Cause and Cure - Deterioration in Accuracy of CFD Simulations with Use of High-Aspect-Ratio Triangular/Tetrahedral Grids

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Outline

- Motivation
- Theoretical Development
- Numerical Results
- Conclusions

Motivation (I)

- High-aspect ratio triangular/tetrahedral elements are generally avoided in the near-wall region by CFD researchers
  - Reduced accuracy of gradients
  - Causes Numerical instability
  - Prismatic/Quadrilateral elements can replace high-aspect ratio tetrahedral/triangular elements in the near-wall region
    - ✦ Mesh generation becomes complicated (compared to generation of pure triangles/tetrahedrons)

- To achieve maximal accuracy, efficiency and robustness, triangular/tetrahedral elements are mandatory grid building blocks for the space-time conservation and solution element (CESE) method

Motivation (II)

With requirements of the CESE method in mind,

Primary Objective:

Develop a rigorous mathematical framework that identifies the reason behind the difficulties in use of high-aspect ratio triangular/tetrahedral mesh elements and thereby, help overcome the difficulty.

Key Outcomes

- Accuracy deterioration of gradient computations involving triangular elements is tied to the elements shape factor

$$\gamma \stackrel{\text{def}}{=} \sin^2\alpha_1 + \sin^2\alpha_2 + \sin^2\alpha_3$$

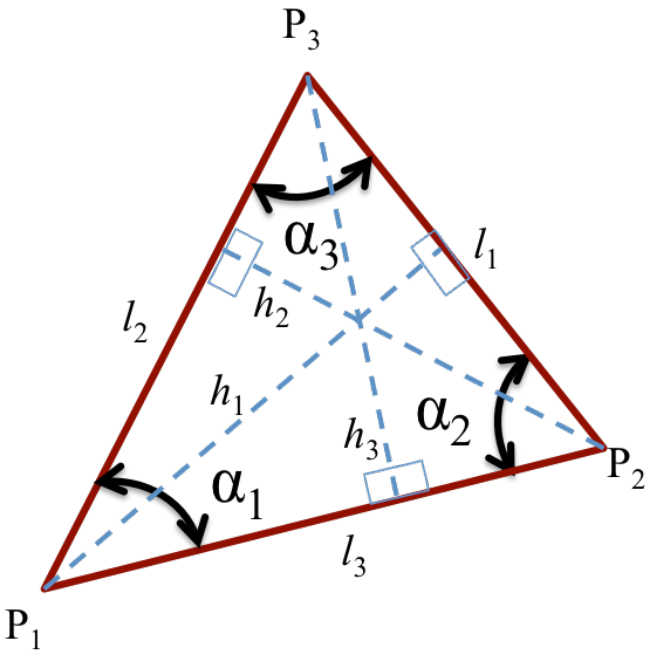
$$\alpha_1, \alpha_2 \text{ and } \alpha_3 = \text{ internal angles of the element}$$

- Degree of accuracy deterioration in gradient computation increases monotonically as the value of γ decreases monotonically from its maximal value of 9/4 (attained only by an equilateral triangle) to its minimal limit value of 0^+ (approached only a high obtuse triangle)

- Independent of its aspect ratio, the shape factor of right-angled triangle has a value of 2, very close to the maximal value of 9/4. Hence a grid built from high-aspect ratio right-angled triangles is much better for accurate computations of gradients than that built from high-aspect-rato and highly obtuse triangles

- Preliminary extensions to 3D

Aspect Ratio of Triangle (I)



Area $A(\Delta P_1 P_2 P_3) > 0$

For each $k = 1, 2, 3$

$\alpha_k =$ Internal angle associated with vertex P_k

$l_k =$ Length of the side facing vertex P_k

$h_k =$ Length of the altitude originating from vertex P_k

$$\pi > \alpha_1, \alpha_2, \alpha_3 > 0 \text{ and } \alpha_1 + \alpha_2 + \alpha_3 = \pi$$

$$l_k > 0, \quad h_k > 0, \text{ and } A = \frac{1}{2} l_k . h_k > 0, \quad k = 1, 2, 3$$

Aspect ratio = maximum ratio of edge length to the altitude associated with it

$$\eta \overset{\text{def}}{=} \max\left\{\frac{l_1}{h_1}, \frac{l_2}{h_2}, \frac{l_3}{h_3}\right\} > 0$$

