New Directions in High-Order Adaptive Methods for Computational Fluid Dynamics

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Introduction

Complex CFD simulations made possible by

- Increasing computational power
- Improvements in numerical algorithms

New liability: ensuring accuracy of computations

- Management by expert practitioners is not feasible for increasingly-complex flow fields
- Reliance on best-practice guidelines is an open-loop solution: numerical error is unchecked for novel configurations
- Output calculations are not yet sufficiently robust, even on relatively standard simulations

⇒ research into adaptive methods that can “close the loop”
Successful adaptive methods require

1. Accurate error estimation
   - How much error is present?
   - Where is it coming from?
   ⇒ **Approach:** *adjoint-weighted residual*

2. Efficient adaptation
   - How should degrees of freedom be introduced?
   - Can scheme approximation properties be improved?
   - Is the scheme itself adequate?
   ⇒ **Approach:** *a diverse set of adaptation strategies*
Why not just adapt “obvious” regions?

Fishtail shock in $M_\infty = 0.95$ inviscid flow over a NACA 0012 airfoil
A typical output-adaptive result

![Diagram illustrating output-adaptive iterations](image)

- Initial mesh
- Adapted mesh
- adaptive iterations
- ±$\epsilon$ (error est.)
- raw output
- corrected output
- exact output value
- output
- cost (degrees of freedom)
- corrected output

Adaptive mechanics: the role of high order

- High-order methods: errors converge faster than 2nd-order
- Typically choose high-order methods for “smooth” problems, where we expect to see convergence plots that look like:

\[
\text{log(error)} = \begin{cases} 
  p = 1 & \text{one uniform ref.} \\
  p = 2 & \text{two uniform refs.} \\
  p = 3 & \text{initial mesh}
\end{cases}
\]

\[
\text{log(dof)}
\]
Can aero applications benefit from high order?

- Question considered by recent high-order CFD workshops
- Aerospace applications usually have both smooth and singular features (shocks, trailing edges)
- Singularities can limit observed rates

Mach numbers (0–0.7), Euler flow over a NACA 0012 airfoil

Drag error convergence

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High-order in mesh adaptation

- $h$-Adaptation can isolate singularities with small elements
- In many high-order methods, local $p$-enrichment is possible
- High-order just becomes another refinement tool for efficiently improving accuracy
We have done many $h/p$ adaptive runs

**Transonic RANS flow over a NACA 0012**

23.1: Initial mesh (1740 elements)

23.2: Mach number contours

23.3: 6\textsuperscript{th} adapted mesh, isotropic (8,736 elements)

23.4: 10\textsuperscript{th} adapted mesh, anisotropic (4,816 elements)
We have done many $h/p$ adaptive runs.
We have done many $h/p$ adaptive runs

Staggered pitching/plunging airfoils; ALE, dynamic $p$
We have done many $h/p$ adaptive runs.

Flapping wing; ALE, dynamic $p$
Novel adaptive strategies (for FEM)

- **Automatic hp**: choice driven by error indicator
- **Node movement**: warp elements to improve approximation
- **Trial space tailoring**: better than polynomials
- **Test space optimization**: not just Galerkin
- \ldots

\begin{align*}
\log(\text{error}) & \\
\log(\text{dof}) & \\
\text{adaptive } h & \\
\text{uniform } h & \\
\text{adaptive } hp & \\
\text{adaptive } hp \text{ and node movement} & \\
\end{align*}
Polynomial approximation spaces are popular

\[ u(\vec{x}) = \sum_j U_j \phi_j(\vec{x}), \quad \phi_j(\vec{x}) \subset \mathcal{P}^p \]

But they are not always the most efficient

In FEM, we can tailor \( \{ \phi_j(\vec{x}) \} \) to each element

One application: \( p \)-multigrid coarse spaces

- Typically \( \mathcal{P}^{p-1}, \mathcal{P}^{p-2}, \ldots \)
- We consider \emph{arbitrary} subspaces \( \mathcal{V}_H \subset \mathcal{P}^p \)
- Similar to algebraic multigrid, locally on each element

