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Updates to Implicit Edge-Based Gradient Methods

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Lessons Learned

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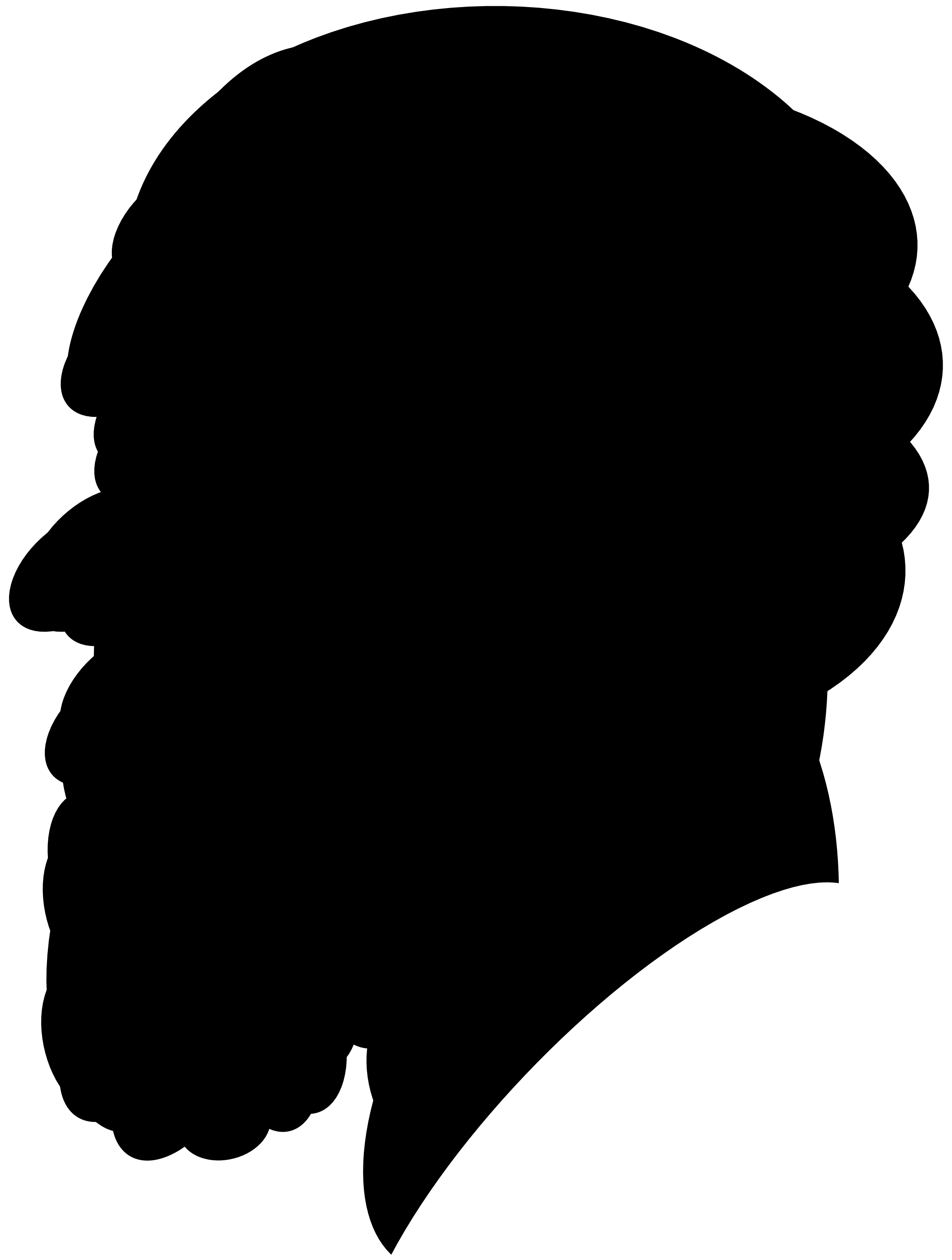

Lesson 1: *Forget that you think you know.*

Lesson 2: *See it for yourself.*

Lesson 3: *Understand limits.*

Lesson 1: *Forget that you think you know.*

Economical 3rd-Order Methods

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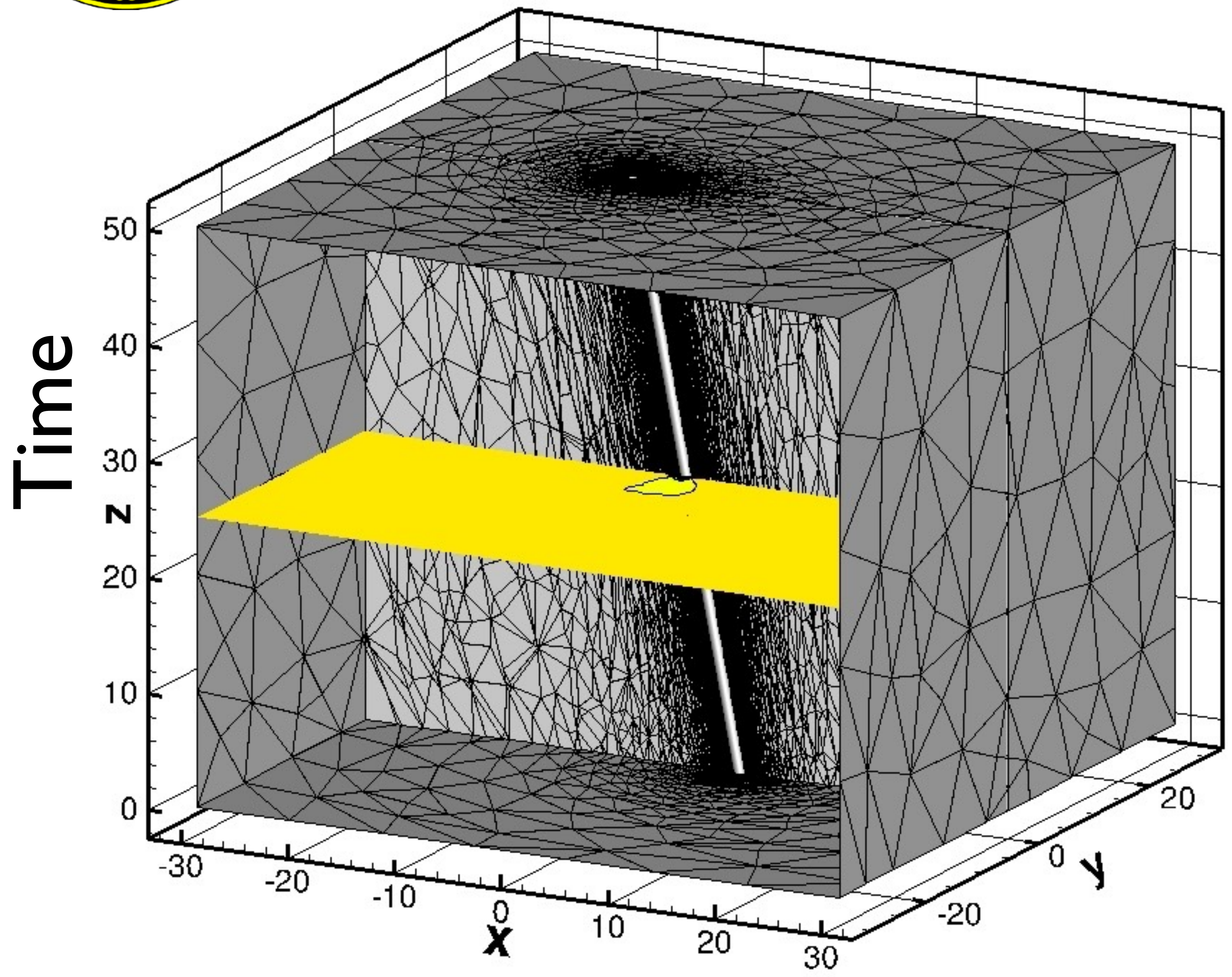
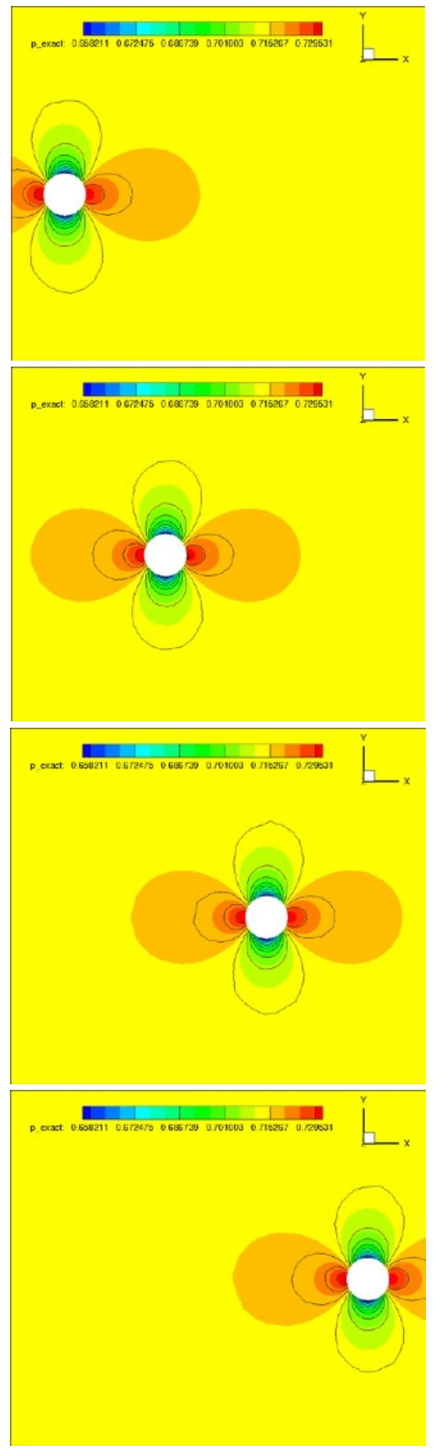
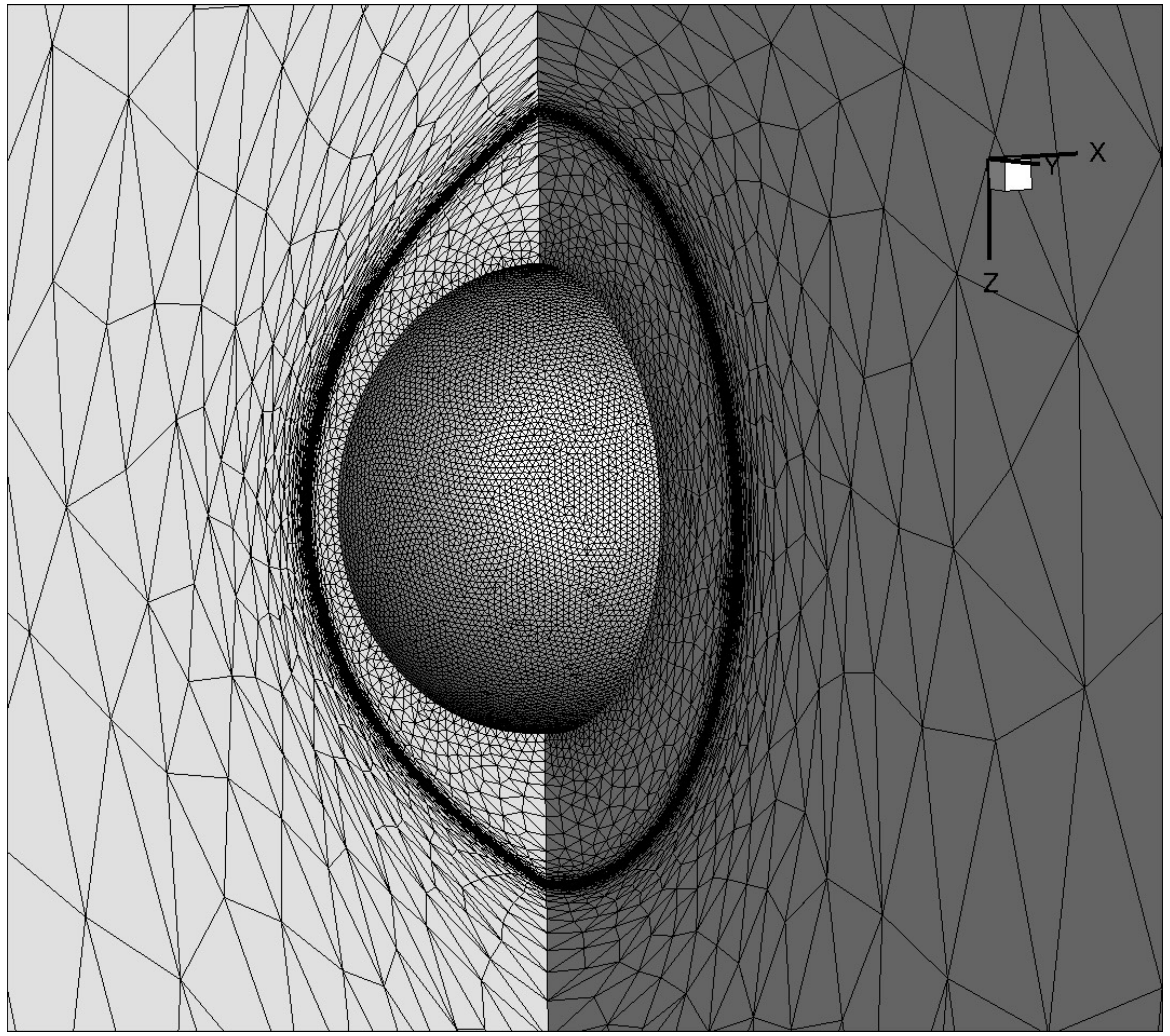
Exploring Space-Time Hyperbolic NS