- It can also be shown that, the largest side is always associated with the shortest altitude
- This definition is also applicable to highly obtuse triangles (usual definition of aspect ratio being ratio of lengths of longest and shortest side doesn't work for such triangles)

Aspect Ratio of Triangle (II)

$$\text{(i) } \eta \geq \eta_{min} \stackrel{\text{def}}{=} \frac{2}{\sqrt{3}}$$

$$\text{(ii) } \eta = \eta_{min} \text{ if and only if } \alpha_1 = \alpha_2 = \alpha_3 = \frac{\pi}{3}$$

$$\text{(iii) } \lim_{\min(\alpha_1,\alpha_2,\alpha_3)\to 0^+} \eta = +\infty$$

$$\text{and (iv) } \eta \gg 1 \quad \text{if and only if} \quad \min\{\alpha_1, \alpha_2, \alpha_3\} \ll 1$$

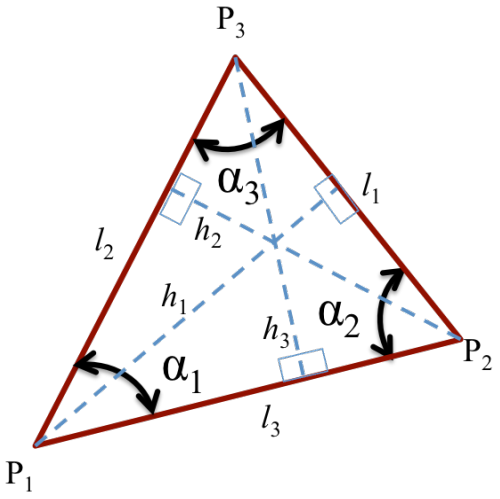
Aspect ratio η

- Attains its minimal value when the triangle is equilateral
- Attains a large value when one of the internal angles of the triangle has a very small value

Shape Factor of a Triangle

Shape factor, γ, of a triangle is defined as

$$\gamma \overset{\text{def}}{=} \sin^2\alpha_1 + \sin^2\alpha_2 + \sin^2\alpha_3$$



It can be shown that:

(i) $0 < \gamma \leq \dfrac{9}{4}$

(ii) $\gamma = \gamma_{max} \overset{\text{def}}{=} \dfrac{9}{4} \Leftrightarrow \alpha_1 = \alpha_2 = \alpha_3 = \dfrac{\pi}{3} \Leftrightarrow l_1 = l_2 = l_3 > 0$

(iii) $\gamma \to 0^+ \Leftrightarrow \max\{\alpha_1, \alpha_2, \alpha_3\} \to \pi^- \Leftrightarrow \min\{\alpha_1, \alpha_2, \alpha_3\} \to 0^+ \Rightarrow \eta \to +\infty$

and (iv) if one of $\{\alpha_1, \alpha_2, \alpha_3\} = \dfrac{\pi}{2} \Rightarrow \gamma = 2$ (even if one of $\{\alpha_1, \alpha_2, \alpha_3\} \ll 1$ and thus $\eta \gg 1$)

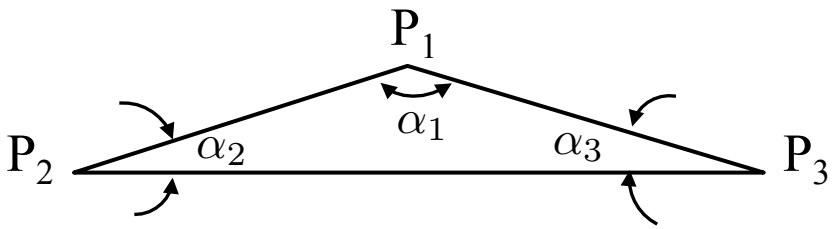
Note:

$\Leftrightarrow$ means "if and only if"

$\Rightarrow$ means "implies that"

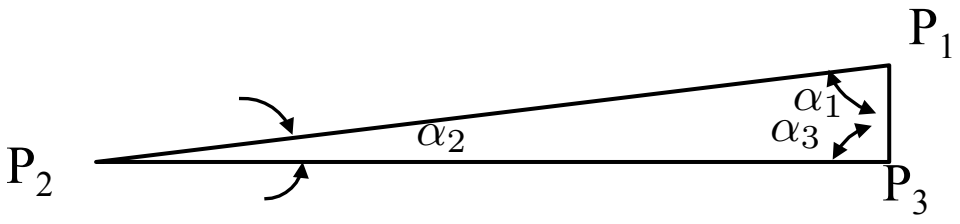
- Shape factor of a high aspect ratio right-angled triangle ($\gamma = 2$) not far from that of an equilateral triangle (γ =9//4)

