Adaptive Differential
Discontinuous High-Order Methods in CFD

Z.J. Wang (zjwang.com)
Spahr Professor and Chair
Department of Aerospace Engineering
University of Kansas, Lawrence, U.S.A.
Outline

➢ Lecture 1:
  ▪ Introduction and review
  ▪ Extending a 1\textsuperscript{st} order scheme to higher-order
    ○ Discontinuous Galerkin
    ○ Spectral volume
    ○ Spectral difference
    ○ Correction procedure via reconstruction or flux reconstruction

➢ Lecture 2:
  ▪ Extension to multiple dimensions
  ▪ Extension to viscous problems
Outline (cont.)

➢ Lecture 3:
  ▪ Boundary conditions
  ▪ Shock capturing
    ○ Limiter
    ○ Artificial viscosity

➢ Lecture 4:
  ▪ Solution based hp-adaptations
  ▪ Sample demonstration problems
  ▪ Remaining research issues
Outline

Lecture 1:

- Introduction and review
- Extending a 1st order scheme to higher-order
  - Discontinuous Galerkin
  - Spectral volume
  - Spectral difference
  - Correction procedure via reconstruction or flux reconstruction
My Philosophy

- To present key ideas in 1D, not dwell on implementation details
- To show how these ideas were developed so you can develop new ones
- Highlight the similarities and differences, pros and cons wherever possible
Introduction

\[ \frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0, \quad c > 0 \]
Introduction – Approximation

How to approximate an unknown solution with possibly infinite number of degrees of freedom (nDOFs) with a limited nDOFs

- Piece-wise polynomials (FD, FV, FE, …)
- A global expansion composed of discrete sine and cosine functions (spectral method)
- A global high-order polynomial?
- …
Degrees of Freedom

- Finite difference (FD)
  - Nodal values on a set of discrete points
  - Local polynomial approximation
  - Discontinuous?

- Finite volume (FV)
  - Control volume averages
  - Local polynomial approximation
  - Discontinuous

- Finite element (FE)
  - Nodal or modal
  - Local polynomial approximation
  - Either continuous or discontinuous
Let’s Start from the Very Beginning

- 1\textsuperscript{st} order FD upwind scheme

\[ \frac{\partial u_i}{\partial t} + c \frac{(u_i - u_{i-1})}{\Delta x} = 0 \]

- 1\textsuperscript{st} order FV upwind scheme

\[ \frac{\partial \overline{u}_i}{\partial t} + c \frac{\overline{u}_i - \overline{u}_{i-1}}{\Delta x} = 0 \]
How to Extend to Higher Order

- Extend the stencil

- Add more degrees of freedom in element

\[ u_i(x) \in P^2 \]
Extending Stencil vs. More Internal DOFs

- Simple formulation and easy to understand for structured mesh
- Complicated boundary conditions: high-order one-sided difference on uniform grids may be unstable
- Not compact

- Boundary conditions trivial with uniform accuracy
- Non-uniform and unstructured grids
  - Reconstruction universal
- Scalable
  - Communication through immediate neighbor
Review of the Godunov FV Method

Consider

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

Integrate in \( V_i \)

\[
\int_{V_i} \left( \frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} \right) dx = \frac{\partial \bar{u}_i}{\partial t} \Delta x_i + \int_{i-1/2}^{i+1/2} \frac{\partial f}{\partial x} dx
\]

\[
= \frac{\partial \bar{u}_i}{\partial t} \Delta x_i + (f_{i+1/2} - f_{i-1/2}) = 0
\]
Godunov FV Method (cont.)

- Assume the solution is piece-wise constant, or a degree 0 polynomial.
- However, a new problem is created. The solution is discontinuous at the interface.
- How to compute the flux?
  \[ f_{i+1/2} = \frac{[f(u_i) + f(u_{i+1})]}{2} \]
- A “shock-tube” problem solved to obtain the flux by Godunov.
- Other Riemann solvers developed for efficiency.
Discontinuous Galerkin Method

- Originally developed in 1970s and popular since 1990s (Cockburn & Shu, Bassi & Rebay, …)
- Each cell has enough DOFs so that neighboring data are not used in reconstructing a higher-degree polynomial
- Assume we choose \( a, b \) and \( c \) as the DOFs so that

\[
U_i(x) = a_i + b_i x + c_i x^2, \quad x \in V_i
\]
Discontinuous Galerkin Method (cont.)

- However, at each cell we need to update 3 DOFs! How?
- Finite volume update

\[
\int_{V_i} 1 \left( \frac{\partial U}{\partial t} + \frac{\partial f}{\partial x} \right) dx = 0
\]

- Two more equations based on weighed residual

\[
\int_{V_i} x \left( \frac{\partial U}{\partial t} + \frac{\partial f}{\partial x} \right) dx = 0
\]
\[
\int_{V_i} x^2 \left( \frac{\partial U}{\partial t} + \frac{\partial f}{\partial x} \right) dx = 0
\]

- Then

\[
\int_{V_i} \phi \left( \frac{\partial U}{\partial t} + \frac{\partial f}{\partial x} \right) dx = \int_{V_i} \phi \frac{\partial U}{\partial t} dx + (\phi \hat{f}_{Riem})_{i+1/2} - \int_{V_i} f \frac{\partial \phi}{\partial x} dx = 0
\]
Spectral Volume Method

- Develop in early 2000s (Wang, Liu, …)
- Each cell has again enough DOFs so that neighboring data are not used in reconstructing a higher-degree polynomial
- The DOFs are sub-cell averages. The number of sub-cells is $k+1$ in 1D
- The polynomial at each cell is reconstructed from the sub-cell averages

\[
C_{i,j} \quad i,j-1/2 \quad i,j+1/2
\]
Spectral Volume Method (cont.)