Improving Unstructured-Grid Methods







Common interest: *Economical 3rd-order methods* with a single flux per face/edge, not requiring 2nd derivatives at all, towards automated CFD with fully adaptive tetrahedral grids.

2nd/3rd-Order Edge-Based (EB) Discrtetizations

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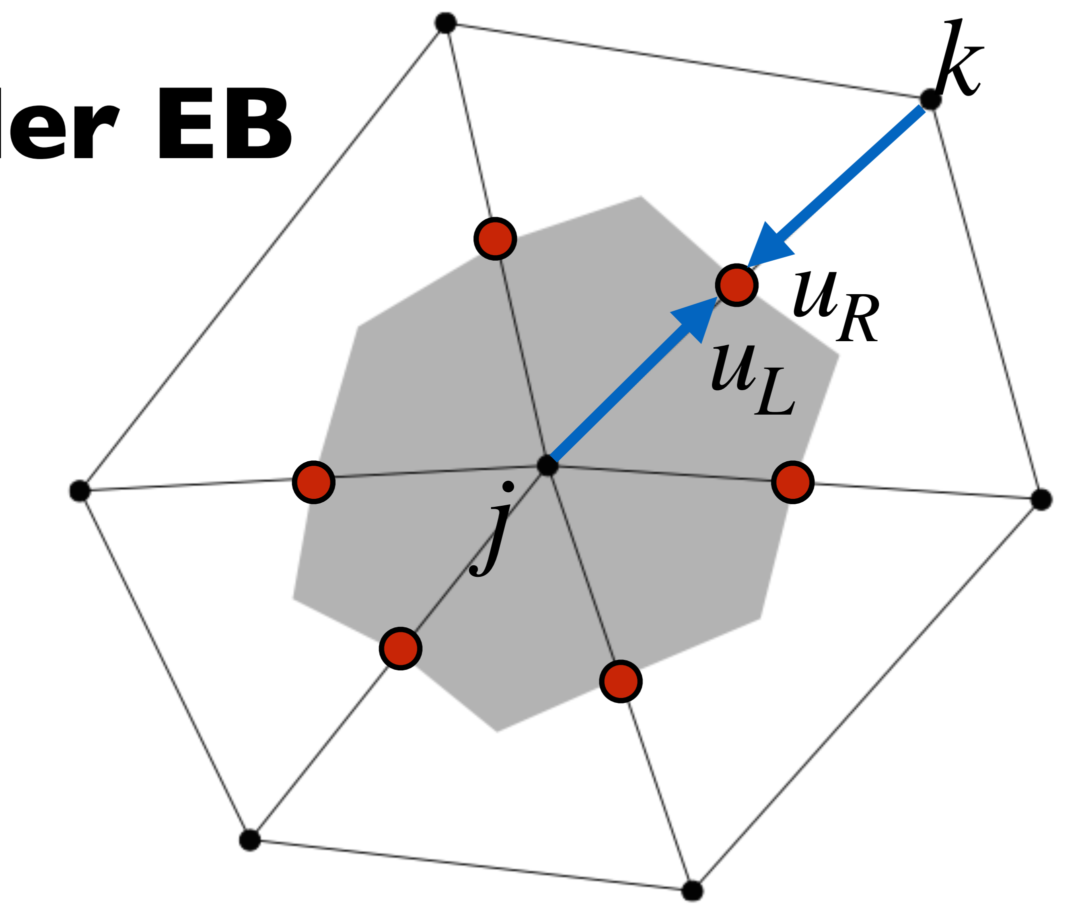
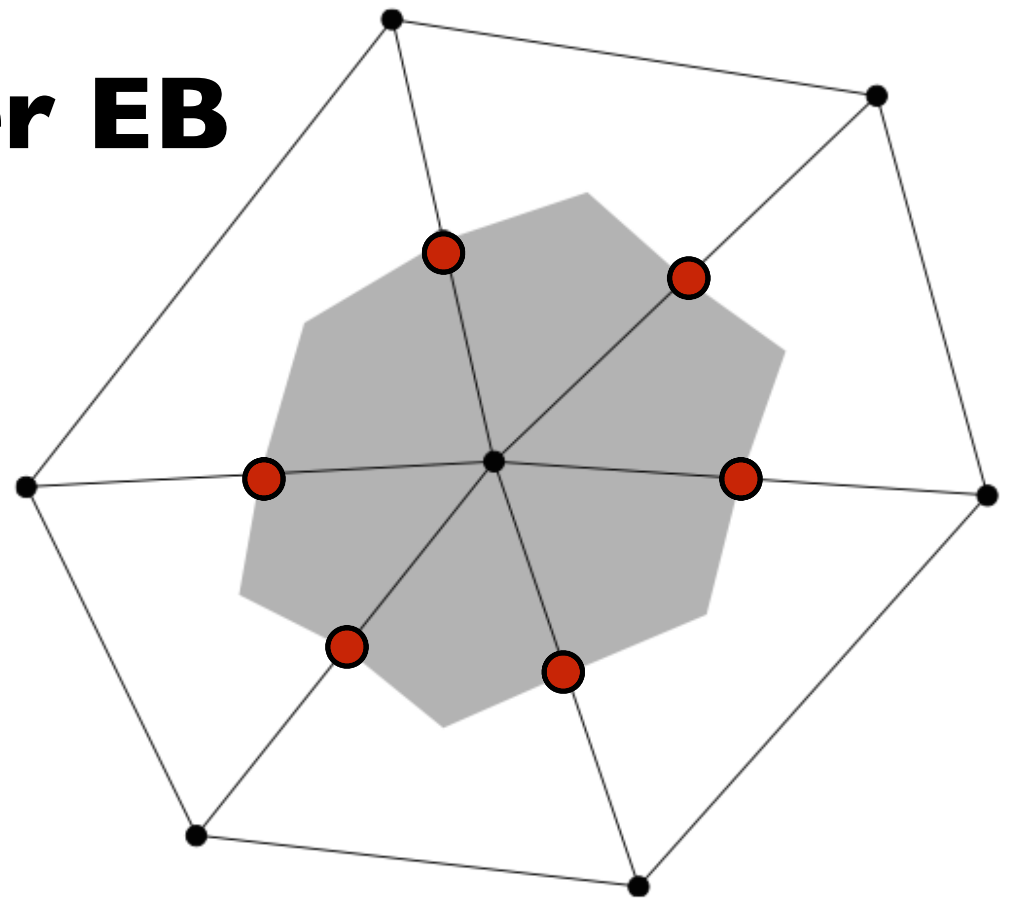
2nd-order EB



3rd-order EB



Edge-Based Schemes : *A single flux per edge*

$$\frac{1}{V_j} \sum_{k \in \{k_j\}} \phi_{jk}(u_L, u_R) \, |\mathbf{n}_{jk}| = s(\mathbf{x}_j)$$

$$u_L = u_j + \frac{1}{2} \mathbf{g}_j \cdot \Delta \mathbf{r}_{jk} , \quad u_R = u_k - \frac{1}{2} \mathbf{g}_k \cdot \Delta \mathbf{r}_{jk} , \quad \Delta \mathbf{r}_{jk} = \mathbf{x}_k - \mathbf{x}_j$$

3rd-order accurate (Katz&Sankaran2011, Diskin&Thomas2012) with

- Linear solution/flux reconstruction with **quadratic LSQ gradients**.
- Accuracy-preserving source quadrature Nishikawa&Liu JCP2017.

-> <u>2nd derivatives not needed.</u>

for arbitrary triangular/tetrahedral grids.

