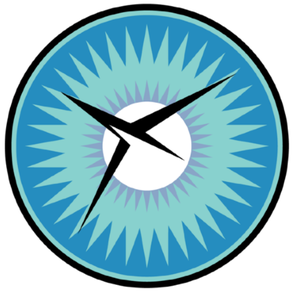
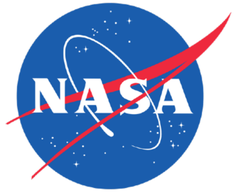


Towards Robust and Accurate Implicit Gradient Methods for Second- and Third-Order Nodal-Gradient Cell-Centered Finite-Volume Discretizations on Tetrahedral Grids

Hiroaki Nishikawa, *National Institute of Aerospace*

11:10am, in Academic Ballroom 412, AIAA Aviation,
Tuesday, July 30, 2024



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Economical 3rd-Order Methods

Economical 3rd-Order Methods

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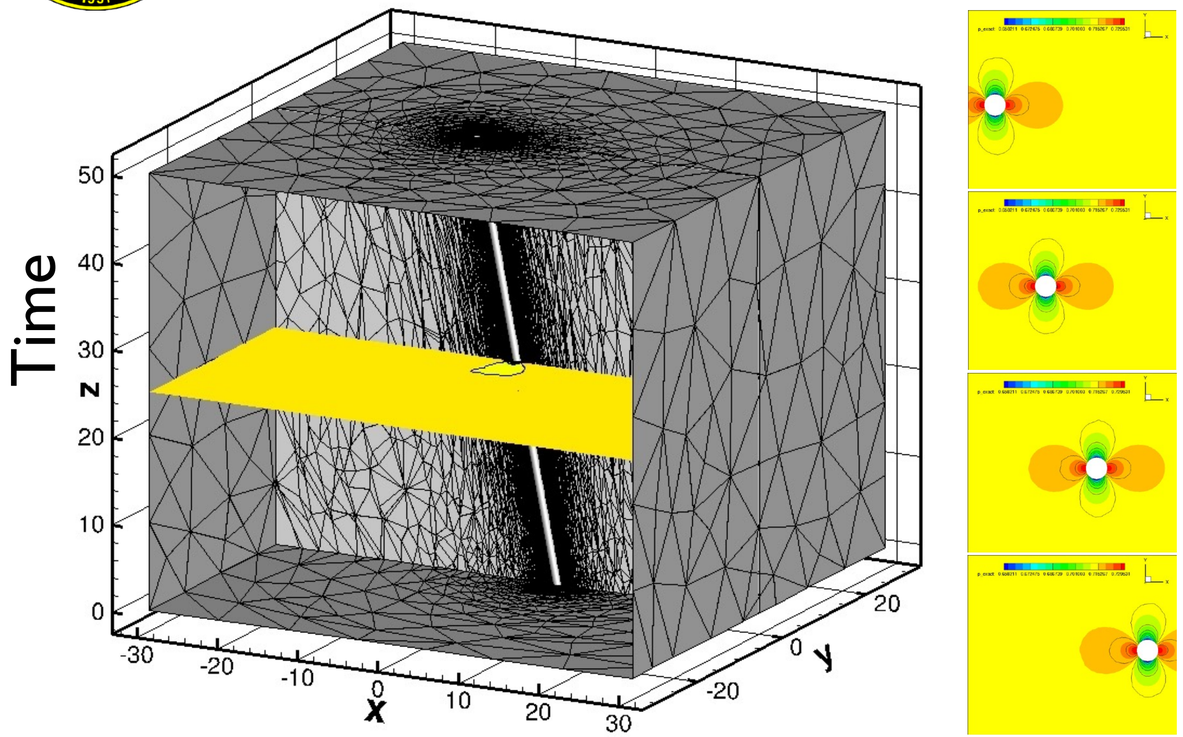
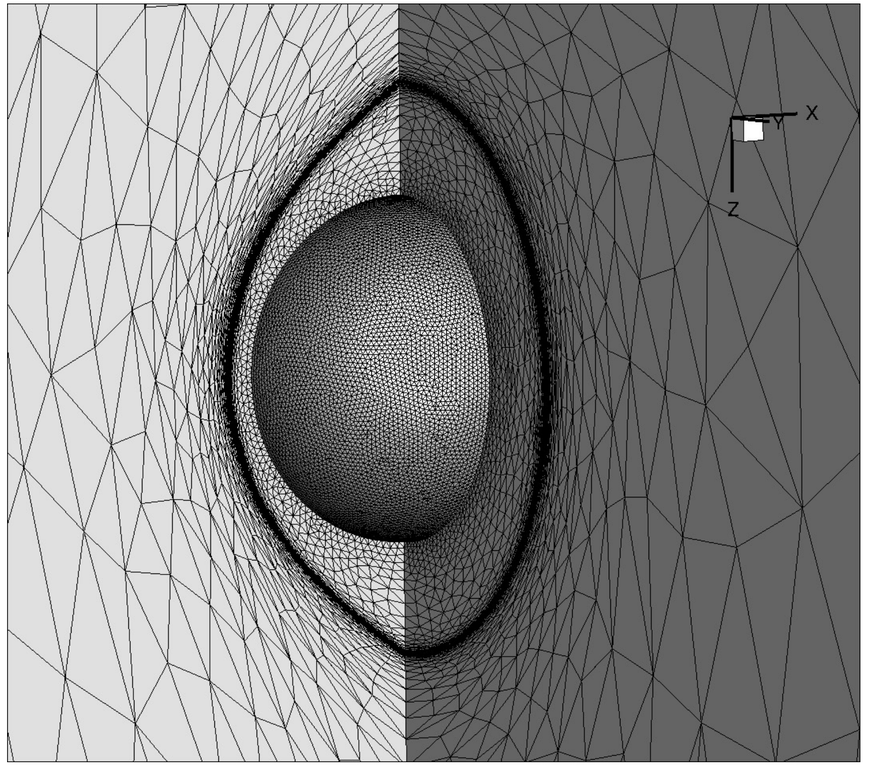
Exploring Space-Time Hyperbolic NS



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.