- The sub-cell averages are updated using a FV method on the sub-cell

\[
\frac{d\bar{u}_{i,j}}{dt} \Delta x_{i,j} + (f_{i,j+1/2} - f_{i,j-1/2}) = 0
\]

- Riemann fluxes are only used across the cell interfaces

- Reconstruction universal
SD/Correction Procedure via Reconstruction

- SD developed by Y. Liu et al. in 2005 and CPR Developed by Huynh in 2007 and extended to simplex by Wang & Gao in 2009, ...

- It is a differential formulation like “finite difference”

\[
\frac{\partial U_i(x)}{\partial t} + \frac{\partial F_i(x)}{\partial x} = 0, \quad U_i(x) \in P^k, \quad F_i(x) \in P^{k+1}
\]

- The DOFs are solutions at a set of “solution points”
**CPR (cont.)**

- Find a flux polynomial \( F_i(x) \) one degree higher than the solution, which minimizes

\[
\| \tilde{F}_i(x) - F_i(x) \|
\]

- The use the following to update the DOFs

\[
\frac{du_{i,j}}{dt} + \frac{dF_i(x_{i,j})}{dx} = 0
\]
If the new flux polynomial goes through the flux values at the flux points, the resultant scheme is spectral difference/volume.
If the following equations are satisfied

\[
\int_{V_i} \left[ \tilde{F}_i(x) - F_i(x) \right] dx = 0
\]

\[
\int_{V_i} \left[ \tilde{F}_i(x) - F_i(x) \right] x dx = 0
\]

The scheme is DG!
1D – P1 SV/SD and DG Schemes

\[
\begin{align*}
\frac{du_{i,2}}{dt} + \frac{c}{\Delta x/2} (u_{i,2} - u_{i,1}) &= 0 \\
\frac{du_{i,1}}{dt} + \frac{c}{\Delta x} (u_{i,2} + u_{i,1} - 3u_{i-1,2} + u_{i-1,1}) &= 0
\end{align*}
\] SV/SD

\[
\begin{align*}
\frac{du_{i,1}}{dt} + \frac{c}{4\Delta x} (3u_{i,2} + 7u_{i,1} - 15u_{i-1,2} + 5u_{i-1,1}) &= 0 \\
\frac{du_{i,2}}{dt} + \frac{c}{4\Delta x} (9u_{i,2} - 11u_{i,1} + 3u_{i-1,2} - 5u_{i-1,1}) &= 0
\end{align*}
\] DG
Outline

Lecture 2:
- Extension to multiple dimensions
- Extension to viscous problems
CPR in 2D

Consider

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

The weighted residual form is

\[
\int_{V_i} \left( \frac{\partial Q}{\partial t} + \nabla \cdot \vec{F}(Q) \right) W dV = \int_{\partial V_i} \frac{\partial Q}{\partial t} W dV + \int_{\partial V_i} W \vec{F}(Q) \cdot \vec{n} dS - \int_{V_i} \nabla W \cdot \vec{F}(Q) dV = 0.
\]

Let \( Q^h \) be the discontinuous approximate solution in \( P^k \).

The face flux integral replaced by a Riemann flux

\[
\int_{V_i} \frac{\partial Q_i^h}{\partial t} W dV + \int_{\partial V_i} W \vec{F}_n^\ast (Q_i^h, Q_{i+}^h, \vec{n}) dS - \int_{V_i} \nabla W \cdot \vec{F}(Q_i^h) dV = 0.
\]
Performing integration by parts to the last term
\[ \int \frac{\partial Q_i^h}{\partial t} W dV + \int W \nabla \cdot \tilde{F}(Q_i^h) dV + \int W \left[ \tilde{F}^n(Q_i^h, Q_{i+1}^h, \tilde{n}) - F^n(Q_i^h) \right] dS = 0. \]

Introduce the lifting operator
\[ \int W \delta_i dV = \int W \left[ \tilde{F} \right] dS \]

where \( \delta_i \in P^k \), \( \left[ \tilde{F} \right] = \left[ \tilde{F}^n(Q_i^h, Q_{i+1}^h, \tilde{n}) - F^n(Q_i^h) \right] \) Then we have
\[ \int \frac{\partial Q_i^h}{\partial t} W dV + \int W \nabla \cdot \tilde{F}(Q_i^h) dV + \int W \delta_i dV = 0, \]
CPR in 2D (cont.)