-> *perfect for adaptive grids.*

Explicit and Implicit Gradient Methods

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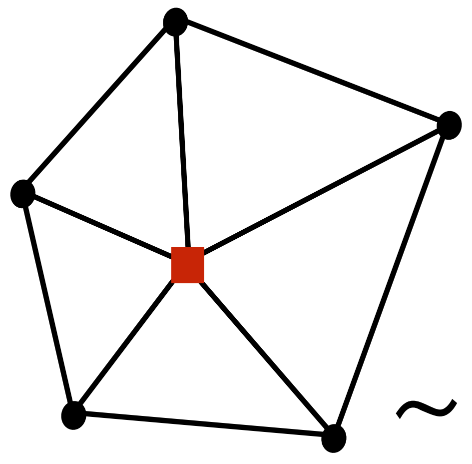
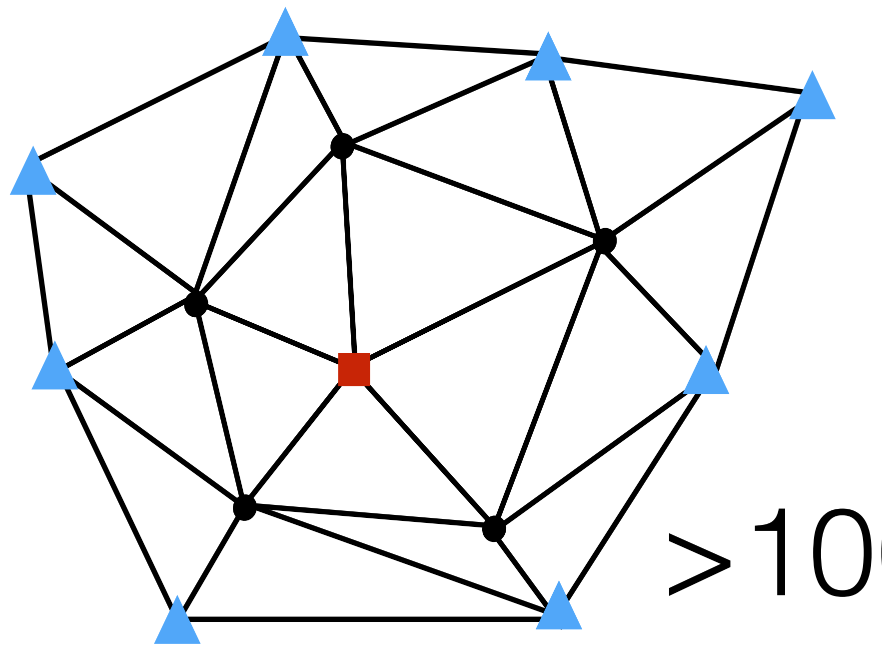
Explicit:

$\mathbf{g}_j^{Linear\ LSQ}$



~14 in 3D

$\mathbf{g}_j^{Quadratic\ LSQ}$



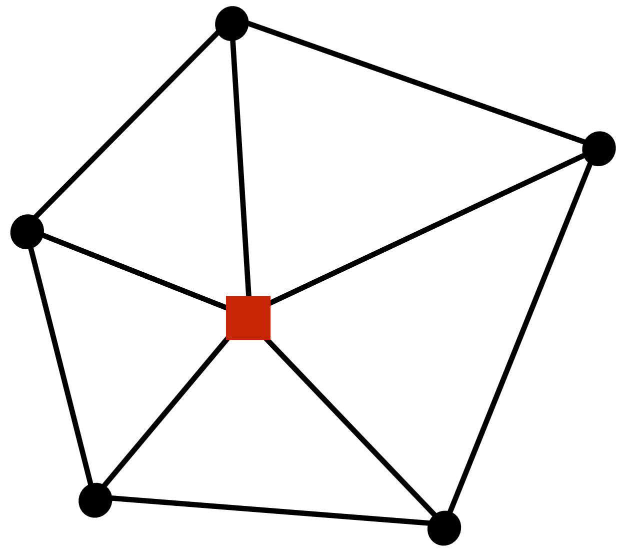
>100 in 3D

Large stencil: a solver gets more robust but less accurate.

Haider&Croisille&Courbet NM2009

Implicit:

$$\mathbf{M}_{jj}\mathbf{g}_j + \sum_{k\in\{k_j\}} \mathbf{M}_{jk}\mathbf{g}_k = GG$$



Galerkin: Löhner(1994)

Variational Reconstruction: Wang et. al., JCP2017

Implicit GG: Nishikawa, JCP2019

Implicit EB gradient: Nishikawa, AIAA2020

Advantages of Implicit Gradients

- Flow solver is more stable with a huge gradient stencil.
- Superior gradient accuracy.
- Per-relaxation cost can be lower than LSQ gradients with hundred of neighbors

Linear/Quadratic IEBG (AIAA2020)

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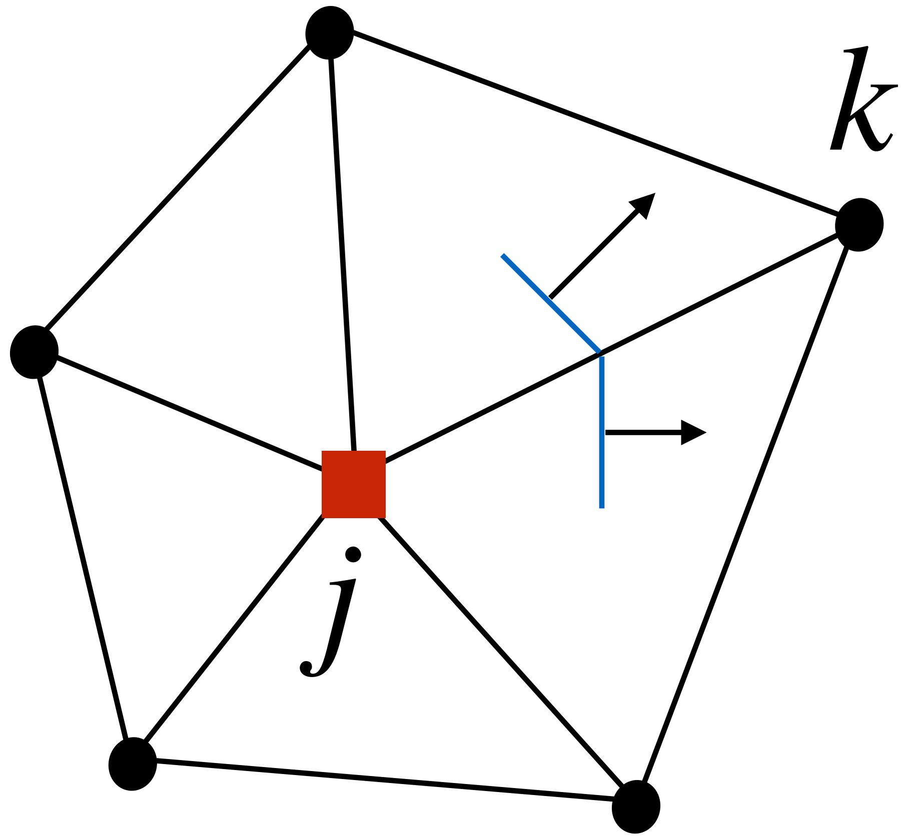
$$\frac{1}{V}\int_V \nabla u \, dV = \frac{1}{V}\int_V \mathbf{g} \, dV$$

Accuracy-preserving source quadrature

Nishikawa&Liu JCP2017

$$\frac{1}{V}\oint_{\partial V} u \, d\mathbf{n} = \frac{1}{V}\int_V \mathbf{g} \, dV \quad \longrightarrow \quad \frac{1}{V_j}\sum_{k\in\{k_j\}} \frac{u_L+u_R}{2}\mathbf{n}_{jk} = \frac{1}{V_j}\sum_{k\in\{k_j\}} \left\{ c\,\mathbf{g}_j + (2-c)\,\mathbf{g}'_k \right\} V_{jk}$$

$$\mathbf{g}'_k = \mathbf{g}_k - \nabla \mathbf{g}_j^{LLSQ}(\mathbf{x}_k - \mathbf{x}_j)$$



with

$$u_L = \kappa \frac{u_j+u_k}{2} + (1-\kappa)[u_j + \mathbf{g}_j \cdot (\mathbf{x}_k - \mathbf{x}_j)]$$

$$u_R = \kappa \frac{u_j+u_k}{2} + (1-\kappa)[u_k - \mathbf{g}_k \cdot (\mathbf{x}_k - \mathbf{x}_j)]$$

Linear IEBG: Two free parameters: κ and c.

Quadratic IEBG: Remains compact and 3x3 blocks (not 9x9 with 2nd derivatives like others), but no free parameters: $\kappa = 0$ and $c = 13/5$.

Not very robust… I couldn't adjust anything…

Numerical results show O(h^2) for other values of c

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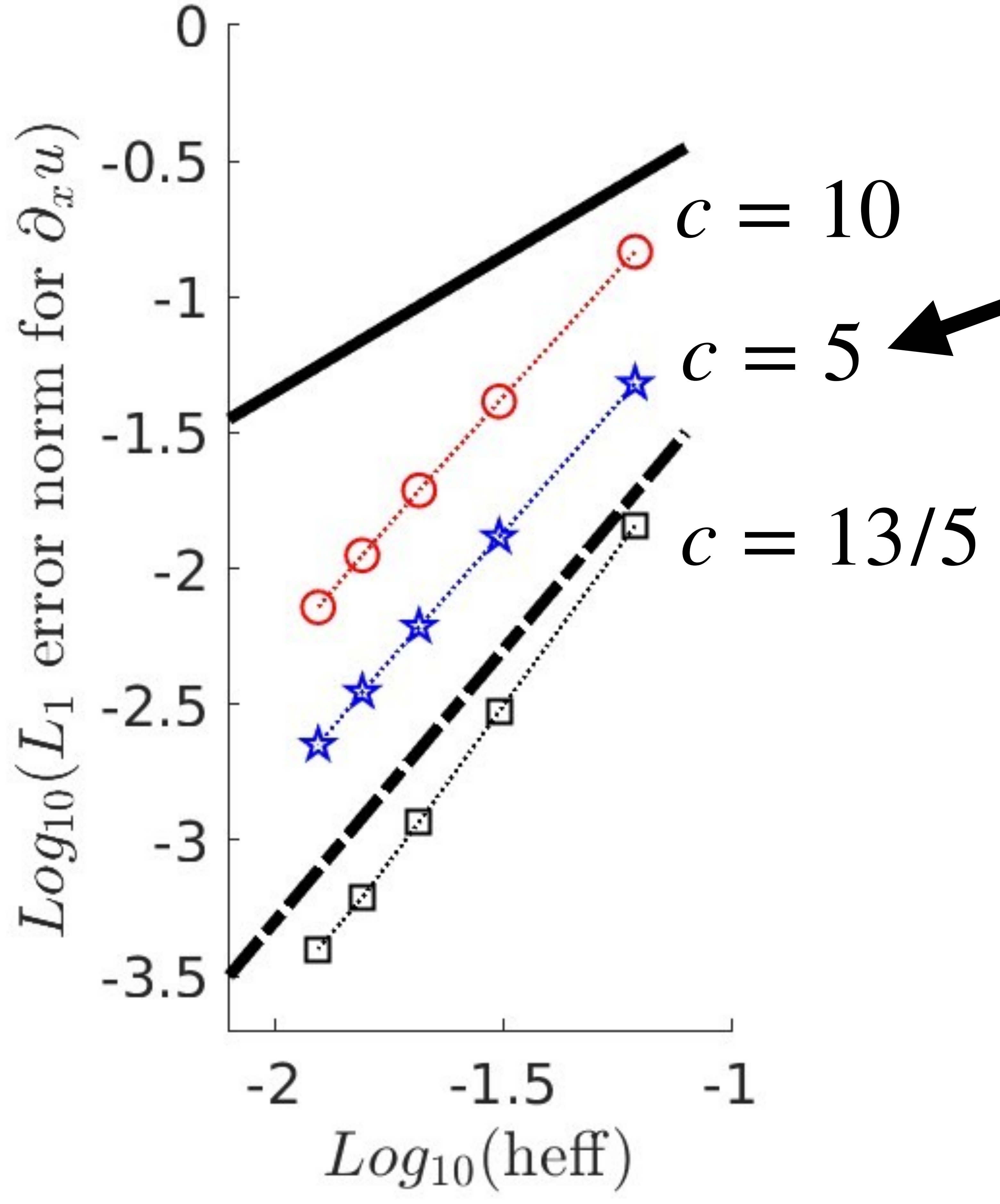
Emmett Padway (NASA) observed 2nd-order gradient accuracy for different values of c (2022).