Economical 3rd-Order NGCC Discretization

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This paper focuses on a 3rd-order cell-centered method:

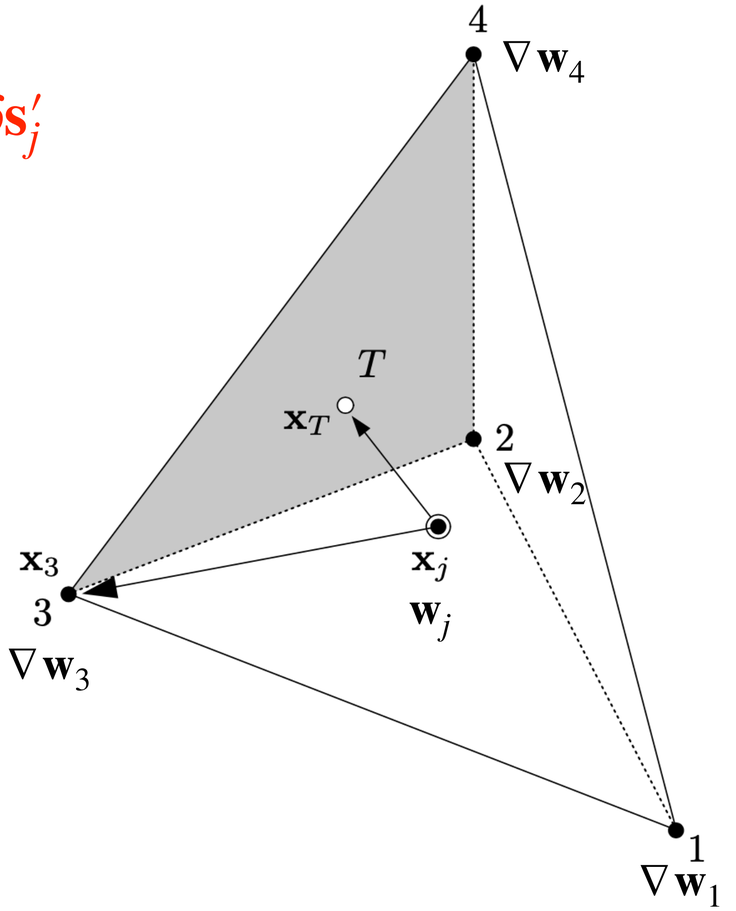
$$V_j \frac{\partial \mathbf{u}_j}{\partial t} + \sum_{k \in \{k_j\}} \Phi_{jk}(\mathbf{w}_L, \mathbf{w}_R) \, |\mathbf{n}_T| - \mathbf{s}_j V_j = \delta \mathbf{f}_j + \delta \mathbf{s}'_j$$

where $\mathbf{u}_j$ is a vector of point-valued solutions at cell center, and

Quadratic interpolation:
$$\mathbf{w}_L = \mathbf{w}_j + \frac{1}{2}\left(\overline{\nabla \mathbf{w}}_T + \overline{\nabla \mathbf{w}}_j\right)(\mathbf{x}_T - \mathbf{x}_j)$$

Flux correction:
$$\delta \mathbf{f}_j = \frac{1}{24} \sum_{k \in \{k_j\}} \sum_{i=1}^{3} \left(\frac{\partial \mathbf{f}}{\partial \mathbf{w}}\right) \nabla \mathbf{w}_i (\mathbf{x}_i - \mathbf{x}_T) \, |\mathbf{n}_T|$$

Source correction:
$$\delta \mathbf{s}'_j = \frac{1}{40} \sum_{i=1}^{4} \nabla \mathbf{s}'_i (\mathbf{x}_i - \mathbf{x}_j) V_j \qquad \mathbf{s}' = \mathbf{s}_j - \frac{\partial \mathbf{u}}{\partial t}$$



We only need gradients at nodes for 3rd-order accuracy: no second derivatives required.

Explicit and Implicit Gradient Methods $\mathbf{g} = \left[\partial_x u, \partial_y u, \partial_z u\right]$

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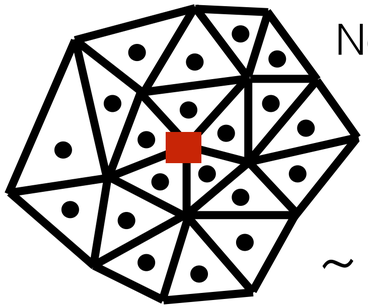
Explicit:

Linear LSQ

$$\mathbf{g}_j = \sum_{k \in nghbrs} C_{jk} u_k$$

Quadratic LSQ

$$\mathbf{g}_j = \sum_{k \in nghbrs} C_{jk} u_k$$



Node-nghbr aug

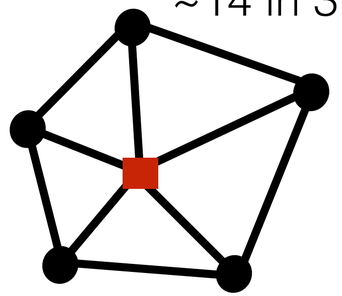
~ 200 in 3D

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

Haider&Croisille&Courbet NM2009

Implicit:

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



~14 in 3D

Galerkin: Löhner(1994)