Or

\[ \int_{V_i} \left( \frac{\partial Q_i^h}{\partial t} + \nabla \cdot \tilde{F}(Q_i^h) + \delta_i \right) WdV = 0, \]

which is equivalent to

\[ \frac{\partial Q_i^h}{\partial t} + \nabla \cdot \tilde{F}(Q_i^h) + \delta_i = 0. \]

In the new formulation, the weighting function completely disappears! Note that $\delta_i$ depends on $W$. 
Lifting Operator – Correction Field

Obviously, the computation of $\delta_i$ is the key. From

$$\int_{V_i} W \delta_i \, dV = \int_{\partial V_i} W [\tilde{F}] \, dS,$$

If $[\tilde{F}], \delta_i \in P^k$ $\delta_i$ can be computed explicitly given $W$. Define a set of “flux points” along the faces, and set of solution points, where the “correction field” is computed as shown. Then

$$\delta_{i,j} = \frac{1}{|V_i|} \sum_{f \in \partial V_i} \sum_l \alpha_{j,f,l} [\tilde{F}]_{f,l} S_f,$$

$\alpha_{j,f,l}$: lifting coefficients independent of $Q$
Finally the following equation is solved at the solution point $j$ (collocation points)

$$\frac{\partial Q^h_{i,j}}{\partial t} + \nabla \cdot \vec{F}(Q^h_{i,j}) + \frac{1}{|V_i|} \sum_{f \in \partial V_i} \sum_l \alpha_{j,f,l} [\tilde{F}]_{f,l} S_f = 0.$$ 

The first two terms correspond to the differential equation, and the 3rd term is the correction term.
Arrangement of SPs and FPs

\[ P = 2 \]

\[ P = 3 \]

\[ P = 2 \]
Extension to High-Order Elements

Transform an iso-parametric element to the standard element

\[ \mathbf{r} = \sum_{j=1}^{N} M_j(\xi, \eta) \mathbf{r}_j \]

Then

\[ \frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = 0 \]

becomes

\[ \frac{\partial \tilde{Q}}{\partial t} + \frac{\partial \tilde{E}}{\partial \xi} + \frac{\partial \tilde{F}}{\partial \eta} = 0 \]
Extension to High-Order Elements (cont.)

where

\[ \tilde{Q} = |J|Q \]
\[ \tilde{E} = |J|(E\xi_x + F\xi_y) \]
\[ \tilde{F} = |J|(E\eta_x + F\eta_y) \]

and

\[ J = \frac{\partial(x, y)}{\partial(\xi, \eta)} = \begin{bmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{bmatrix} = \begin{bmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{bmatrix}^{-1} \]
Extension to High-Order Elements (cont.)

Apply CPR to the transformed equation on the standard element

\[
\frac{\partial Q_{i,j}^h}{\partial t} + \nabla \cdot \bar{F}(Q_{i,j}^h) + \frac{2}{|J_{i,j}|} \sum_{f \in \partial V_i} \sum_{l} \alpha_{j_f,l} [\tilde{F}]_{f,l} S_{f,l} = 0.
\]

For quadrilateral element, the CPR scheme is 1D in each coordinate direction!
Mixed Grids

- In order to minimize data reconstruction and communication, solution points coincide with flux points.
- For quadrilateral elements, the corrections are one-dimensional!
- Mass matrix is $I$ for all cell-types.

\[ [\hat{F}]_{f,1}, [\hat{F}]_{f,2}, [\hat{F}]_{f,3} \]
Extension to Viscous Flows

- How to deal with the second order derivative?
- Second Order FV Method:
  - The solution gradients at an interface are sometimes computed by averaging the gradients of the neighboring cells sharing the face.
- High Order Method:
  - Local Discontinuous Galerkin (Cockburn and Shu), motivated by the numerical results of Bassi and Rebay
  - Internal Penalty
Simplest Case First - SV

Consider the 1D heat equation

\[ u_t - u_{xx} = 0, \quad x \in [0, 2\pi] \quad \text{periodic boundary condition} \]

\[ u(x,0) = \sin(x) \]

Integrating in a CV to obtain

\[
\frac{d\bar{u}_{i,j}(t)}{dt} h_{i,j} - (u_x|_{i,j+1/2} - u_x|_{i,j-1/2}) = 0
\]

with

\[
\bar{u}_{i,j}(t) = \frac{\int_{x_{i,j-1/2}}^{x_{i,j+1/2}} u(x, t) dx}{h_{i,j}}
\]
Formulation for 1D Heat Equation

Because the solution is SV-wise continuous, \( u_x \) not well defined at SV boundaries. Therefore it is replaced by a “numerical flux” \( \hat{u}_x \)

\[
\frac{d\bar{u}_{i,j}(t)}{dt} - \frac{1}{h_{i,j}} (\hat{u}_x|_{i,j+1/2} - \hat{u}_x|_{i,j-1/2}) \approx 0
\]

Formulation 1-Naïve SV Formulation

\[
\hat{u}_x|_{i,j+1/2} = \frac{1}{2} \left[ (u_x)^+_{i,j+1/2} + (u_x)^-_{i,j+1/2} \right]
\]
Behaviors of the Naïve SV Formulation

$t = 0.7$

This formulation converges to the wrong solution!
Similar result by Cockburn and Shu
Formulation 1 - Local DG Formulation

Introducing an auxiliary unknown \( q = u_x \)

\[
\begin{align*}
u_t - q_x &= 0 \\
q - u_x &= 0
\end{align*}
\]

Integrating in a CV

\[
\begin{align*}
\frac{d\bar{u}_{i,j}}{dt} - \frac{1}{h_{i,j}} ( \hat{q}|_{i,j+1/2} - \hat{q}|_{i,j-1/2} ) &= 0 \\
\bar{q}_{i,j} - \frac{1}{h_{i,j}} ( \hat{u}|_{i,j+1/2} - \hat{u}|_{i,j-1/2} ) &= 0.
\end{align*}
\]

Selecting “numerical flux” following LDG

\[
\begin{align*}
\hat{u}|_{i,j+1/2} &= u^+|_{i,j+1/2} \\
\hat{q}|_{i,j+1/2} &= q^-|_{i,j+1/2}
\end{align*}
\]
Computational Results of LDG

\[(k+1)\text{-th order achieved for a degree } k \text{ polynomial reconstruction}\]
Formulation 2 – Penalty Formulation