Later, the author observed the same with his code (2023).

Something is wrong.

Not a bug in a code.
Not a problem in the algorithm.

The problem is that I thought I knew…

Simple if I knew nothing about source quadrature

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Forget the source formula and derive:

IEBG system

$$\mathbf{A}_h \mathbf{G}_h = \mathbf{b} \quad \longrightarrow$$

Gradient error

$$\mathbf{G}_h - \mathbf{G}_{exact} = \mathbf{A}_h^{-1} TE$$

$O(1)$

Gradient accuracy order matches TE order.

meaning that QIEBG must have TE=$O(h^2)$. It actually does for *any* c :

$$\frac{1}{V_j} \sum_{k \in \{k_j\}} \frac{u_L + u_R}{2} \mathbf{n}_{jk} - \frac{1}{V_j} \sum_{k \in \{k_j\}} \left\{ c\, \mathbf{g}_j + (2-c)\, \mathbf{g}'_k \right\} V_{jk} = \nabla u - \mathbf{g} + \underline{\underline{O(h^2)}}$$

So, we have 2nd-order gradient accuracy for any c.

That's good news: I can try to adjust it for robustness.

So, what was wrong?

Let me skip this to avoid confusion.

(Please read the paper or ask me.)

Better understanding by forgetting that I think I know.

Lesson 2: *See it for yourself.*

Computed by Automatic Differentiation (AIAA2020)

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$$\frac{1}{V_j}\sum_{k\in\{k_j\}}\frac{u_L+u_R}{2}\mathbf{n}_{jk}=\frac{1}{V_j}\sum_{k\in\{k_j\}}\left\{c\,\mathbf{g}_j+(2-c)\mathbf{g}'_k\right\}V_{jk}$$

In 2020, I computed $\mathbf{M}_{jj}$ and $\mathbf{M}_{jk}$ by automatic differentiation

$$\longrightarrow \quad \mathbf{M}_{jj}\mathbf{g}_j+\sum_{k\in\{k_j\}}\mathbf{M}_{jk}\mathbf{g}_k=GG$$

Solve the linear system by a relaxation scheme: e.g., Gauss Seidel.

$$\mathbf{g}_j^{n+1}=-\mathbf{M}_{jj}^{-1}\left[\sum_{k\in\{k_j\}}\mathbf{M}_{jk}\mathbf{g}_k^n\right]+\mathbf{M}_{jj}^{-1}GG$$

This relaxation fails for some sets of parameters κ and c. Why? I didn't know…

Then, in 2023

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To gain some insight on how IEBG fails when it fails,
I decided to derive the block matrix $\mathbf{M}_{jj}$ and see what it looks like.

Linear IEBG:

$$\mathbf{M}_{jj} = \frac{\kappa - 1}{4V_j} \sum_{k \in \{k_j\}} (\mathbf{n}_{jk} \otimes \Delta \mathbf{r}_{jk}) + \frac{c}{2V_j} \sum_{k \in \{k_j\}} V_{jk}\, \mathbf{I}$$

$$= \frac{\kappa - 1}{2V_j} V_j \mathbf{I} + \frac{c}{2V_j} V_j \mathbf{I}$$

$$= \left(\frac{c + \kappa - 1}{2} \right) \mathbf{I}$$

$$\frac{1}{2} \sum_{k \in \{k_j\}} (\mathbf{n}_{jk} \otimes \Delta \mathbf{r}_{jk}) = V_j \mathbf{I}$$

for arbitrary triangular/tetrahedral grids:

Not a matrix but a scalar! Very easy to invert: $\mathbf{M}_{jj}^{-1} = \left(\frac{2}{c + \kappa - 1} \right) \mathbf{I}$ (similarly for QIEBG).

Oh, it fails when $c + \kappa - 1 = 0$!

True also at boundary nodes

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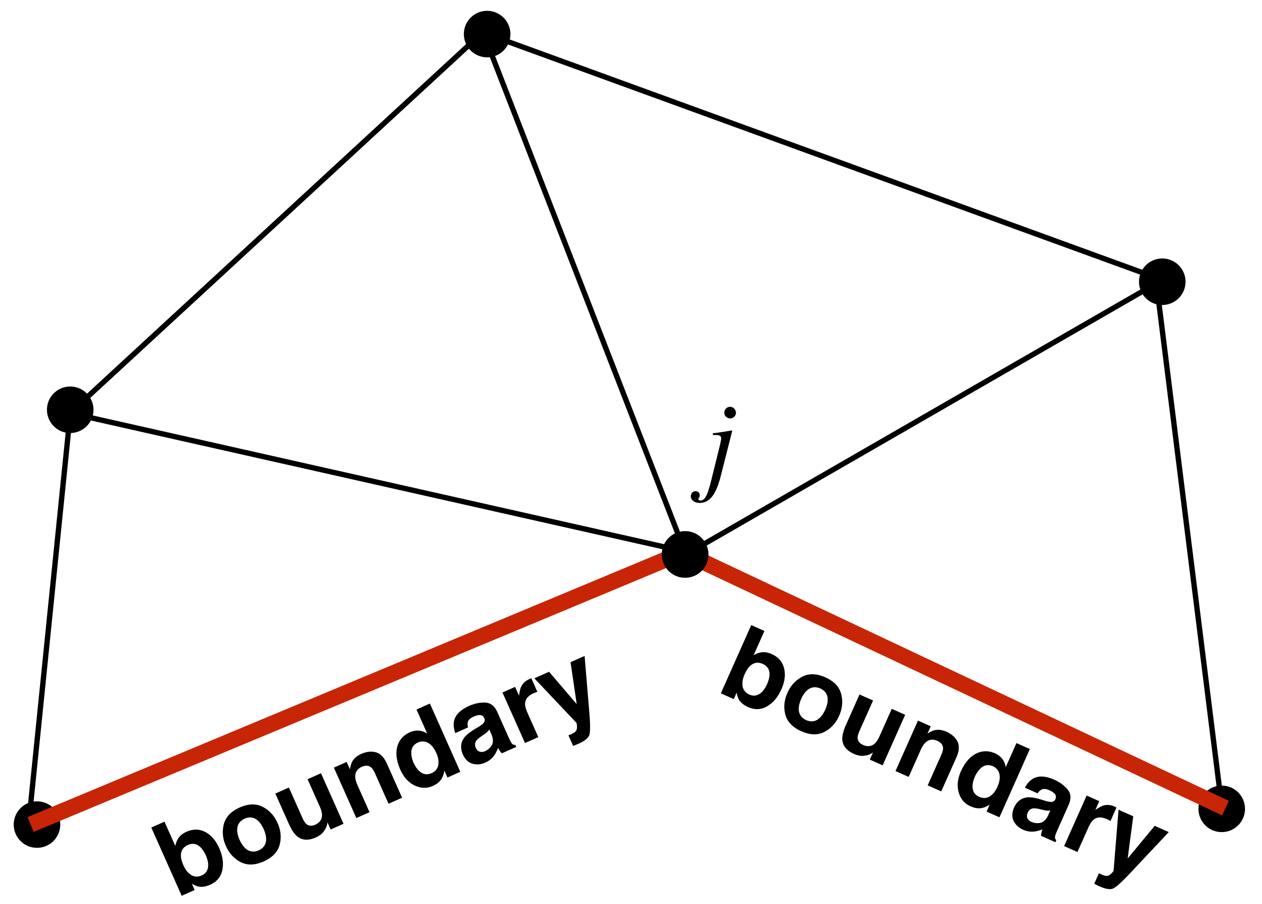
This remains true while an edge is collapsed:

$$\mathbf{M}_{jj} = \left(\frac{c + \kappa - 1}{2} \right) \mathbf{I}$$



Achieved great simplification by seeing it for myself.

Lesson 3: *Understand limits.*

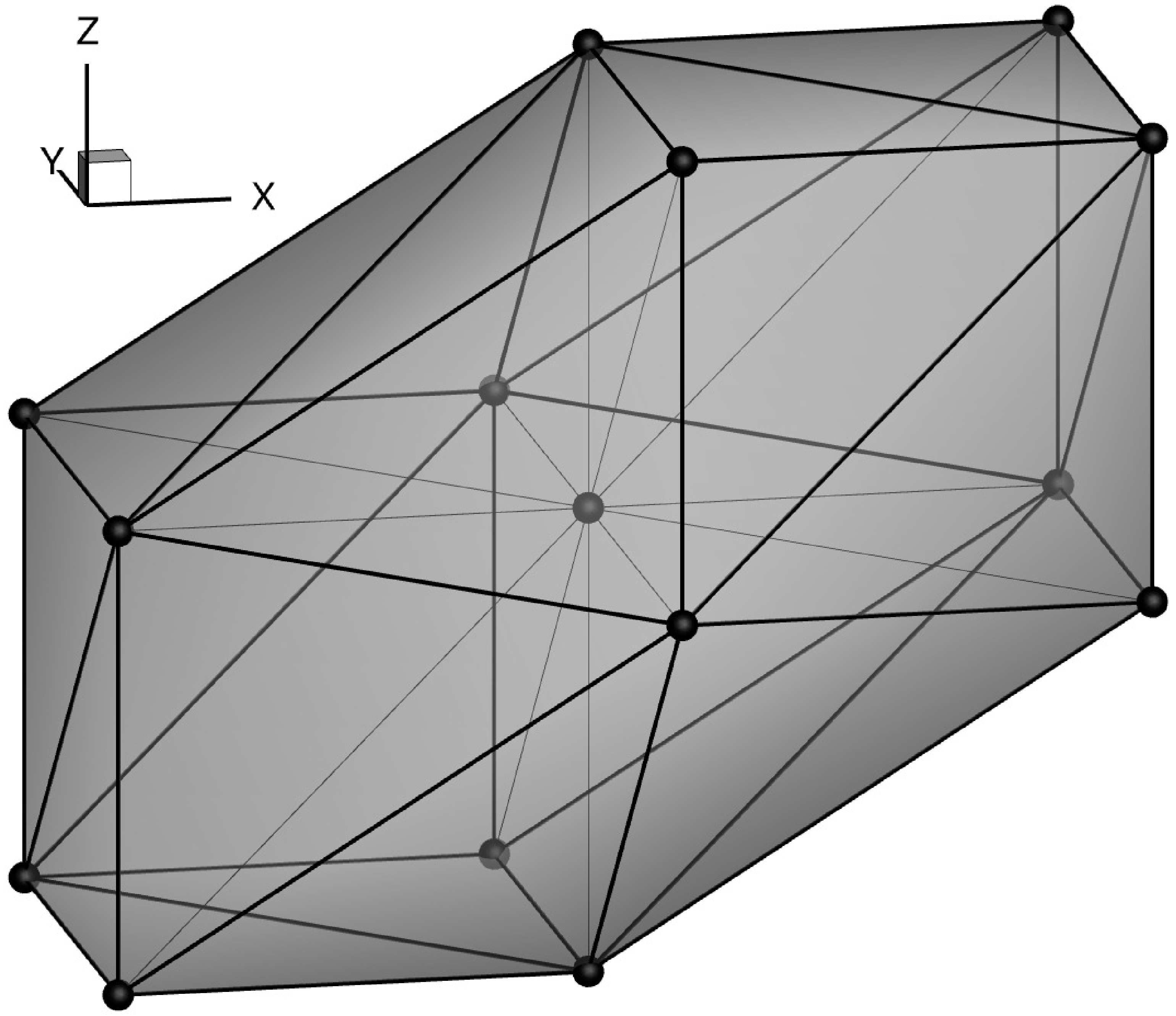
What values are allowed for κ and c ? I didn't know well…

-> Look at accuracy and stability.