Variational Reconstruction: Wang et. al., JCP2017

Implicit GG: Nishikawa, JCP2019

Implicit EB gradient: Nishikawa, AIAA2020

Advantages of Implicit Gradients

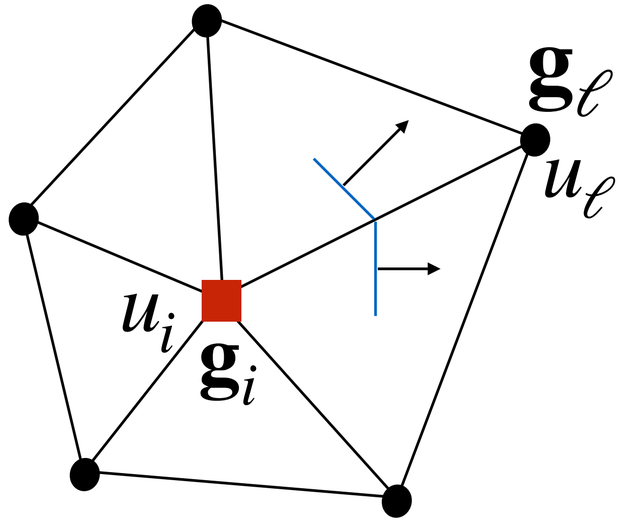
- Flow solver is more stable with a huge gradient stencil.
- Superior gradient accuracy.
- Per-relaxation cost can be lower than LSQ gradients with hundred of neighbors

Implicit Gradients

IEBG2 (AIAA2024) $\mathbf{g} = \left[\partial_x u, \partial_y u, \partial_z u\right]$

IEBG2 system: Exact for quadratic functions

$$\mathbf{M}_{ii}\mathbf{g}_i + \sum_{\ell \in \{\ell_i\}} \mathbf{M}_{i\ell}\mathbf{g}_\ell = \frac{1}{V_j} \sum_{\ell \in \{\ell_i\}} \frac{u_i + u_\ell}{2}\mathbf{n}_{i\ell} \qquad \mathbf{g}_i = \begin{bmatrix} \partial_x u_i \\ \partial_y u_i \\ \partial_z u_i \end{bmatrix}$$



We can solve the system by a relaxation scheme:

$$\mathbf{g}_i^{m+1} = \mathbf{g}_i^m - \mathbf{M}_{ii}^{-1}\left(\sum_{\ell \in \{\ell_i\}} \mathbf{M}_{i\ell}\mathbf{g}_\ell^m + \frac{1}{V_j} \sum_{\ell \in \{\ell_i\}} \frac{u_i + u_\ell}{2}\mathbf{n}_{i\ell} \right)$$

Successfully demonstrated for their 3rd-order EB discretization method.

IEBG2 is very efficient and perfect for the 3rd-order EB because it does not require second derivatives.

Can we develop something similar to our 3rd-order CCFV method?

Implicit Nodal-Gradient Cell-Solution Method

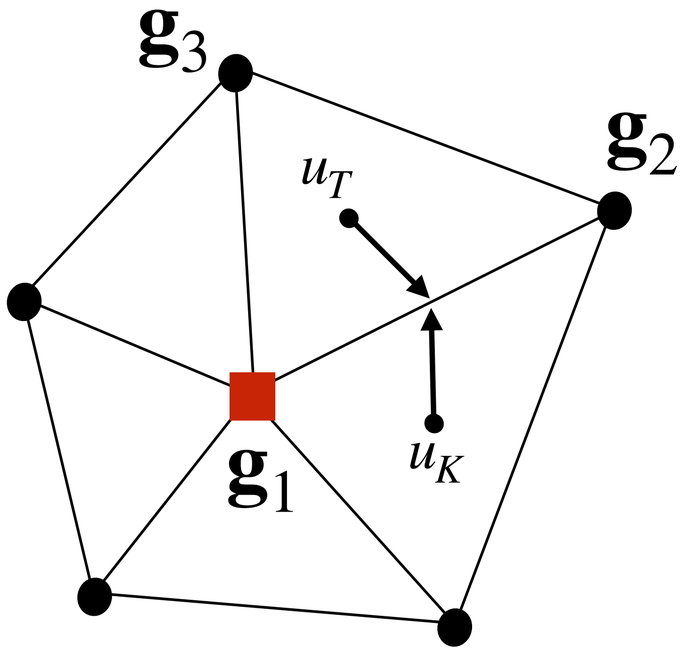
Yes, we can. First, define the cell discretization:

$$\mathbf{g} = \nabla u \longrightarrow \int_{V_T} \mathbf{g}\, dV = \oint_{\partial V_T} u\, \hat{\mathbf{n}} ds$$

3rd-order NG-CCFV

No 2nd derivatives

$$\longrightarrow \mathbf{Res}_T = \frac{\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3}{3} - \sum_{K \in \{K_T\}} \left[\phi_{TK} + \delta\phi_{TK}\right] |\mathbf{n}_{TK}|$$



Then, minimizing the cell residuals in the LSQ sense:

$$\mathscr{F} = \frac{1}{2} \sum_{\text{all cells}} \mathbf{Res}_T^2 \longrightarrow \frac{\partial \mathscr{F}}{\partial \mathbf{g}_i} \equiv \mathbf{Res}_i = \sum_{T \in \{T_i\}} \left(\frac{\partial \mathbf{Res}_T}{\partial \mathbf{g}_i} \right)^t \mathbf{Res}_T = \mathbf{0}$$