Aspect Ratio and Shape Factor of a Triangle



$0 < \pi - \alpha_1 \ll 1$ and $0 < \alpha_2, \alpha_3 \ll 1$

(a) $\eta \gg 1$ and $\gamma \ll 1$

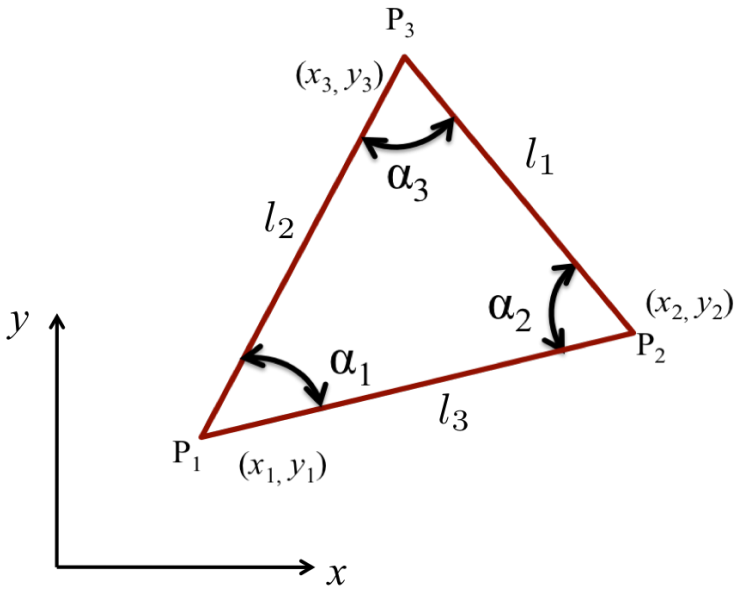


$\alpha_1 \approx \alpha_3 \approx \pi/2$ and $0 < \alpha_2 \ll 1$

(b) $\eta \gg 1$ and $\gamma \approx 2$

- Both triangles shown above have high aspect ratios (η), because one of their internal angles is very small (<< 1)
  - But their shape factors (γ) are vastly different
- Because the value of α_1 is close to π and therefore $\alpha_2, \alpha_3 \ll 1$, the triangle depicted in left (a) has a high aspect ratio, and is also highly obtuse and thus has a very small value of shape factor
  - Accuracy of gradient computation from this triangle will be poor in comparison to the one from right (b)

Gradient Vector and Directional Derivatives

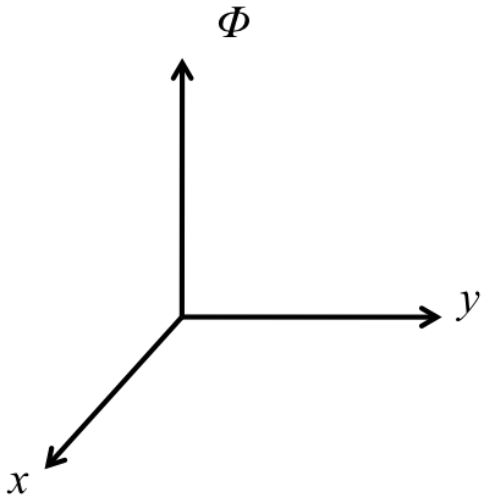


$$A(\Delta P_1 P_2 P_3) = |\delta|/2 > 0$$

where,

$$\delta \overset{\text{def}}{=} \begin{vmatrix} x_2 - x_1 & y_2 - y_1 \\ x_3 - x_1 & y_3 - y_1 \end{vmatrix}$$

$$= (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1) \neq 0$$



For each $k = 1, 2, 3$, let
(i) ϕ_k be a scalar value assigned to the spatial point P_k, and
(ii) $\hat{P}_k$ denote a point in the $x - y - \phi$ space with coordinates (x_k, y_k, ϕ_k).