Accuracy: Good to find special values

On a regular tetrahedral grid: Linear IEBG = Quadratic IEBG

$$\mathbf{Res}_j = \frac{5}{36}\left(c - \frac{13-9\kappa}{5}\right)\left(\partial_{xx} + \partial_{yy} + \partial_{zz} - \partial_{xy} - \partial_{yz} + \partial_{zx}\right)(\nabla u)\, h^2 + O(h^4)\,.$$



Regular tetrahedral grid

$$\boxed{c = \frac{13-9\kappa}{5}}$$

<- 4th-order accurate.

In this work, we set $\kappa = 0$ and $c = \dfrac{13}{5}$,

but a larger value $c = 5$ was needed for robustness.

Is it supposed to work?

Stability: Good to understand limits

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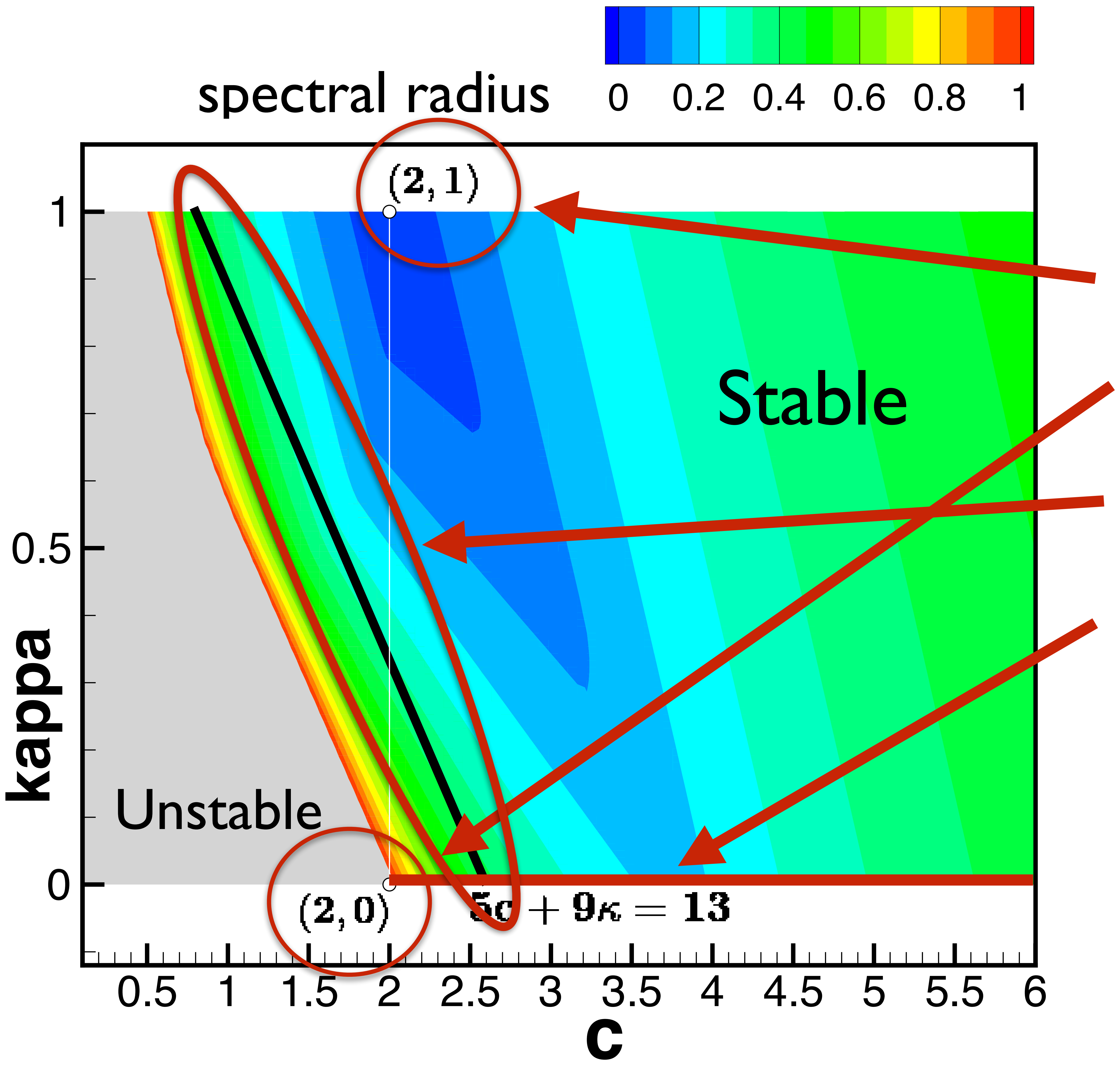
Performed a Fourier stability analysis for the Gauss-Seidel scheme.



So, we see

- Explicit at $(c, \kappa) = (2,1)$. Zero spectral radius!
- Linear IEBG is 2nd-order accurate at (2,0) but unstable.
- 4th-order IEBG is stable: $5c + 9\kappa = 13$
- Quadratic IEBG ($\kappa = 0$) is stable for $c > 2$.

So, we can safely set $c = 5$.

A better guide on how to choose parameters.

Results

Mach 0.3 smooth bump

(Accuracy verification and supersonic/hypersonic problems in the paper.)

Mach 0.3 Subsonic Flow over a smooth bump

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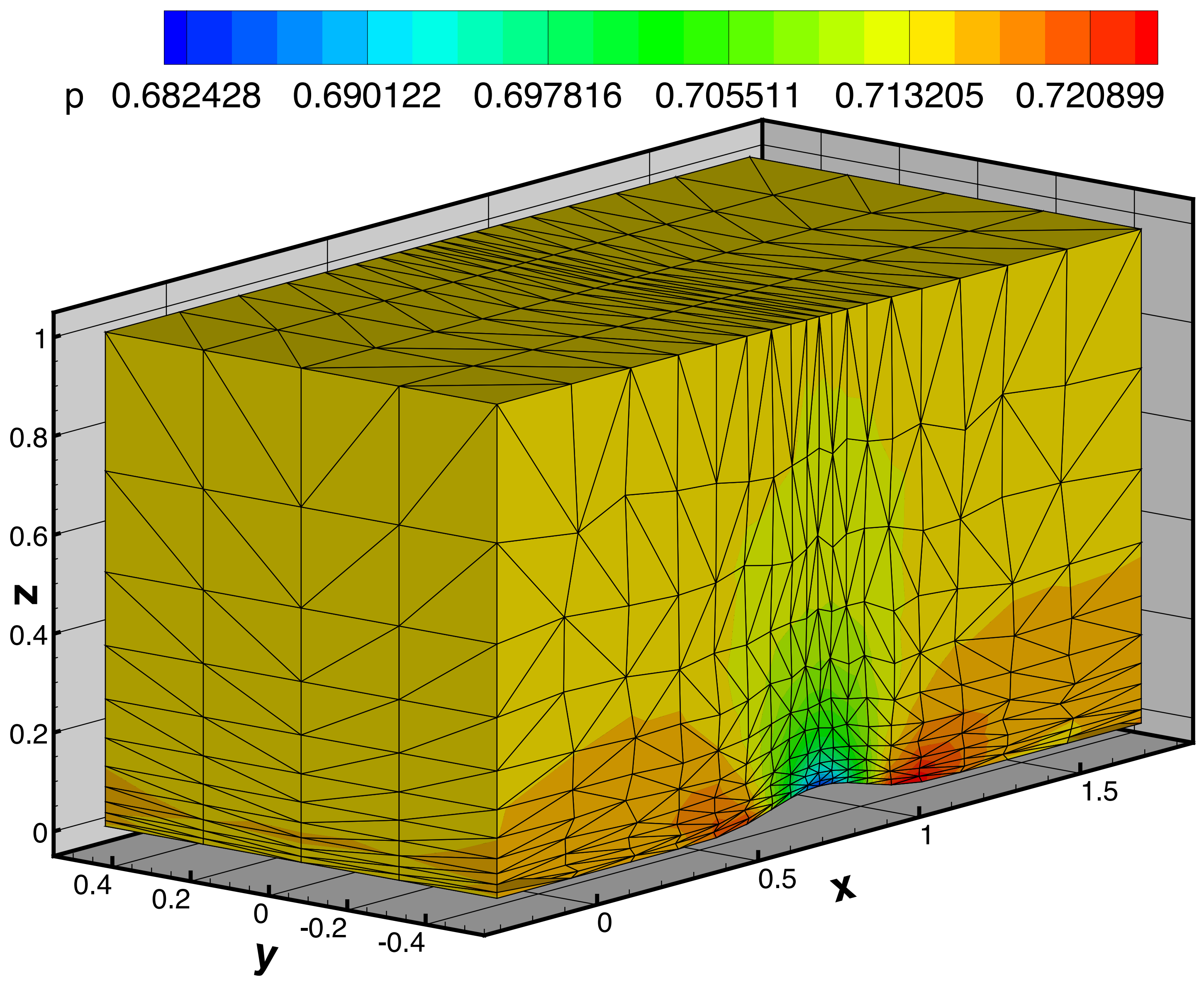
Solve Euler by 2nd/3rd-order EB methods:

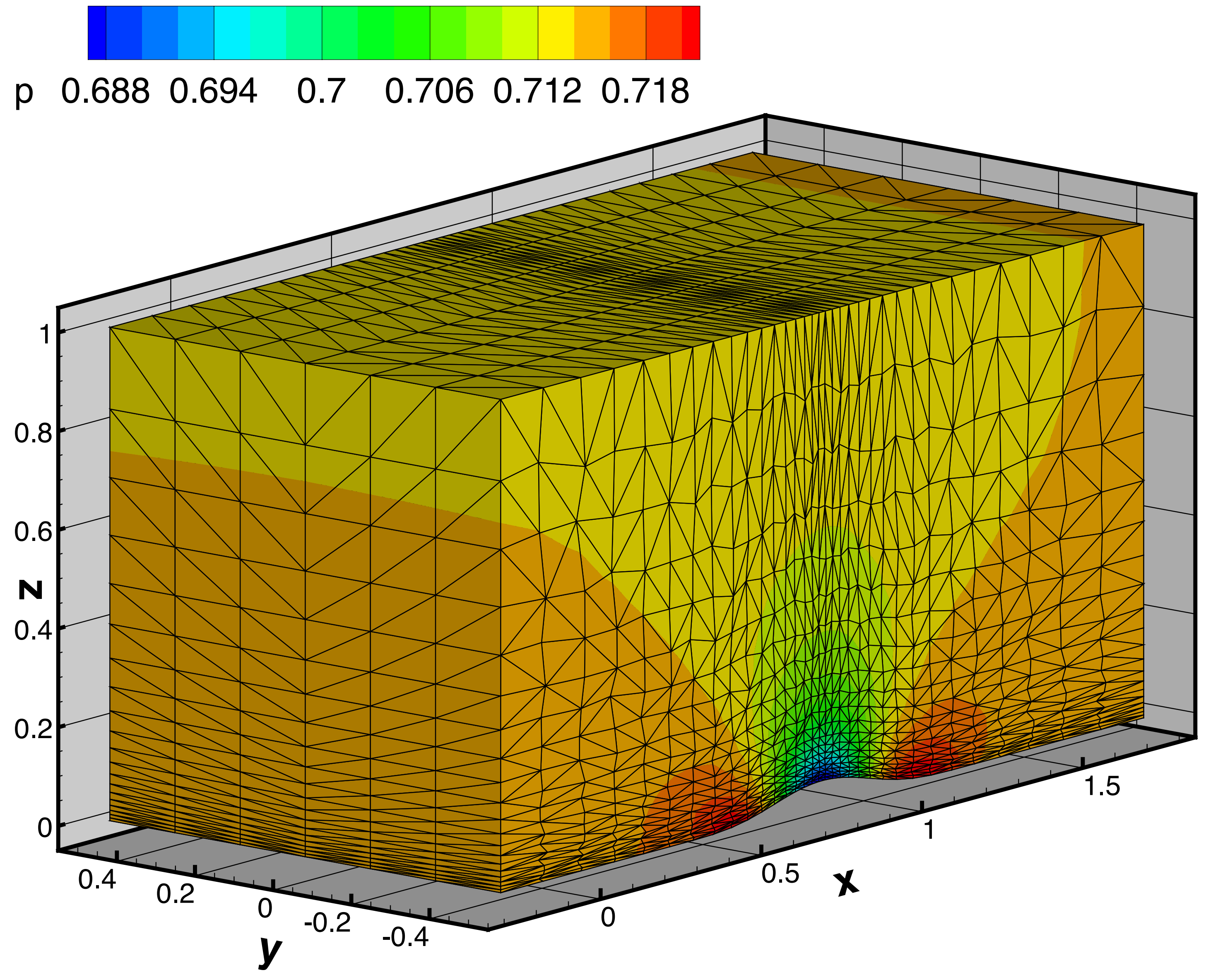
(1) $\mathbf{G}^{n+1} = \mathbf{G}^{n} + \Delta\mathbf{G}$: Update gradients by one Gauss-Seidel relaxation.

(2) $\mathbf{U}^{n+1} = \mathbf{U}^{n} + \Delta\mathbf{U}$: Update solutions by one iteration of implicit Euler solver.

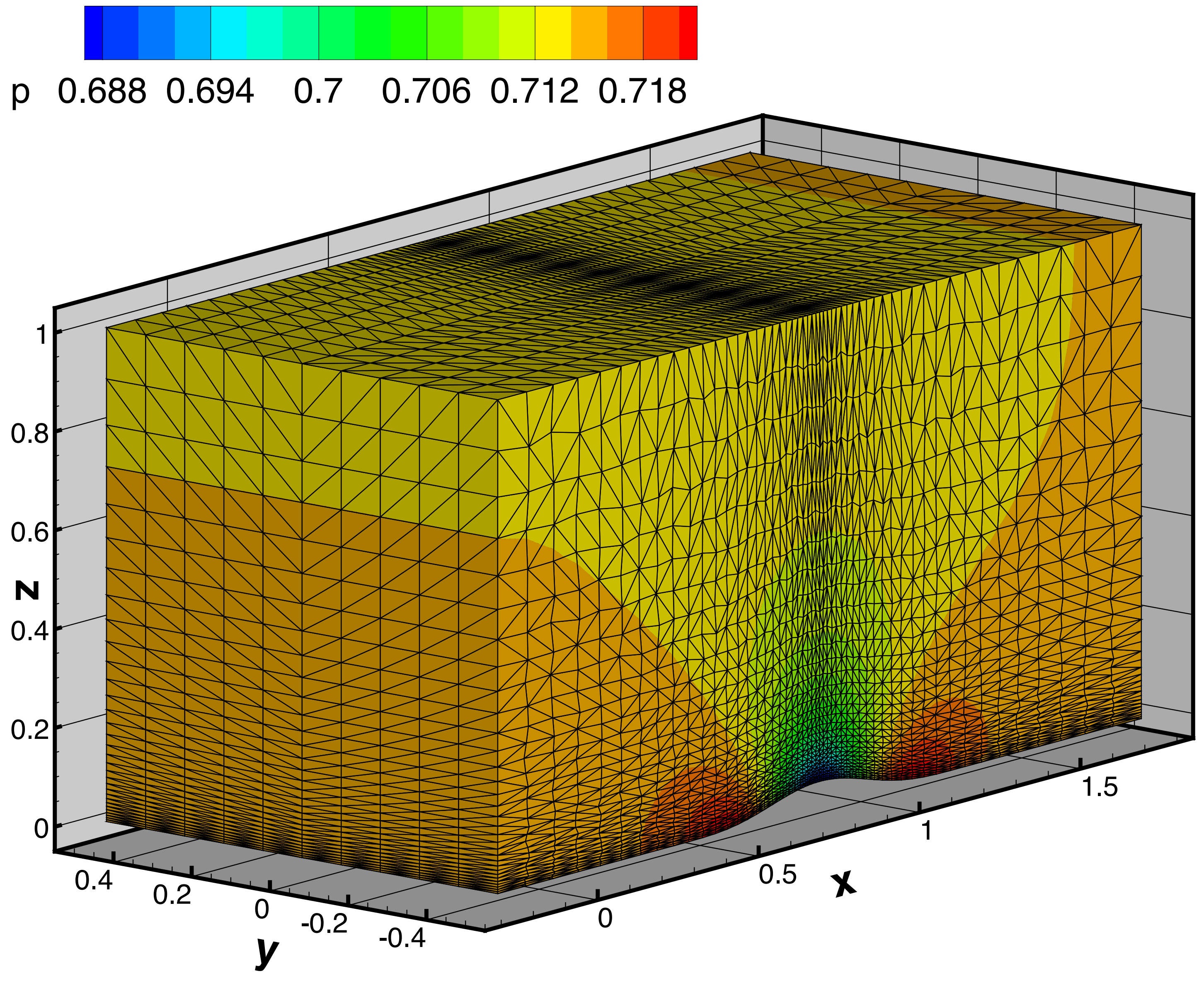
Grid 1



Grid 2



Grid 3



Subsonic Flow: $\kappa = 0$ and $c = 5$

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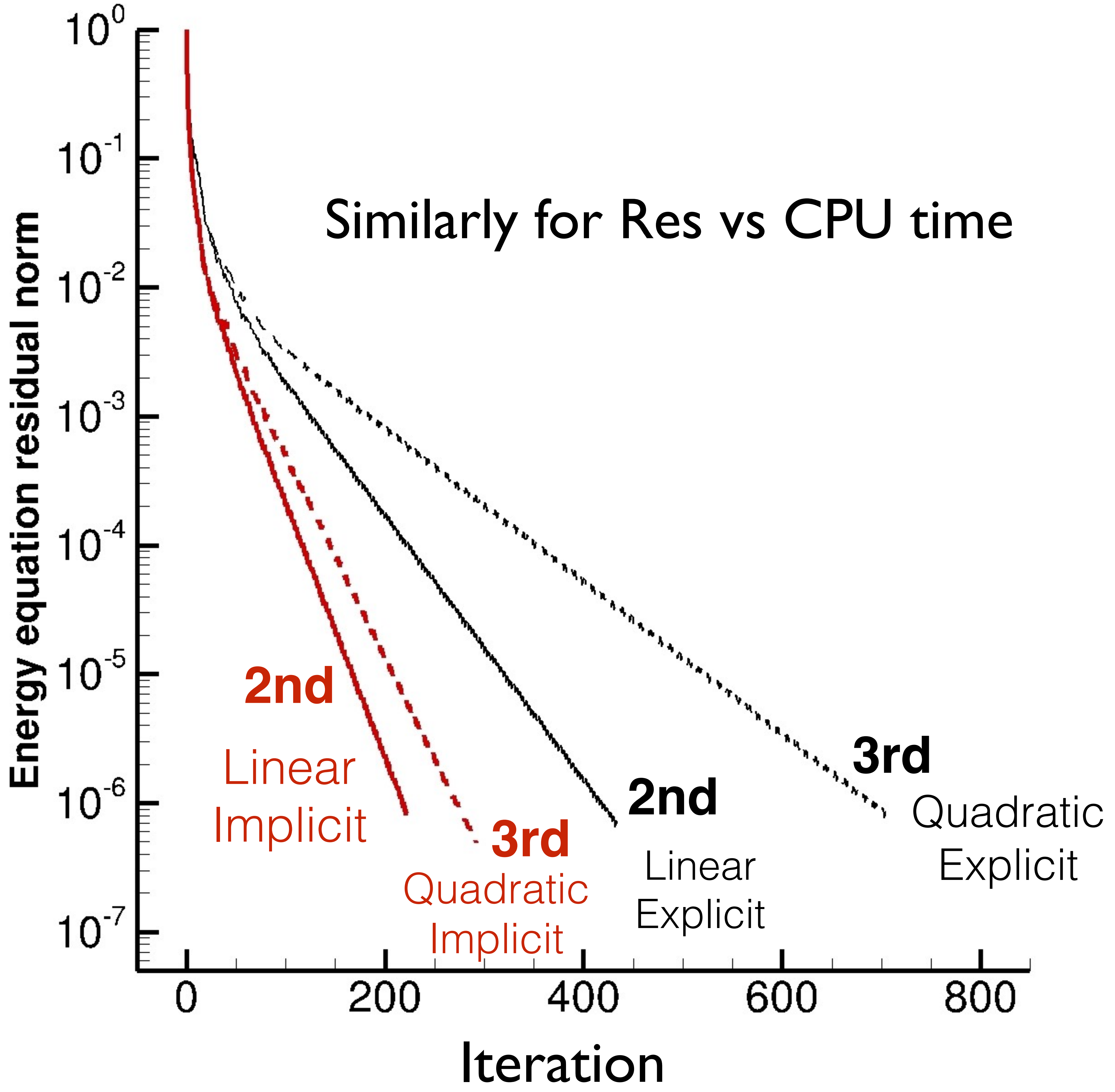
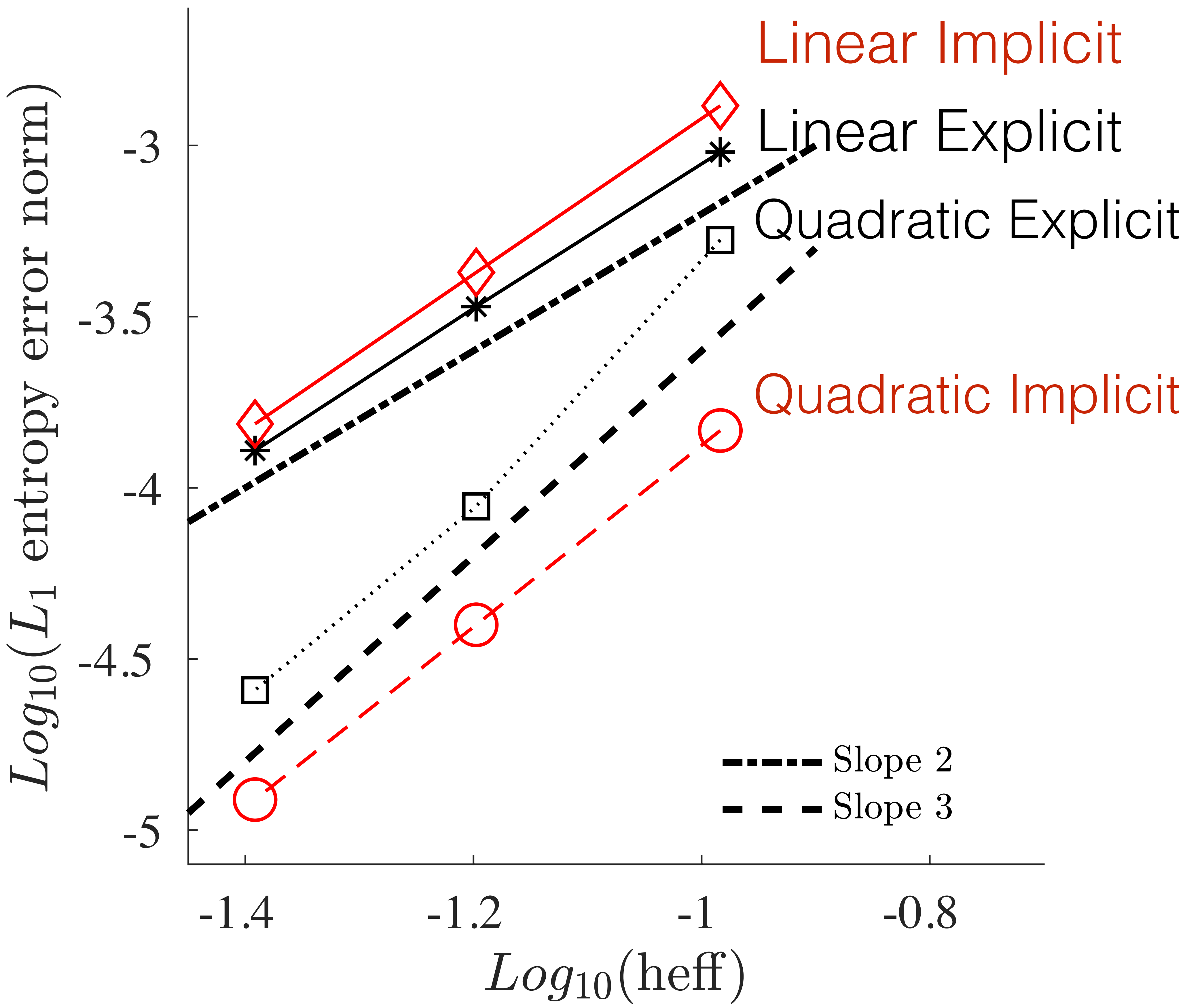
(1) Residual norm vs iteration