The resulting system is second-derivative-free as desired, but not robust…

Worked very hard to make it robust, but couldn't get it done successfully…

IEBG2 for NG-CCFV Method

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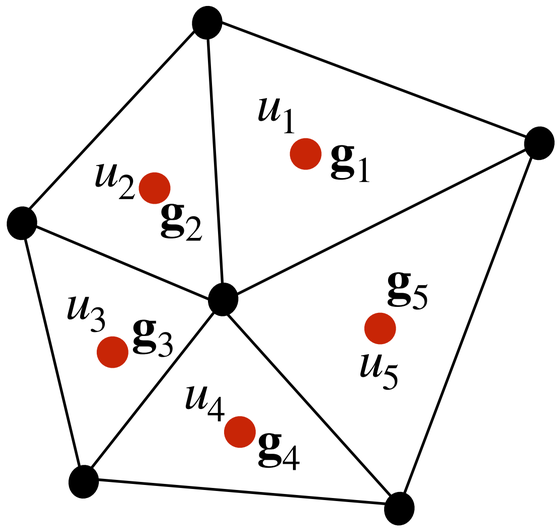
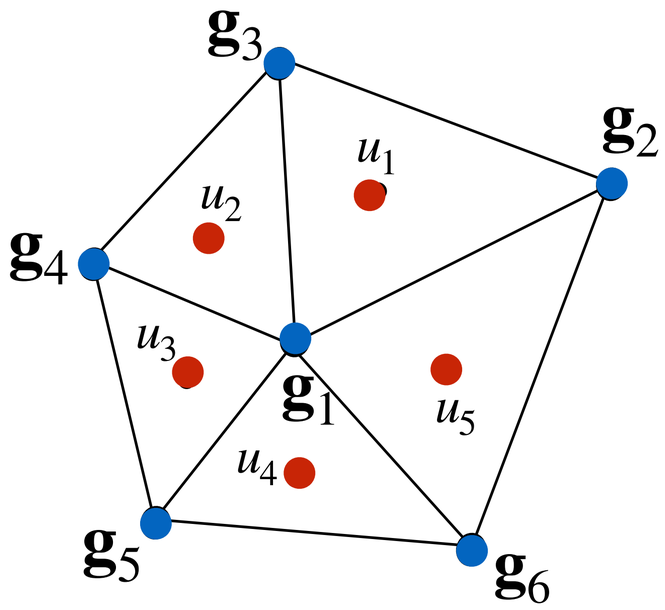
Realize that NG-CCFV is somewhere between CCFV and NCEB:

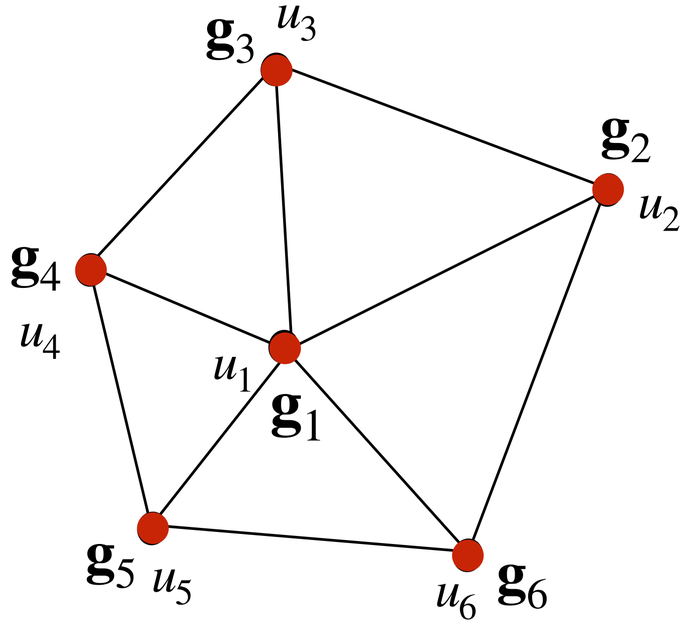
Cell-Centered



Nodal-Grad Cell-Centered



Node-Centered



$$\mathbf{M}_{ii}\mathbf{g}_i + \sum_{\ell \in \{\ell_i\}} \mathbf{M}_{i\ell}\mathbf{g}_\ell = \frac{1}{V_j} \sum_{\ell \in \{\ell_i\}} \frac{u_i + u_\ell}{2} \mathbf{n}_{i\ell}$$

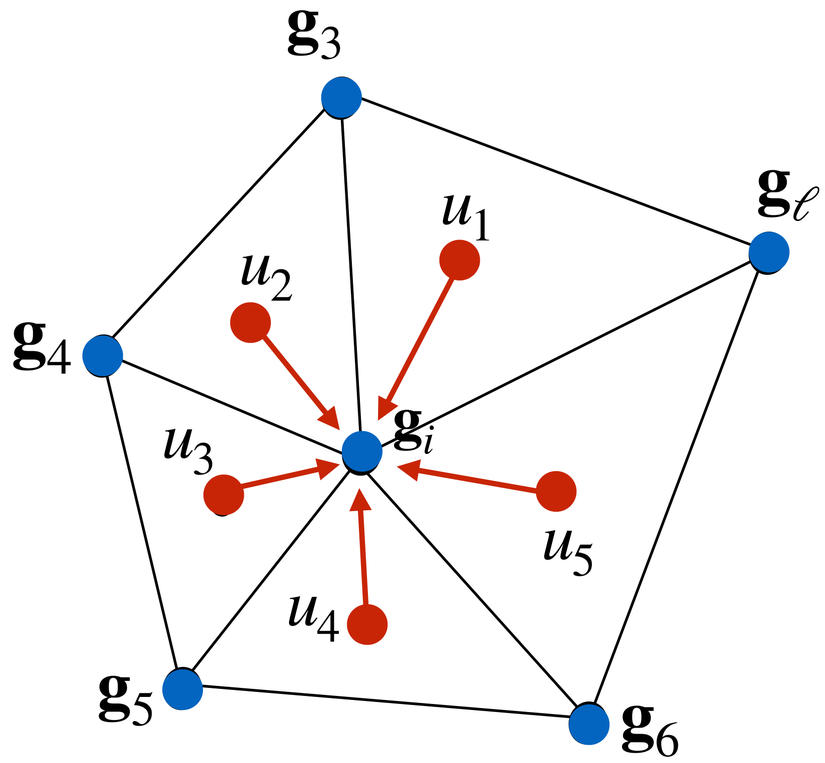
IEBG2 can be directly employed if the solution values can be transferred from cells to nodes.