Numerical flux given by

\[
\hat{u}_x |_{i,j+1/2} = \frac{1}{2} \left[ (u_x)^+_{i,j+1/2} + (u_x)^-_{i,j+1/2} \right] + \frac{\varepsilon}{h_{i,j}} (u^+_{i,j+1/2} - u^-_{i,j+1/2})
\]

where \( \varepsilon \) is a constant. A Fourier analysis performed to choose the value \( \varepsilon \). It was found \( \varepsilon = 1 \) gives the highest order of accuracy for linear reconstruction.
Results of the Penalty Formulation

\[(k+1)\text{-th order achieved for a degree } k \text{ polynomial if } k \text{ odd, otherwise } k\text{-th order.}\]
CPR Formulation for Computing Gradients

Introduce another variable

\[ R = Q_x \]

Apply weighted residual to the above equation

\[
\int_{V_i} RW_i dx = \int_{V_i} WQ_x dx = \int_{V_i} [(WQ)_x - QW_x] dx
\]

\[
= (WQ_{com})|_L^R - \int_{V_i} QW_x dx = [W(Q_{com} - Q)]|_L^R + \int_{V_i} WQ_x dx
\]

Let

\[
\int_{V_i} \delta W_i dx = [W(Q_{com} - Q)]|_L^R
\]

Then

\[
R_{i,j} = (Q_i)_x,j + \alpha_{L,j}(Q_{com,L} - Q_L) + \alpha_{R,j}(Q_{com,R} - Q_R)
\]
CPR Formulation for Computing Gradients

Need to compute gradient

\[ \vec{R} = \nabla Q \]

Applying CPR to the above equation, we obtain

\[
R_{i,j} = \left( \nabla Q_i^h \right)_j + \frac{1}{|V_i|} \sum_{f \in \partial V_i} \sum_{l} \alpha_{j,f,l} \left[ Q_{f,l}^{com} - Q_{i,f,l} \right]_{f,l} \vec{n}_f s_f
\]
LDG on 2D Convection-Diffusion Equations

Consider

\[ u_t + \nabla \cdot (\mathbf{b} u) - \nabla \cdot (\mu \nabla u) = 0 \]

Introducing auxiliary variables

\[ q = \nabla u \]

Integrating in a CV to obtain

\[ \bar{q}_{i,j} - \frac{1}{V_{i,j}} \sum_{r=1}^{K} \int_{A_r} \hat{u} \cdot n dA = 0 \]

\[ \frac{d\bar{u}_{i,j}}{dt} + \frac{1}{V_{i,j}} \left\{ \sum_{r=1}^{K} \int_{A_r} (\mathbf{b}\hat{u} \cdot n) dA - \sum_{r=1}^{K} \int_{A_r} \mu \hat{q} \cdot n dA \right\} = 0 \]
Numerical Flux Computation

Upwind for inviscid flux

\[ \tilde{u} = \begin{cases} u_L & \beta \cdot n > 0 \\ u_R & \beta \cdot n < 0 \end{cases} \]

Alternate directions for viscous and auxiliary “numerical fluxes”

or

\[ \hat{u} \approx u_R \quad \hat{q} \approx q_L \]

\[ \hat{u} \approx u_L \quad \hat{q} \approx q_R \]
Results for 2D Convection-Diffusion Equations

\[ u_t + (u_x + u_y) - 0.01(u_{xx} + u_{yy}) = 0, \quad (x, y) \in [-1,1] \times [-1,1] \]

\[ u(x, y, 0) = \sin(\pi(x + y)) \]
Numerical Experiments on NS Equations

- Couette Flow
- Laminar Flow along a Flat Plate
- Subsonic Flow over a Circular Cylinder
- Laminar Subsonic Flow around NACA0012 Airfoil
Couette Flow - Convergence

Convergence History
Laminar Flow along a Flat Plate

Flow Conditions:
- Free stream Ma = 0.3, Re = 10000
- Adiabatic plate, length = 1.0

The Thickness of Boundary Layer (at x=1.0):

\[
\delta \bigg|_{x=1.0} = 5 \cdot \sqrt{\frac{\mu \cdot x}{\rho_\infty \cdot u_\infty}} \bigg|_{x=1.0} = 5 \cdot \frac{x}{\sqrt{\text{Re}} \bigg|_{x=1.0}} = 0.05
\]
Computational Domain

$[-1, 1] \times [0, 1]$
Mesh

Coarse mesh - 208 cells (8 cells along the plate)
Medium mesh - 832 cells (16 cells along the plate)
Fine mesh - 3328 cells (32 cells along the plate)
u-velocity Profiles with Different SVs

Linear SV

Cubic SV
Skin Fraction Coefficient along the plate

Linear SV
Skin Fraction Coefficient (con’d)

Quadratic SV

- **Blasius solution**
- **Coarse mesh**
- **Medium mesh**
- **Fine mesh**
Skin Fraction Coefficient (con’d)

Cubic SV

Cf

Blasius solution
Coarse mesh
Medium mesh
Fine mesh

x
Subsonic Flow over a Circular Cylinder

Flow Conditions: $Ma = 0.2$, $Re = 75$

Mesh Near the Cylinder
Schematic Structure and Mesh

- **Adiabatic wall**
- **Fix every thing**
- **Fix pressure**
Interested Phenomena

- The Von Karmen Vortex Street (generated by the cylinder)
  - Mach contours
  - Entropy contours
  - Vorticity contours