Fewer iterations and faster time-to-solution

IEBG methods are not expensive.

(2) Entropy error convergence



2nd- and 3rd-order convergence

Lower 3rd-order error by QIEBG.

Supersonic/Hypersonic Flow: $\kappa = 0$ and $c = 5$

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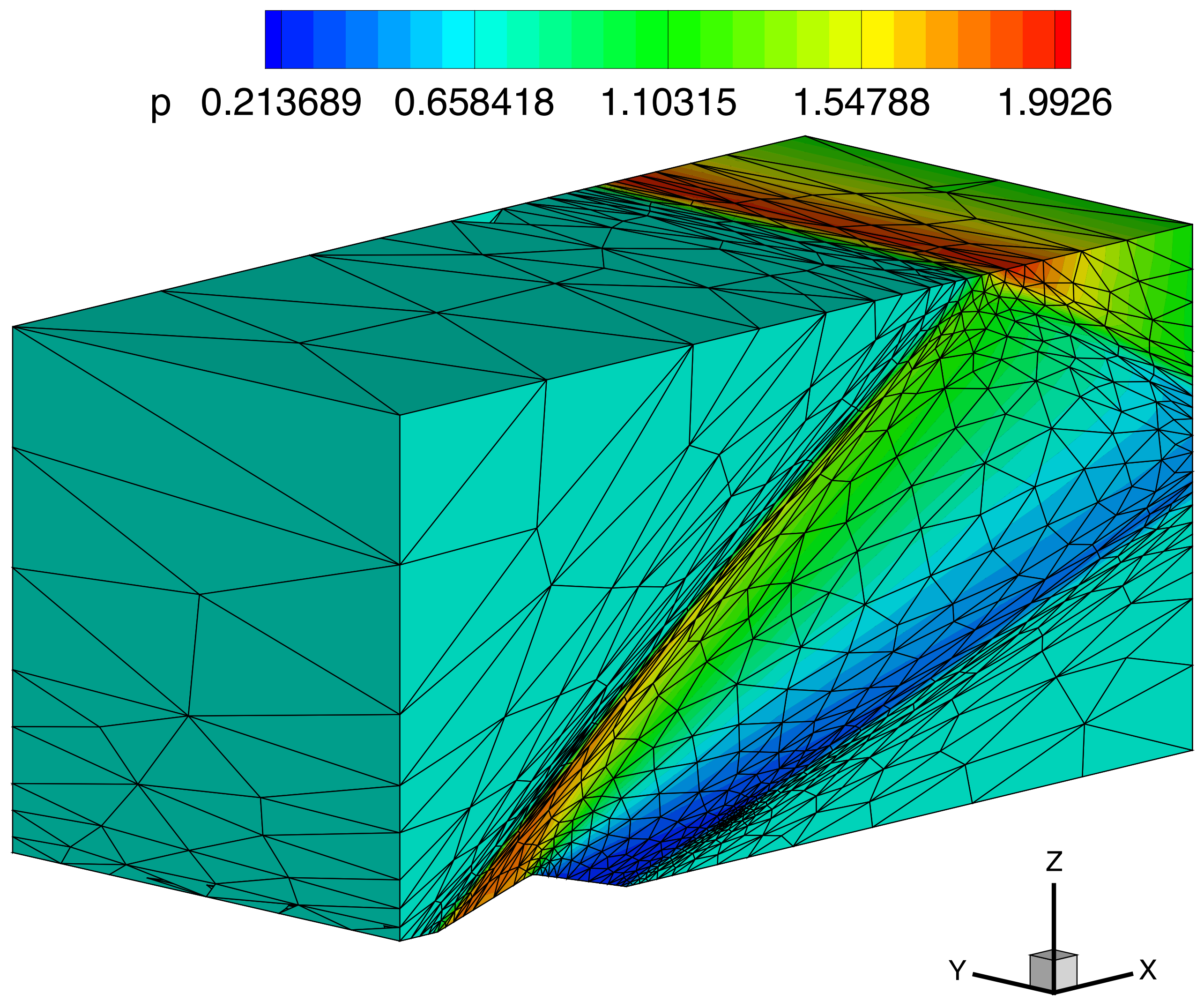
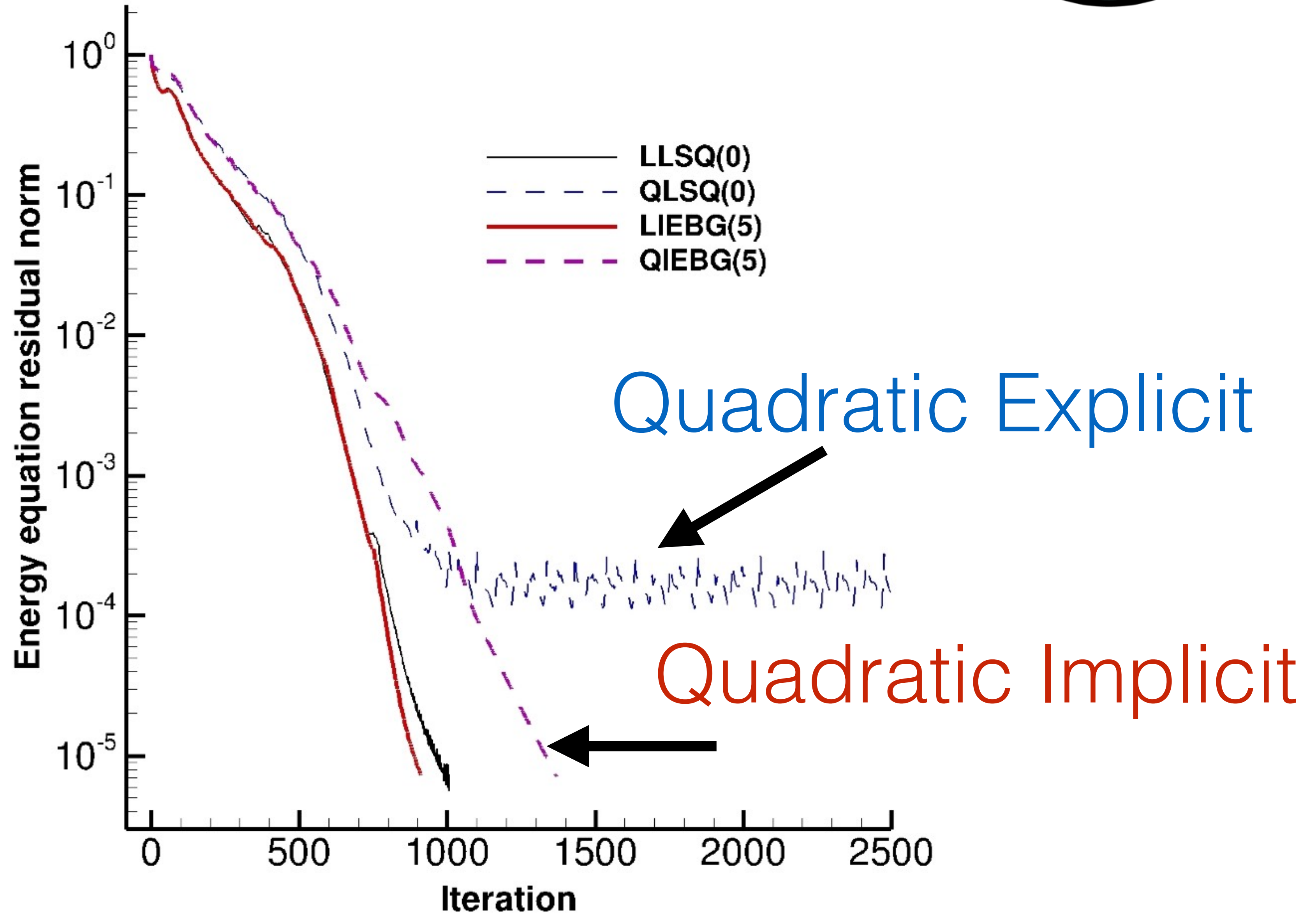
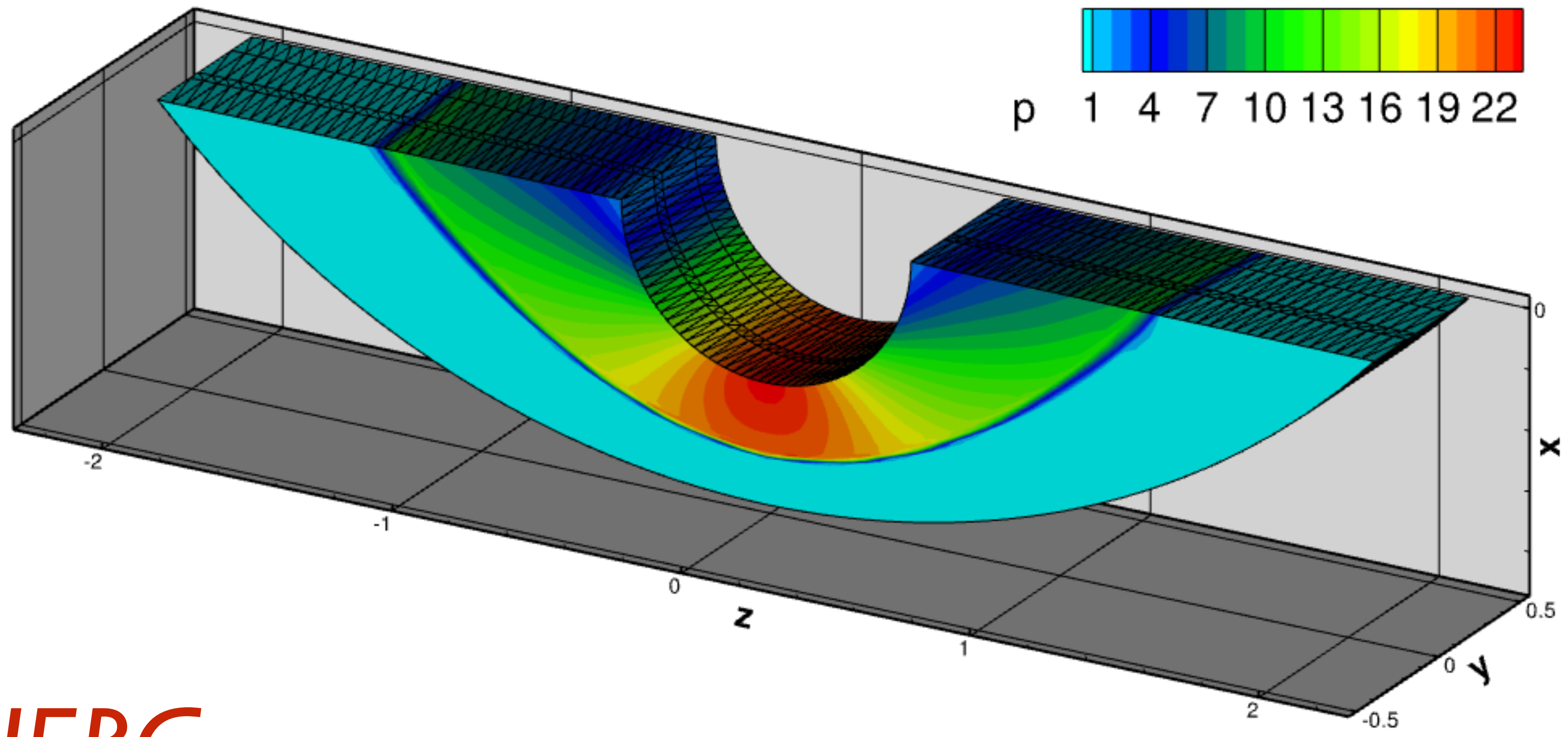
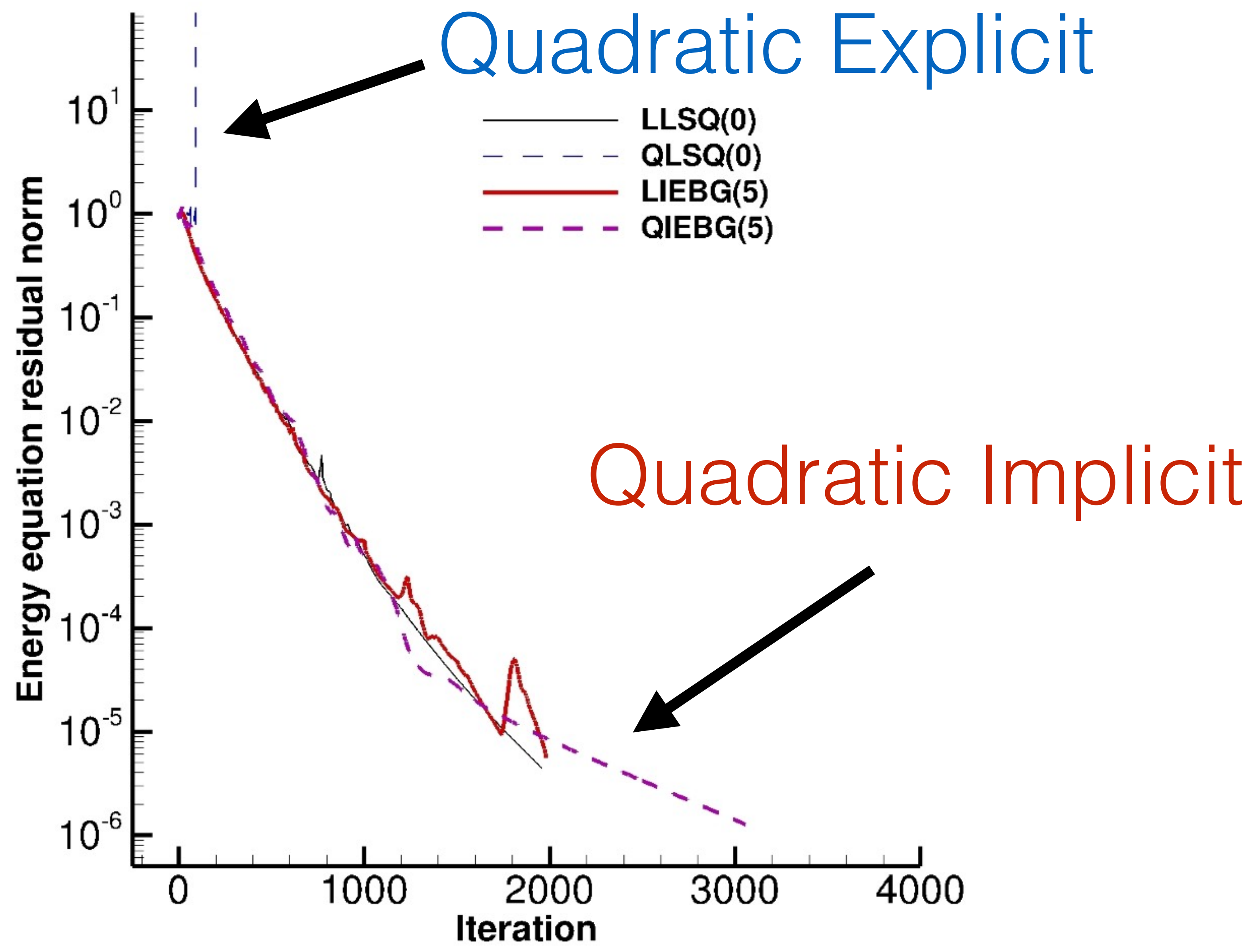
Mach 2.5 flow over a triangular bump.