IEBG2 for NG-CCFV Method

Just interpolate the solution from cells to nodes:

$$u_i = \frac{1}{N_{c_i}} \sum_{j \in \{c_i\}} \left[u_j + \left\{ C\mathbf{g}_i + (1-C)\overline{\mathbf{g}}_j \right\} \cdot (\mathbf{x}_i - \mathbf{x}_j) \right]$$

where C=1/2 for quadratic interpolation, otherwise linear.



Then, IEBG2 can be directly employed:

$$\mathbf{M}_{ii}\mathbf{g}_i + \sum_{\ell \in \{\ell_i\}} \mathbf{M}_{i\ell}\mathbf{g}_\ell = \frac{1}{V_j} \sum_{\ell \in \{\ell_i\}} \frac{u_i + u_\ell}{2} \mathbf{n}_{i\ell}$$

Right hand side depends on the nodal gradients —> Defect correction iteration.

Defect-Correction Iteration

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Define the residual:

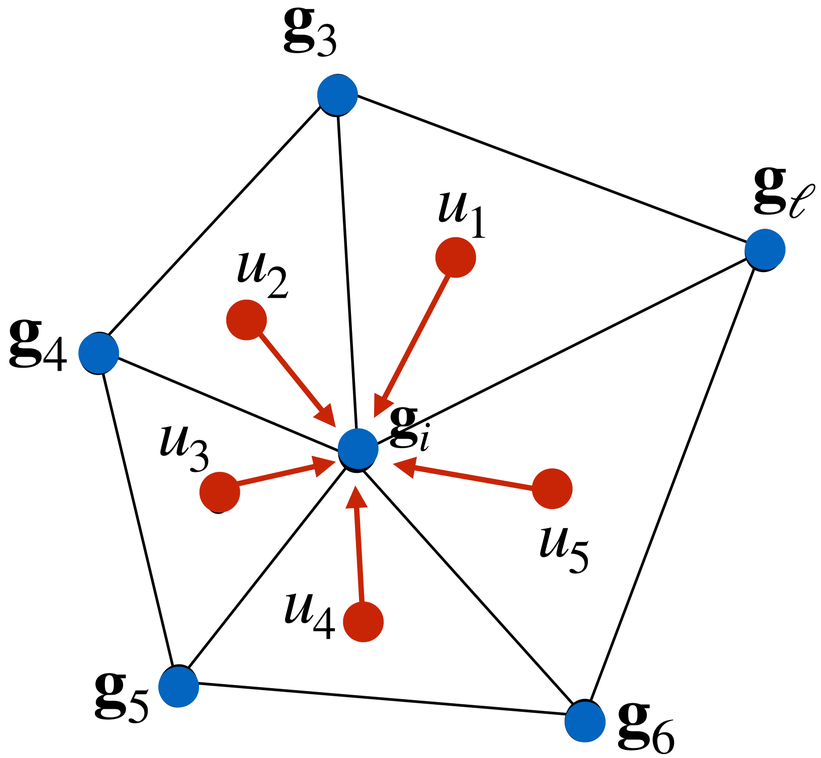
$$\mathbf{r}_i = \mathbf{M}_{ii}\mathbf{g}_i + \sum_{\ell\in\{\ell_i\}} \mathbf{M}_{i\ell}\mathbf{g}_\ell - \frac{1}{V_j}\sum_{\ell\in\{\ell_i\}} \frac{u_i + u_\ell}{2}\mathbf{n}_{i\ell} \qquad u_i = \frac{1}{N_{c_i}}\sum_{j\in\{c_i\}}\left[u_j + \left\{C\mathbf{g}_i + (1-C)\overline{\mathbf{g}}_j\right\}\cdot(\mathbf{x}_i - \mathbf{x}_j)\right]$$

Then, we can solve it by the defect-correction iteration:

$$\mathbf{g}_i^{n+1} = \mathbf{g}_i^n + \Delta\mathbf{g}_i$$

$$\Delta\mathbf{g}_i^{m+1} = \Delta\mathbf{g}_i^m - \mathbf{M}_{ii}^{-1}\left(\sum_{\ell\in\{\ell_i\}} \mathbf{M}_{i\ell}\Delta\mathbf{g}_\ell^m + \mathbf{r}_i\right) \qquad m = 0,1,2,3,4$$

5 preconditioner relaxations (Gauss-Seidel)



This algorithm can be easily implemented if IEBG is already available.

Implicit Solver for Euler

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Starting from the initial values:

$$\mathbf{g}_i^0 = (0,0,0), \quad i = 1,2,3,\cdots,N_{nodes} \qquad \mathbf{w}_j^0 = (\rho_\infty, u_\infty, v_\infty, w_\infty, p_\infty,), \quad j = 1,2,3,\cdots,N_{cells}$$

Then, iterate for $n = 0,1,2,3,\cdots$, until convergence,

Update gradients at all nodes i=1,2,3,…, for all variables: $\mathbf{g} = (\nabla\rho, \nabla u, \nabla v, \nabla w, \nabla p)$

$$\mathbf{g}_i^{n+1} = \mathbf{g}_i^n + \Delta\mathbf{g}_i \qquad \Delta\mathbf{g}_i^{m+1} = \Delta\mathbf{g}_i^m - \mathbf{M}_{ii}^{-1}\left(\sum_{\ell\in\{\ell_i\}} \mathbf{M}_{i\ell}\Delta\mathbf{g}_\ell^m + \mathbf{r}_i\right) \qquad m = 0,1,2,3,4$$

Update solutions:

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta\mathbf{U} \qquad \left(\mathbf{D} + \frac{\partial\overline{\mathbf{Res}}}{\partial\mathbf{U}}\right)\Delta\mathbf{U} = -\mathbf{Res}(\mathbf{U}^n)$$ *<- Relax by GS*

This is a loosely-coupled iteration between gradients and solutions.