- The Periodic Nature of the Flow
  - Pressure histories at different locations
  - The period of oscillations corresponds to a Stroual number of 0.151
Instantaneous Mach Contours

\( M = 0.2 \) flow over a circular cylinder at \( Re = 75 \)
Instantaneous Entropy Contours

$M = 0.2$ flow over a circular cylinder at $Re = 75$
Instantaneous Vorticity Contours

$M = 0.2$ flow over a circular cylinder at $Re = 75$
Pressure History at Point (1,1)
Pressure History at Point (5,1)
Pressure History at point (10,1)
Outline

Lecture 3:

- Boundary conditions
- Discontinuity capturing
  - Limiter
  - Artificial viscosity
**Subsonic Inlet BC**

The 1D characteristic theory is applied in the normal direction (approximately)

Since \( \nu_n = \vec{v}_\infty \cdot \vec{n} < 0 \), there are two incoming and one outgoing characteristics

The three incoming Riemann invariants are:

\[
p / \rho^\gamma, \nu_t, \nu_n - 2c / (\gamma - 1)
\]

which can be fixed at the free stream value. The outgoing invariant \( \nu_n + 2c / (\gamma - 1) \) is computed at the interior point 1.
Subsonic Inlet BC (cont.)

Since the tangential velocity does not affect the normal flux, the following equations are sufficient to determine the flux:

\[ p / \rho^\gamma = p_\infty / \rho_\infty, \]
\[ \nu_n - 2c / (\gamma - 1) = \nu_{\infty,n} - 2c_\infty / (\gamma - 1) \]
\[ \nu_n + 2c / (\gamma - 1) = \nu_{1,n} + 2c_1 / (\gamma - 1) \]

Alternatively, the incoming acoustic invariant can be replaced by the total enthalpy:

\[ (E + p) / \rho = (E_\infty + p_\infty) / \rho_\infty \]

Finally the flux is computed using full flux \( F^n(U_b) \)
Subsonic Outlet BC

There are 3 outgoing and 1 incoming characteristics since \( v_n = \bar{v} \cdot \hat{n} > 0 \), only one physical condition can be fixed. One can either fix the incoming acoustic invariant or the exit pressure

\[
p / \rho^\gamma = p_1 / \rho_1^\gamma
\]

\[
v_n + 2c / (\gamma - 1) = v_{2,n} + 2c_2 / (\gamma - 1)
\]

\[
v_n - 2c / (\gamma - 1) = v_{\text{exit},n} - 2c_{\text{exit}} / (\gamma - 1) \text{ or } p = p_{\text{exit}}
\]

Then the full flux is computed using the computed solution

\[
F^n(U_b)
\]
Symmetry BC

For a symmetry BC, in order to achieve full compatibility with interior cells, split flux is used, i.e.,

\[ \tilde{F}(U_{in}, U_b, \n) \]

where \( U_{in} \) is the reconstructed solution at the boundary face from the interior cell, and \( U_b \) is computed based on the symmetry condition, i.e.,

\[
\begin{align*}
    P_b &= P_{in} \\
    \rho_b &= \rho_{in} \\
    \bar{v}_b &= \bar{v}_{in} - 2(\bar{v}_{in} \cdot \n)\n
\end{align*}
\]
Either full or split flux can be used for a wall BC.

- At a wall, since the normal velocity vanishes, only a pressure term remains in the momentum flux. We could set the wall pressure to

\[ p_b = p_{in} \]

- An inviscid wall is identical to the symmetry boundary condition using a split flux.

- For a viscous wall assuming no-slip BC, the velocity is set at

\[ \vec{v}_b = -\vec{v}_{in} \]
Shock Capturing

- Solution truly discontinuous
- Smooth features look like discontinuities due to a lack of resolution
- There are two approaches
  - Limiter – reconstruct the troubled cells to remove oscillations
  - Artificial viscosity – by adding a dissipation term near the shock wave
Problem:

- How to capture discontinuity sharply while preserving accuracy at local extrema?

\[ p = 1 \text{ (2nd order scheme)} \]

\[ S_i = \frac{1}{\Delta x} \min \text{mod}(\bar{u}_{i+1} - u_i, u_i - \bar{u}_{i-1}) \]
Gibbs Phenomenon

\[ P = 2 \]
Gibbs Phenomenon (cont.)

\[ P = 5 \]
Parameter-Free AP-TVD Marker

- Troubled cell method: Marker + Limiter

![Graph showing solution points, marks, and reconstruction with a circle indicating troubled cell.]
Parameter-Free Accuracy-Preserving TVD Marker

1) \( \bar{u}_{\text{max},i} = \max(\bar{u}_{i-1}, \bar{u}_i, \bar{u}_{i+1}) \) and \( \bar{u}_{\text{min},i} = \min(\bar{u}_{i-1}, \bar{u}_i, \bar{u}_{i+1}) \)

If \( u_{j,i} > 1.001 \cdot \bar{u}_{\text{max},i} \) or \( u_{j,i} < 0.999 \cdot \bar{u}_{\text{min},i} \), \( (j = 1, p + 2) \)

then cell \( i \) is considered as a possible troubled cell.