Mach 5.0 flow over a circular cylinder.





More robust with QIEBG.

Conclusions

Conclusions and Future Work

Lesson 1: *Forget that you think you know.*

2nd-order accurate gradient for any c

$$\mathbf{Res}(c) = \nabla u - \mathbf{g} + O(h^2)$$

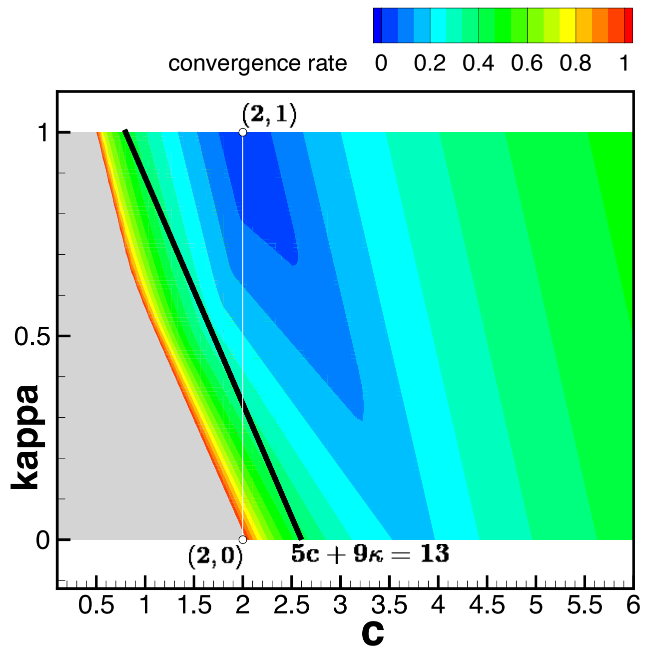
Robust with $c = 5$.

Lesson 2: *See it for yourself.*

Simplified:

$$\mathbf{M}_{jj} = \left(\frac{c+\kappa-1}{2}\right)\mathbf{I}$$

Lesson 3: *Understand limits.*

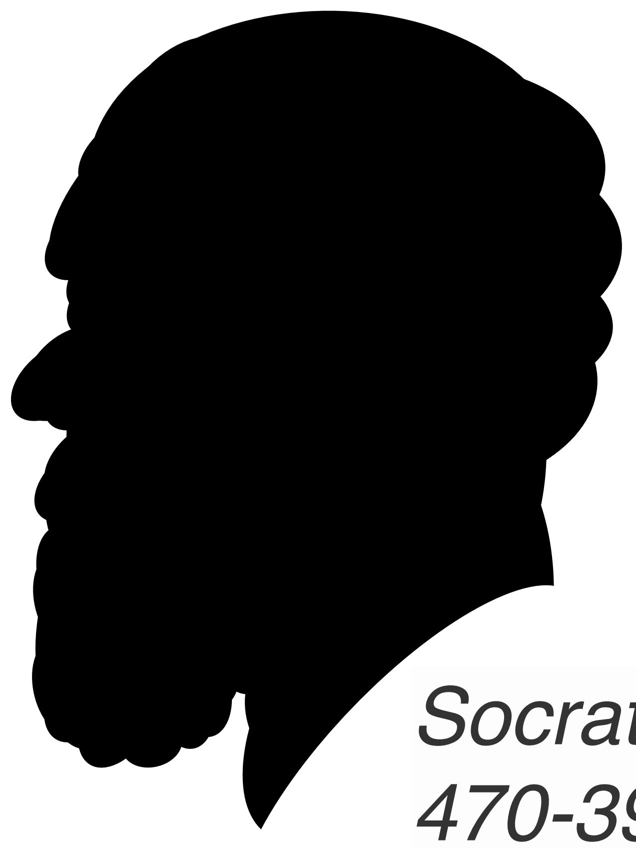


4th-order with $c = (13 - 9\kappa)/5$

Stable with $c > 2$ *(QIEBG* $\kappa = 0$*)*

Results: IEBG demonstrated for subsonic/supersonic/hypersonic flows.
Lower 3rd-order errors and more robust iterative convergence than with quadratic LSQ.

Future work: Applications to space-time viscous problems and cell-centered nodal-gradient finite-volume methods.



Socrates
470-399 B.C.

"I neither know nor think that I know" *(in Plato, Apology 21d).*

I had to realize and admit I didn't know, or this work would have been far less complete.
3rd-order EB scheme is now made more robust.

*“The really important thing is not to live,
but to live well.”*

***Socrates**,*
470-399 B.C.

*The really important thing is not to develop CFD algorithms,
but to develop them well.*

*Always seek a better understanding, a further simplification,
and a better guide on how to choose parameters.*