Results

Accuracy Verification

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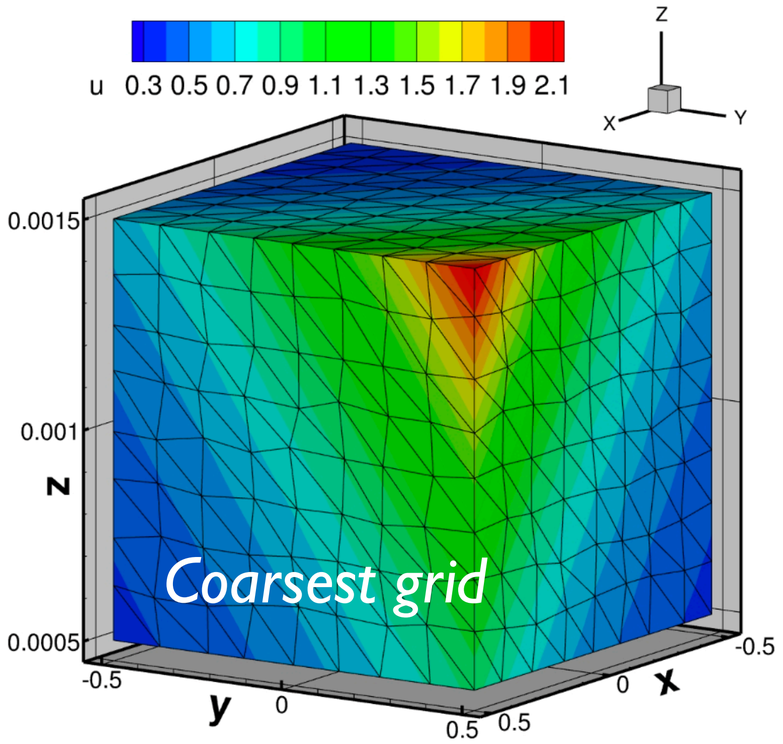
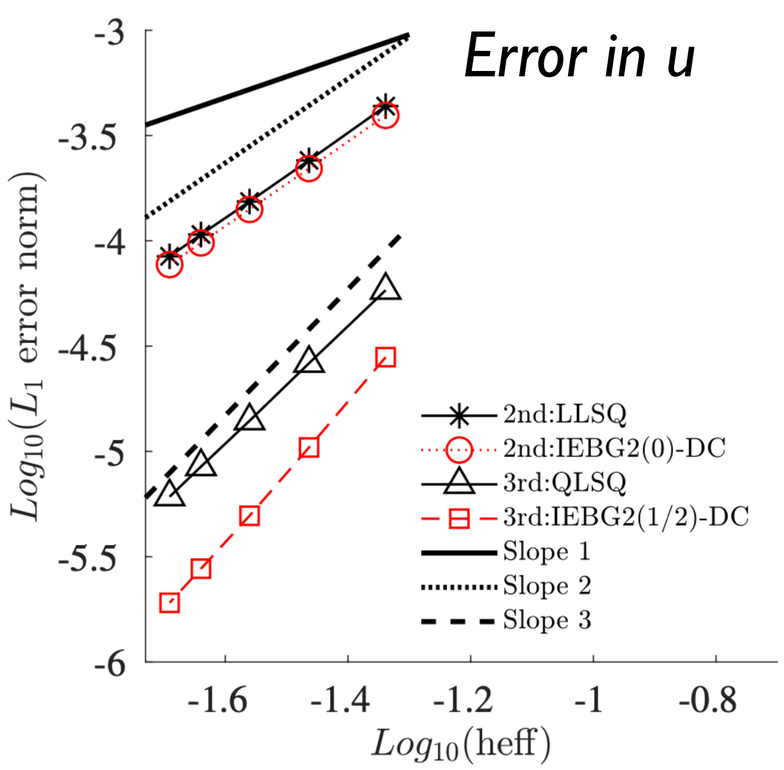
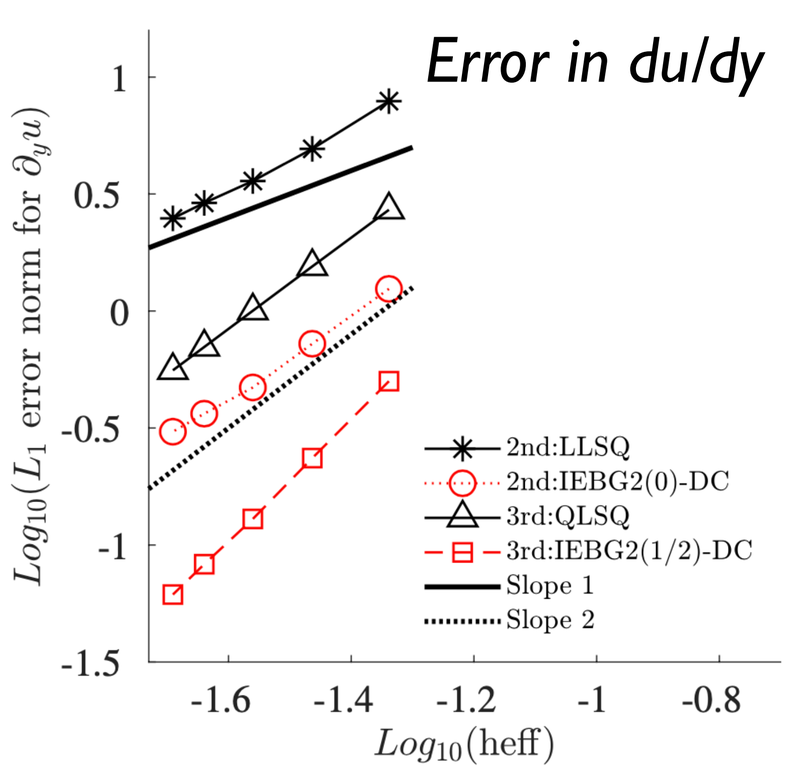
Solve Euler by 2nd- and 3rd-order NG-CCFV methods with LSQ and IEBG2 gradients over 5 levels of grids and measure the solution error, using manufactured solutions.







