discretizations and implicit time-integration schemes ($\Delta t = 0.05$, $CFL_{max} = 85$)

DG $p = 1$ and BDF2 schemes

- Implicit versus explicit schemes
  - Ratio of the smallest to largest cell area is 1:1425 (current mesh)
  - Local CFL number is defined as

$$\mathrm{CFL}_k = \frac{\Delta t}{vol_k} \sum_{j=1}^{\text{faces}} (|\mathbf{u} \cdot \mathbf{n}| + c)_j$$

  - Correspond to an explicit CFL ratio of 38:1
  - Comparison between second-order BDF2 scheme and second-order explicit forward Euler (FD2) scheme (fixed spatial scheme of $p = 3$)

$$\tilde{\mathbf{U}}_h^{n+1} = \frac{4}{3}\tilde{\mathbf{U}}_h^{n} - \frac{1}{3}\tilde{\mathbf{U}}_h^{n-1} - \frac{2}{3} M^{-1} \Delta t \mathbf{R}(\tilde{\mathbf{U}}_h^{n})$$

Shedding Flow over a Triangular Wedge

- Implicit versus explicit schemes
  - Ratio of the smallest to largest cell area is 1:1425 (current mesh)
  - Local CFL number is defined as

$$\mathrm{CFL}_k = \frac{\Delta t}{vol_k} \sum_{j=1}^{\mathrm{faces}} \left(|\mathbf{u} \cdot \mathbf{n}| + c \right)_j$$

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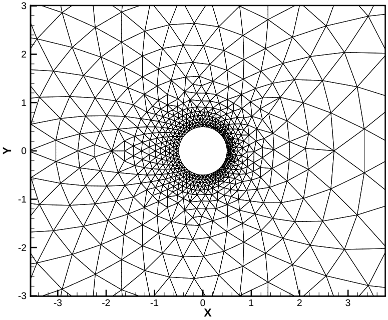
  - Comparison between second-order BDF2 scheme and second-order explicit forward Euler (FD2) scheme (fixed spatial scheme of $p = 3$)

$$\tilde{\mathbf{U}}_h^{n+1} = \frac{4}{3}\tilde{\mathbf{U}}_h^n - \frac{1}{3}\tilde{\mathbf{U}}_h^{n-1} - \frac{2}{3}M^{-1}\Delta t \mathbf{R}(\tilde{\mathbf{U}}_h^n)$$

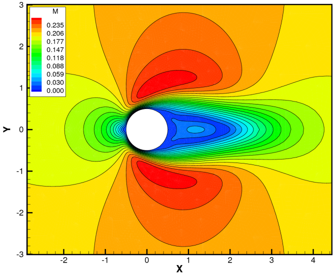
$t = 2.5$	Time-step size	Time steps	Convergence limit	CPU time (s)
Implicit (BDF2)	$\Delta t = 0.05$	50	7 orders	5160
Explicit (FD2)	$\Delta t = 5 \times 10^{-5}$	50000	–	22920

  - A speedup of 4.5 is obtained through the use of the implicit time-integration scheme (significant improvement for long-term integration problems).

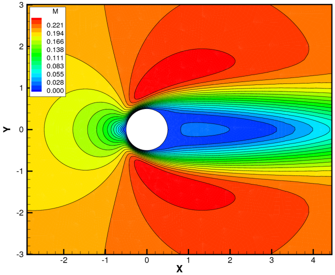
- $Re_D = 40$, $M_\infty = 0.2$ and $AOA = 0^\circ$
  - Adiabatic and no-slip wall boundary condition
  - Various orders of DG discretizations
  - BDF2 scheme with $\Delta t = 0.05$



Computational mesh (N =1622)

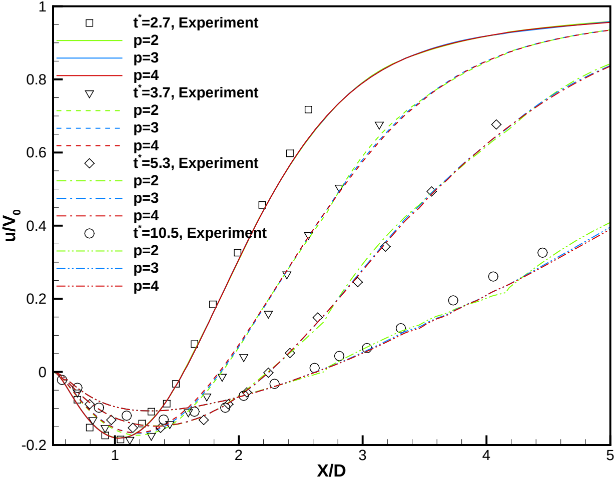


Mach number contours ($p = 4$) at $t = 3.7$



Mach number contours ($p = 4$) at $t = 10.5$

- Comparison of streamwise velocity evolution at the flow axis with experimental data [Coutanceau 1977]



Outline (Lecture 1)

Conclusions

- High-order methods have earned increasing popularity for solving convection, diffusion and convection-diffusion equations, which have wide applications in fluid dynamics.
- Discontinuous Galerkin methods can be viewed as an intermediate approach between finite element and finite volume methods.
- Higher-order temporal schemes are capable of achieving higher accuracy solution over the lower-order counterparts with a fixed time-step size.
- The use of higher-order time-integration schemes aims to balance spatial and temporal errors.
- To make high-order discontinuous Galerkin methods competitive, solution acceleration methods are required, which will be discussed in the next lecture.

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