2) \( \tilde{u}^{(2)}_i = \min \max(\tilde{u}^{(2)}_i, \beta \frac{\bar{u}^{(1)}_{i+1} - \bar{u}^{(1)}_i}{x_{i+1} - x_i}, \beta \frac{\bar{u}^{(1)}_i - \bar{u}^{(1)}_{i-1}}{x_i - x_{i-1}}) \). \( (\text{for } p > 1) \)

If \( \tilde{u}^{(2)}_i = \bar{u}^{(2)}_i \), then cell \( i \) is unmarked as a troubled cell;

Otherwise cell \( i \) is confirmed as a troubled cell.

\( (\beta = 1.5) \)
Parameter-Free AP TVD Marker

- $p=2$
- $p=3$
- $p=4$
- $p=5$
- $p=6$
Parameter-Free AP TVD Marker

\begin{align*}
p=2 & \quad \text{Graph} \\
p=3 & \quad \text{Graph} \\
p=4 & \quad \text{Graph} \\
p=5 & \quad \text{Graph} \\
p=6 & \quad \text{Graph}
\end{align*}
Parameter-Free AP TVD Marker
Generalized Moment Limiter: 1D

If cell $i$ has been marked as a troubled cell, then

(1) Reconstruction

$$u_i(x) = \bar{u}_i + \bar{u}_i'(x - x_i)$$

$$+ \frac{1}{2} \bar{u}_i^{(2)} [(x - x_i)^2 - \frac{1}{12} h_i^2]$$

$$+ \frac{1}{6} \bar{u}_i^{(3)} [(x - x_i)^3 - \frac{1}{4} h_i^2 (x - x_i)]$$

$$+ \frac{1}{24} \bar{u}_i^{(4)} [(x - x_i)^4 - \frac{1}{2} h_i^2 (x - x_i)^2 + \frac{7}{240} h_i^4]$$

$$+ \ldots$$

Functional Equivalent to the original solution polynomial
**Generalized Moment Limiter: 1D**

(2) **Hierachically Limiting**

\[ \bar{Y}_i^{(p)} = \min \{ \bar{u}_i^{(p)}, \beta \frac{\bar{u}_{i+1}^{(p-1)} - \bar{u}_i^{(p-1)}}{x_{i+1} - x_i}, \beta \frac{\bar{u}_i^{(p-1)} - \bar{u}_{i-1}^{(p-1)}}{x_i - x_{i-1}} \} \].

If \( \bar{Y}_i^{(p)} = \bar{u}_i^{(p)} \), then NO limiting for (1).

Otherwise,

\[ \bar{Y}_i^{(k)} = \min \{ \bar{u}_i^{(k)}, \beta \frac{\bar{u}_{i+1}^{(k-1)} - \bar{u}_i^{(k-1)}}{x_{i+1} - x_i}, \beta \frac{\bar{u}_i^{(k-1)} - \bar{u}_{i-1}^{(k-1)}}{x_i - x_{i-1}} \}, \quad (k = p - 1) \]

\[ \bar{Y}_i^{(k)} \begin{cases} = \bar{u}_i^{(k)} & (k = p - 1). \\ \Rightarrow & \text{NO further limiting} \end{cases} \]

YES.  \( \Rightarrow \) NO further limiting

NO.  \( \Rightarrow \) Do limiting and check for \( k = p - 2 \)

............
Generalized Moment Limiter

- $P = 2$

Example:

Original construction

Limited all cells (2) on all cells

Solution points

Reconstruction (1) on all cells

Mark

Solution points

Original construction

Reconstruction (1) on all cells

Limited all cells (2) on all cells
Generalized Moment Limiter

Example: \( p = 5 \)

\[
0 \quad 0.25 \quad 0.5 \quad 0.75 \quad 1
\]

\[
-1.5 \quad -1 \quad -0.5 \quad 0 \quad 0.5 \quad 1 \quad 1.5 \quad 2 \quad 2.5
\]

- Mark
- Solution points
- Original construction
- Reconstruction (1) on all cells
- Limiting (2) on all cells
Numerical Tests

1. Accuracy study

Linear Advection Equation

\[ u_t + u_x = 0 \]

Non-Linear Burgers Equation

\[ u_t + \left( \frac{u^2}{2} \right)_x = 0 \]
Numerical Tests

2. 1D Discontinuity with  \( u_t + u_x = 0 \)
Numerical Tests

3. 1D Burgers Equation \( u_t + (u^2 / 2)_x = 0 \)
Sod Shock Tube Problem

1. $p=1$
2. $p=2$
3. $p=3$
4. $p=4$
Shock Acoustic-Wave Interaction

$p=1$

$p=2$

$p=3$
Numerical Tests

6. 2D shock vortex interaction

3rd-order PFGM Limiter

Linear Limiter

\[
\begin{align*}
\text{t}=0.05 \\
\text{t}=0.2 \\
\text{t}=0.35
\end{align*}
\]
Localized Laplacian Artificial Viscosity

\[
\frac{\partial Q}{\partial t} + \nabla \cdot F^{\text{inv}}(Q) = \nabla \cdot F^{\text{av}}(Q, \nabla Q)
\]

Laplacian: \( F^{\text{av}}(Q, \nabla Q) = \varepsilon \nabla Q \)

For each element \( e \):

\[
\varepsilon_e = \begin{cases} 
\frac{\varepsilon_0}{2} \left( 1 + \sin \frac{\pi (S_e - S_0)}{2\kappa} \right) & \text{if } S_e < S_0 - \kappa \\
0 & \text{if } S_0 - \kappa \leq S_e \leq S_0 + \kappa \\
\varepsilon_0 & \text{if } S_e > S_0 + \kappa.
\end{cases}
\]