The solver took twice as many iteration with IEBG2. Not expected but…

Mach 0.3 Subsonic Flow over a smooth bump

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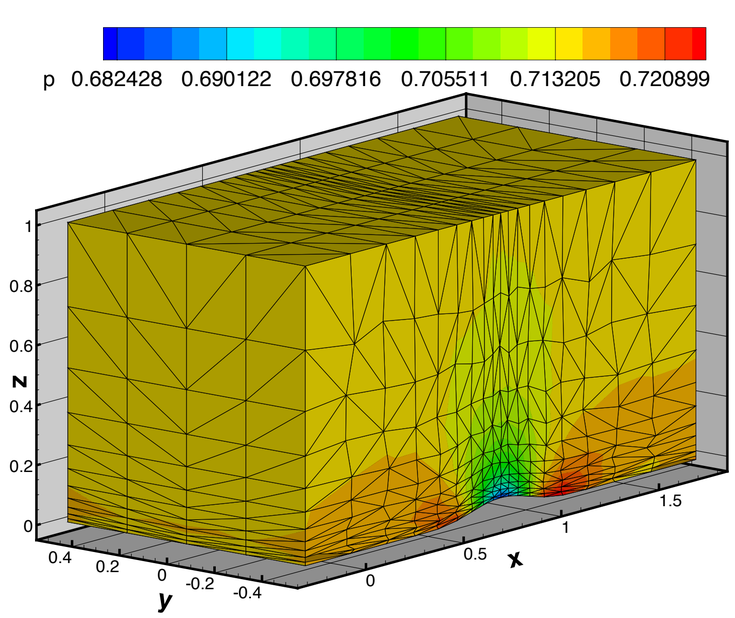
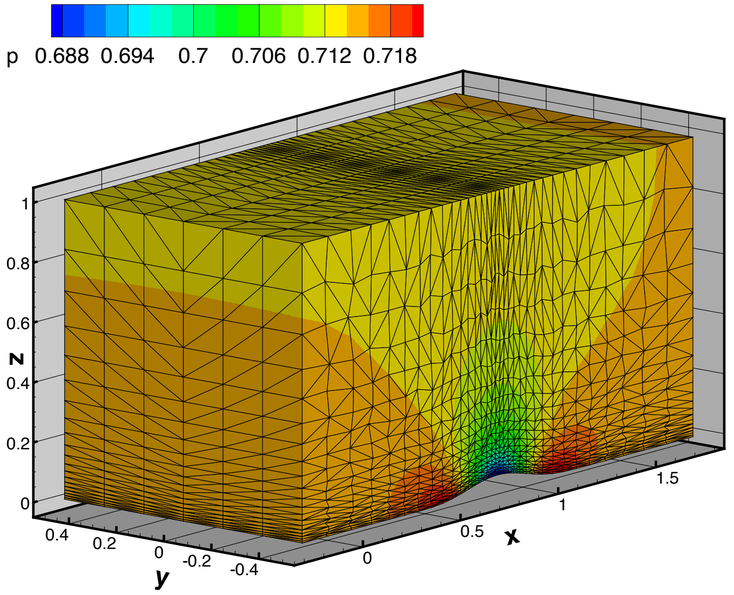
Solve Euler by 2nd- and 3rd-order NG-CCFV methods with LSQ and IEBG2 gradients over 5 levels of grids and measure the spurious entropy error.