First approach: linear \( p \)-multigrid solver acceleration
A closer look at the residual Jacobian matrix

\[ A = \frac{\partial R}{\partial U} = \]

- \( R_i \): the residual on element \( i \)
- \( A_{i,i} \): effect of \( i \)th neighbor state on \( i \)th residual
- \( A_{i,j} \): effect of \( i \)th self state on \( j \)th neighbor residual
- \( A_{j,i} \): effect of \( j \)th self state on \( i \)th neighbor residual

self block

effect of neighbor state on self residual

effect of self state on neighbor residual
Compress the $i^{th}$ block row

Observations:

- Neighbor state perturbations may excite only some residual modes on element $i$
- These modes are typically not excited to the same degree
- Not all neighbor state perturbations affect residuals in element $i$
Apply the SVD

Take the singular value decomposition (SVD) of $A_{i,:}$:

$$\text{SVD}(A_{i,:}) = U \Sigma V^T$$

- $U$ represents the most “excitable” self residual modes.
- $\Sigma$ is the diagonal matrix with the singular values $\sigma_1, \sigma_2, \ldots$.
- $V^T$ represents the ranking of dominant modes based on $\sigma_k$.

$p$-Multigrid: coarse-space test/trial functions from $U$ and $A_{i,:}^{-1}U$.  

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2D advection example

- 2D linear advection (at $25^\circ$)
- Quadrilateral meshes
- Constant inflow state BC
- Random initial condition
- DG Lagrange basis
- Fine space: $p_h = 3 \implies r_h = 16$
- Coarse space: $p_H = 2 \implies r_H = 9$
- Two-grid cycle, $\nu_{\text{pre}} = \nu_{\text{post}} = 2$

- We compare convergence of MG for block, line, SVD smoothers
- Coarse space size of SVD MG is the same size as in block/line
2D advection: convergence rates

One MG iteration is an exact solve with the SVD smoother

Same result at higher orders $p_h$
2D linearized Euler example

- 2D linearized Euler
  \((M = 0.5, \alpha = 2^\circ)\)
- Quadrilateral curved meshes
- Random initial condition
- DG Lagrange basis
- Fine space: \(p_h = 3 \Rightarrow r_h = 64\)
- Coarse space: \(p_H = 2 \Rightarrow r_H = 36\)
- Two-grid cycle

- We compare convergence of MG for block, line, SVD smoothers
- Coarse space size of SVD MG is the same size as in block/line
2D linearized Euler: singular values, convergence

Singular values

- (# nonzero singular values) > \( r_H \)
- Now need more than one MG-SVD iteration
- Significantly fewer MG iterations compared to block or line

Residual convergence

\( r_H = 36 \)
Another way to adapt

So far
- Standard “general-purpose” numerical scheme (DG/HDG)
- Output-based mesh adaptation

Another direction
- Optimize the numerical scheme itself
- Specifically, we optimize the FEM test space

\[ \int_{\Omega} v^T r(u) \, d\Omega = 0 \quad \text{for } u \in \mathcal{P}^p, \ v \subset \mathcal{P}^{p_{\text{test}}} \]

Results in a Petrov-Galerkin method
- Our focus: boundary accuracy for engineering outputs
- Applied to HDG \(\rightarrow\) HDPG
Optimal test functions

Key idea

Choose test functions that make FEM weighted residual look like an error minimization equation

Example: 1D advection on one element

\[ Lu \equiv a \frac{\partial u}{\partial x} = f, \quad a > 0, \quad u(x_L) = u_L \]

Discrete weight. residual: \[ \int_{\Omega} v_h (Lu_h - f) \, dx = 0 \]

- exact weight. residual: \[ \int_{\Omega} v_h L(u_h - u) \, dx = 0 \]

Move \( L \) to test functions:

\[ \int_{\Omega} L^* v_h (u_h - u) \, dx + v_h a(u_h - u) \bigg|_{x_R} = 0 \]
What do we want from the solution? A reasonable error norm is
\[ \|e\|^2 = \int_{\Omega} (u_h - u)^2 \, dx + w_R (u_h - u)^2 \bigg|_{x_R} \]