Parameters in \( \varepsilon_e \):

\[
\varepsilon_0 = f(\Delta \xi_{\text{max}}) \cdot h \cdot |\lambda|_{\text{max}}
\]

\[
S_e = \log_{10} \frac{\langle U - U^p, U - U^p \rangle_e}{\langle U, U \rangle_e}
\]

Adopted in current study by P.-O. Persson & J. Peraire.
2D Explosion

Density at $t=0.25s$  

$P^3$ reconstruction (4th order), $t \in [0, 0.25s]$  
Computational domain $[-1,1] \times [-1,1]$, $100 \times 100$ elements
Double Mach Reflection

Ma = 10, $P^3$ reconstruction (4th order), $t \in [0, 0.2s]$

Computational domain $[0,4] \times [0,1]$, 816 x 204 elements

Artificial viscosity at $t=0.2s$

Density at $t=0.2s$
Ma 3 Wind Tunnel with a Foreword Step

Free stream $Ma = 3$, $P^2$ reconstruction (3rd order), Grid size: 1/80, with clustered elements of size 1/320 near the sharp corner.

Density at $t=4s$

Artificial viscosity at $t=4s$
Shock-Vortex Interaction

Free stream $Ma = 1.1$, $P^3$ reconstruction (4th order), Computational domain: $[0,2] \times [0,1]$, $100 \times 50$ elements.

Small isentropic vortex is superposed to the supersonic flow.
Ma 3 Oblique Shock

Pressure

Artificial viscosity

Ma = 3, $P^2$ reconstruction (3rd order), Grid size 1/20

Ma = 3, $P^4$ reconstruction (5th order), Grid size 1/40
Outline

Lecture 4:
- Verification and Validation
- Solution based hp-adaptations
- Sample demonstration problems
- Summary
Introduction

- Verification: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

- Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. (AIAA G-077-1998) – comparison with experimental data
How to Verify Your Code

- Closure condition of your control volume

\[ \int_{\partial V_i} \vec{n} dS = 0 \]

- Free-stream preservation (extrapolation boundary condition everywhere)

\[ R(Q) = 0 \]

- Exactly preserve a polynomial of a certain degree

- Accuracy study with grid refinement

\[ p = \frac{\ln(\text{Error}_{\Delta x} / \text{Error}_{\Delta x/2})}{\ln(2)} \]
Problems with Analytical Solutions

- Many cases are included in the 1st International Workshop on High-Order CFD Methods (http://zjwang.com/hiocfd.html)
  - Vortex propagation
  - Ringleb flow
  - Subsonic inviscid flow: entropy is constant

- Manufactured solutions
Selected Results – hp-Adaptations

- Discretization error reduction
  - P-enrichment: smooth flow regions (Weierstrass theorem)
  - H-refinement: geometry or flow singularities
  - Anisotropic adaptation: shear layers, shocks,…

- Adaptation criteria/error indicators
  - Feature-based: simple, ad hoc, less rigorous
  - Residual-based: may lead to false refinements
  - Adjoint-based: adapt the mesh in regions affecting the output, and estimate the error in the output
Review of Adjoint-Based Adaptive Methods

Adjoint-based adaptive methods

Dynamically distribute computer resources to regions which are important for predicting engineering outputs

Current status of the output-based adaptation methods

- 2D/3D complex geometry
- Steady/unsteady
- Euler/NS/RANS
- Anisotropic hp-adaptations

[Giles and Pierce, 1997; Becker and Rannacher, 2001; Venditti and Darmofal, 2002; Hartmann and Ouston, 2002; Nielsen et al, 2004; Fidkowski and Darmofal, 2007; Hartmann, 2007; Mani and Mavriplis, 2007; Nemec et al, 2008; Park, 2008; Wang and Mavriplis, 2009; Oliver and Darmofal, 2008; Fdikoswski and Roe, 2009; Ceze and Fdikoswski, 2012; ...]
**Fully Discrete Adjoint**

Let $R_h(Q_h)$ be the residual, $J_h(Q_h)$ be the output. Let $Q$ be the exact solution. The solution error is $\delta Q = Q - Q_h$. Since $R(Q) = R(Q_h + \delta Q) = 0$, we have

$$R(Q_h) + \frac{\partial R_h}{\partial Q_h} \delta Q \approx 0. \quad \delta Q \approx -\left(\frac{\partial R_h}{\partial Q_h}\right)^{-1} R(Q_h)$$

The output error is

$$\delta J_h = J_h(Q) - J_h(Q_h) = \frac{\partial J_h}{\partial Q_h} \delta Q = -\frac{\partial J_h}{\partial Q_h} \left(\frac{\partial R_h}{\partial Q_h}\right)^{-1} R(Q_h)$$

Denote the adjoint $\tilde{\psi}_h^T = -\frac{\partial J_h}{\partial Q_h} \left(\frac{\partial R_h}{\partial Q_h}\right)^{-1}$. Then

$$\delta J_h = \tilde{\psi}_h^T R(Q_h)$$

$$-\frac{\partial J_h}{\partial Q_h} = \tilde{\psi}_h^T \frac{\partial R_h}{\partial Q_h} \quad -\frac{\partial R_h}{\partial Q_h}^T \tilde{\psi}_h = \frac{\partial J_h}{\partial Q_h}^T$$
The Fully Discrete Adjoint for the CPR Method