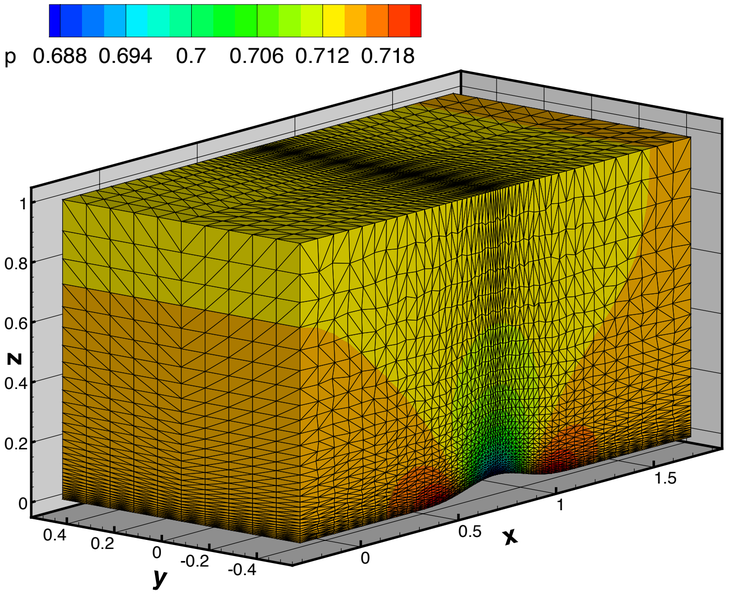
Grid 1



Grid 2



Grid 3



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

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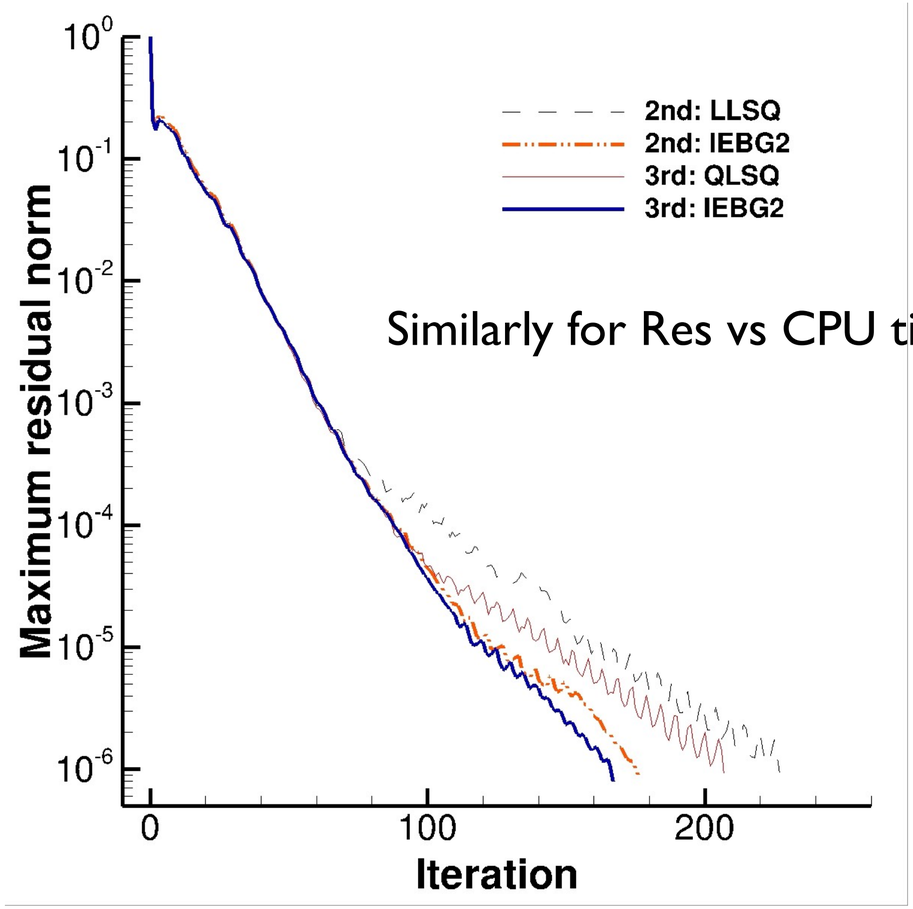
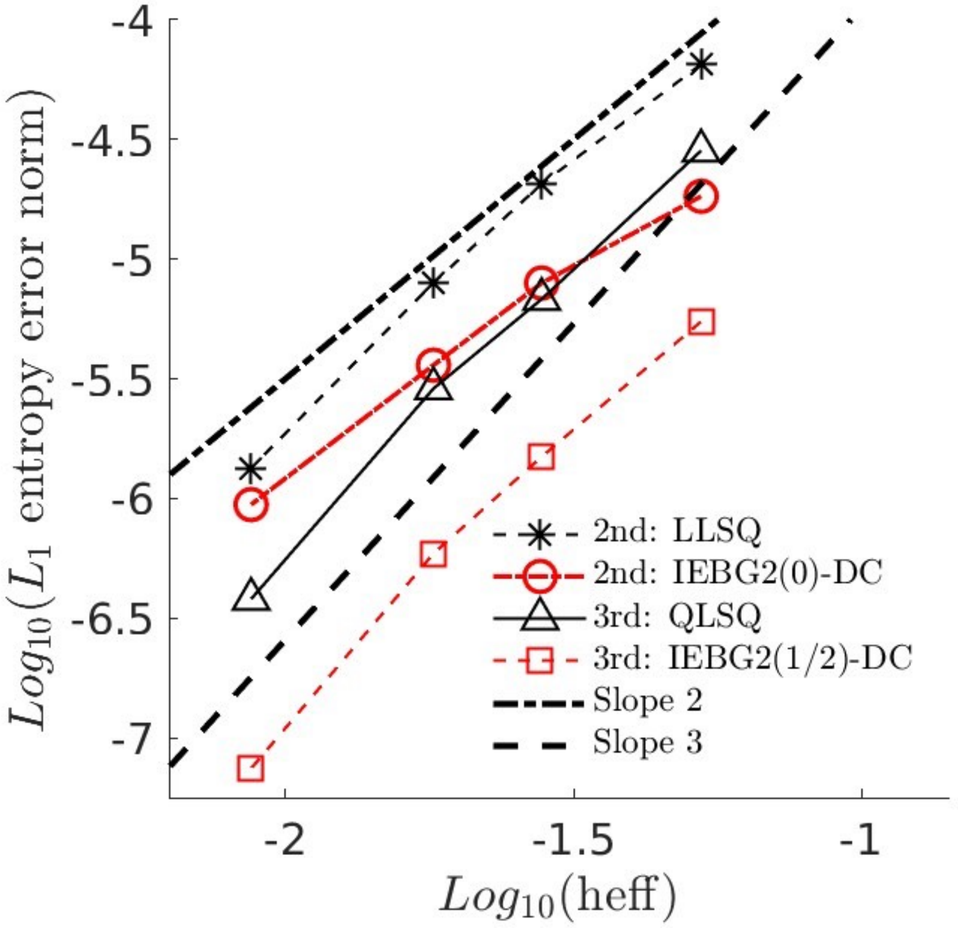
(1) Residual norm vs iteration



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.

Conclusions and Future Work

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Conclusions:

- Developed simple implicit gradient methods for 2nd/3rd-order NG-CCFV methods.
- 3rd-order NG-CCFV method remains 2nd-derivative-free.
- Significantly lower gradient errors by implicit gradient methods.

Future work:

- Compact-stencil version depending only on solutions at cells around a node.
- JFNK solver with gradients added as additional unknowns.
- Further tests needed for more realistic problems with shocks.