For \( u_h = \sum_j U_j \phi_j \), the error minimization equation reads
\[ \frac{\partial \|e\|^2}{\partial U_j} = 0 \quad \rightarrow \quad \int_{\Omega} \phi_j (u_h - u) \, dx + w_R \phi_j (u_h - u) \bigg|_{x_R} = 0 \]

We can make our weighted residual look like this if the test functions, \( v_j \), satisfy an adjoint equation:
\[ L^* v_j = \phi_j \]
\[ v_j \bigg|_{x_R} = \frac{w_R}{a} \phi_j \bigg|_{x_R} \]
Example: 1D advection (ctd.)

Such test functions are adjoints for the outputs,

\[ J_j = \int_\Omega \phi_j u \, dx + w_R \phi_j u \bigg|_{x_R} \]

Our FEM weighted residual is then an adjoint-weighted residual,

\[ \int_\Omega v_i (L u_h - f) \, dx = 0 \quad \rightarrow \quad J_j(u_h) - J_j(u) = 0 \]

By choosing large \( w_R \) we can emphasize boundary accuracy.

Note:
- \( v_j \) must lie in an enriched space (else standard Galerkin)
- For multiple elements we need to localize \( v_j \) calculation
1D scalar result: effect of $W_R$
1D Advection with source

\[ a \frac{\partial u}{\partial x} - cu = 0, \quad u|_{x_L} = 1 \]

- \( a = 1 \) and \( c = 8 \)
- For boundary accuracy, use \( w_R = 1 \times 10^{10} \) and \( p_{test} = 10 \)
- \( p = 0 \) and \( p = 1 \) convergence is shown
1D Advection-diffusion

\[ a \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0 \quad u\big|_{x_L} = 0, \quad u\big|_{x_R} = 1 \]

- \( a/\nu = 20 \)
- \( w_L, w_R = 1 \times 10^{12} \) and \( p_{\text{test}} = 10 \)
- \( p = 1 \) and \( p = 2 \) convergence is shown
Nonlinear systems: Euler equations

- Supersonic Euler, inflow Mach = 2, Dirichlet BCs on left
- Source term $S^T = [0.4\rho^2 \; 0.7(\rho u)^2 \; 0.1(\rho H)^2]$
- $p_{test} = p + 1$, boundary weights = $1 \times 10^7$

\[ p = 0 \]

\[ p = 1 \]

- $2p + 2$ rates are obtained

- Subsonic cases show similar behavior, though with rates of $\approx 2p + 1.75$
Extension to multiple dimensions

Outputs for test function adjoint calculations

\[ J^{k,i} = \int_{\Omega} u_k \, \phi_{k,i} \, d\Omega + \int_{\partial \Omega} \sum_{s=1}^{sr} \left[ w_s \frac{\partial \hat{F}_s}{\partial u_{k,h}} \hat{F}_s(u, \bar{q}) \right] \phi_{k,i} \, ds \]

Similarly for components of \( \bar{q} \) in HDG

Trial space enrichment

- Need accurate test fcns and fluxes
- In 2D, the trial basis needs to be enriched to represent the fluxes
- Enrich the trial space with Lobatto edge functions of order \( p_B \)
- Inside elements: \( p_I < p_B \)
- Total DOF scales linearly with \( p_B \)
HDG for flow over a cylinder: 2D linearized Euler

- Mach number of 0.3
- $p_{\text{test}} = p_b$, boundary weights $= 1 \times 10^{10}$
- HDPG interior order kept at $p_I = 1$, while $p_B$ is enriched

Pressure contours

Cylinder pressure flux

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HDG for flow over a cylinder: 2D linearized Euler

- Here, we compare standard HDG with $p_B = 8$ edge enrichment to HDPG with the same enrichment
- The only difference is the test space
- We see that HDPG achieves much better accuracy

![Graphs showing error vs. number of elements for pressure and x-velocity fluxes for HDG and HDPG with different $p_B$ values.](image)
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