NACA 0012 at $M_\infty = 0.4$, $\alpha = 5^\circ$

- The x-mom of the lift adjoint
- Fully discrete adjoint
- Highly-oscillating adjoint solution

\[
- \frac{\partial R_h}{\partial Q_h}^T \tilde{\psi}_h = \frac{\partial J_h}{\partial Q_h}^T
\]
Dual Consistency

A residual from a differential schemes at SP $j$ of cell $i$

$$R(Q)_{i,j} = \nabla \cdot \bar{f}(Q_i)_j + \frac{1}{|V_i|} \sum_{f \in \partial V_i} \sum_l \alpha_{j,f,l} [F^n]_{f,l} S_f$$

With fully discrete approach

$$- \sum_i \sum_j \frac{\partial R_{i,j}}{\partial Q_k} \psi_i,j = \frac{\partial J}{\partial Q_k}, \quad k = 1, \ldots, N_{DOF}$$

To be dual consistent,

$$- \int_{\Omega} \frac{\partial N(Q)}{\partial Q}^T \psi dV = \frac{\partial J}{\partial Q}^T$$
Discrete Adjoint for the CPR in the Integral Form

\[-\int_\Omega \frac{\partial N(Q)^T}{\partial Q} \psi dV = \frac{\partial J^T}{\partial Q}\]

- Approximate \(\psi_i\) using the basis \(L_j\) from the primal solution space

\[\psi_i = \sum_j L_j \hat{\psi}_{i,j}\]

- Directly discretizing the continuous adjoint eqn

\[-\sum_i \sum_j \frac{\partial R_{i,j}}{\partial Q_k} \omega_j |J_{i,j}| \hat{\psi}_{i,j} = \frac{\partial J}{\partial Q_k}\]

- The difference between \(\tilde{\psi}_{i,j}\) and \(\tilde{\psi}_{i,j}\)

\[\tilde{\psi}_{i,j} = \omega_j |J_{i,j}| \hat{\psi}_{i,j}\]
Comparison of the Adjoint with the CPR Method

NACA 0012 at $M_\infty = 0.4$, $\alpha = 5^\circ$

- The x-mom of the lift adjoint
- Fully discrete adjoint
- Discrete adjoint in the integral form

The inconsistent adjoint  
Dual consistent adjoint
The Adjoint-based Error Estimation

- Output error est.: adjoint solution weighted primal residual
  \[ \delta J_h(Q_h) = J_h(Q_h) - J_h(Q_H) \approx (\hat{\psi}_h)^T R_h(Q_h^H) \]

- Adjoint-based local error indicator
  \[ \eta = \left| (\hat{\psi}_h)^T R_h(Q_h^H) \right| \]

- Multi-p residual-based error indicator
  \[ \eta = \left| R_h(Q_h^H) \right| \]

Local residual distribution  \[ \psi \]  \[ \Rightarrow \]
Adjoint-based error indicator
Accuracy Test of the Adjoint-based Error Est.

NACA 0012 at $M_\infty = 0.5$, $\alpha = 2^\circ$

- The lift as the output $J$
- The effectivity of the error est.

\[ \eta^e_H = \frac{-(\psi_h)^T R_h (Q^H_h)}{J_H (Q_H) - J_h (Q_h)} \]

<table>
<thead>
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<th>Cells</th>
<th>$J_H(Q_H) - J_h(Q_h)$</th>
<th>$-(\psi_h)^T R_h (Q^H_h)$</th>
<th>$\eta^e_H$</th>
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</tbody>
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Subsonic Flow Over a NACA 0012 Airfoil

- Iso/aniso H-adaptation
- Fixed fraction $f = 0.1$
- Inviscid, $M_\infty = 0.5$, $\alpha = 2^\circ$
- 3rd order scheme

Adaptation strategies
- Hanging nodes
- No-hanging nodes
- Error indicators
  - lift adjoint
  - drag adjoint

Initial mesh

Initial solution
Subsonic Flow Over a NACA 0012 Airfoil

- Iso/aniso H-adaptation
- Fixed fraction $f = 0.1$
- Inviscid, $M_\infty = 0.5$, $\alpha = 2^\circ$
- 3rd order scheme

Adaptation strategies
- Hanging nodes
- No-hanging nodes
- Error indicators
  - lift adjoint
  - drag adjoint

Initial mesh

The adapted solution
Subsonic Flow Over a NACA 0012 Airfoil

![Graph showing the relationship between C and sqrt_dof for different refinement methods.]

- **Uniform refinement**
- **iso-hanging**
- **iso-no-hanging**
- **aniso-nohanging**
- **iso-hanging-corr**
- **iso-nohanging-corr**
- **aniso-nohanging-err**
Subsonic Flow Over a NACA 0012 Airfoil
Aniso lift adjoint

Aniso drag adjoint

Iso lift adjoint

Iso drag adjoint
The Supersonic Vortex Transportation Problem

Mesh                           Density

Dual-consistent adjoint        Dual-inconsistent adjoint
The Supersonic Vortex Transportation Problem

Primal sol error

Output error

P1 error estimate

P2 error estimate
Inviscid Flow over the NACA-0012 Airfoil

Initial mesh

Adapted solution

CL-adjoint

CD-adjoint
CL error

CD error
Laminar Flow over NACA-0012 ($\alpha=1^\circ$, Re=5000)

Initial solution

Adapted solution

CL-adjoint

CD-adjoint
Remaining Challenges in High-Order Methods

- High-order grid generation, highly clustered curved meshes near wall
- Error estimates and solution-based hp-adaptations
- Low memory efficient solver
- Shock capturing – to preserve accuracy in smooth regions, convergent and parameter-free