It can be shown that points $\hat{P}_1, \hat{P}_2,$ and $\hat{P}_3$ lie on the plane in the $x - y - \phi$ space defined by

$$\phi = ax + by + c$$

where,

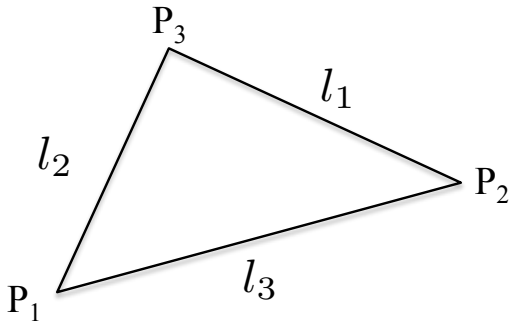
$$a = \frac{\begin{vmatrix} \phi_2 - \phi_1 & y_2 - y_1 \\ \phi_3 - \phi_1 & y_3 - y_1 \end{vmatrix}}{\delta}, \quad b = \frac{\begin{vmatrix} x_2 - x_1 & \phi_2 - \phi_1 \\ x_3 - x_1 & \phi_3 - \phi_1 \end{vmatrix}}{\delta}, \text{ and } \quad c = \frac{\begin{vmatrix} x_1 & y_1 & \phi_1 \\ x_2 & y_2 & \phi_2 \\ x_3 & y_3 & \phi_3 \end{vmatrix}}{\delta}$$

Thus the $x-$ and $y-$ components of $\vec{\nabla}\phi$ on the plane Γ are $\nu_x \overset{\text{def}}{=} \frac{\partial \phi}{\partial x} = a$ and $\nu_y \overset{\text{def}}{=} \frac{\partial \phi}{\partial y} = b \quad (\text{on } \Gamma)$ respectively.

Gradient Vector and Directional Derivatives (III)

Given any two vertices P_i and P_j, the directional derivative $\mu_{i,j}$ along $\overrightarrow{P_{k_1}P_{k_2}}$ is defined by

$$\mu_{i,j} \overset{\text{def}}{=} \frac{\phi_j - \phi_i}{s_{i,j}},\ i \neq j \text{ and } i,j = 1,2,3$$



where,

$$s_{i,j} \overset{\text{def}}{=} \left|\overrightarrow{P_iP_j}\right| = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2} > 0,\ i \neq j \text{ and } i,j = 1,2,3$$

we have

$$l_1 = s_{2,3} = s_{3,2},\ l_2 = s_{3,1} = s_{1,3} \text{ and } l_3 = s_{1,2} = s_{2,1}$$

and

$$-\mu_{2,1} = \mu_{1,2} = \frac{\phi_2 - \phi_1}{l_3},\ -\mu_{3,2} = \mu_{2,3} = \frac{\phi_3 - \phi_2}{l_1} \text{ and } -\mu_{1,3} = \mu_{3,1} = \frac{\phi_1 - \phi_3}{l_2}$$

Gradient Vector and Directional Derivatives (IV)

From earlier equations, we have

$$l_3 \cdot \mu_{1,2} + l_1 \cdot \mu_{2,3} + l_2 \cdot \mu_{3,1} = 0$$

and

$$\mu_{2,1} + \mu_{1,2} = \mu_{3,2} + \mu_{2,3} = \mu_{1,3} + \mu_{3,1} = 0$$

- Six directional derivatives of ϕ are linked by four independent conditions
- Any one of them can be determined in terms of any two independent directional derivatives associated with two different sides of $\Delta P_1 P_2 P_3$

(i) For each $k = 1, 2, 3$, let $\Delta\phi_k$ denote the variation (or numerical error) of ϕ_k at some given time level introduced through a time-marching procedure.

(ii) Let $\Delta\nu_x$ and $\Delta\nu_y$ denote the variations of ν_x and ν_y ($x-$ and $y-$ components of $\vec{\nabla}\phi$) induced by the presence of $\Delta\phi_k$, $k = 1, 2, 3$.

$$\Delta\nu_x = \frac{\begin{vmatrix} \Delta\phi_2 - \Delta\phi_1 & y_2 - y_1 \\ \Delta\phi_3 - \Delta\phi_1 & y_3 - y_1 \end{vmatrix}}{\delta} \quad \text{and} \quad \Delta\nu_y = \frac{\begin{vmatrix} x_2 - x_1 & \Delta\phi_2 - \Delta\phi_1 \\ x_3 - x_1 & \Delta\phi_3 - \Delta\phi_1 \end{vmatrix}}{\delta}$$

(iii) For any pair of i and j with $i \neq j$ and $i, j = 1, 2, 3$, let $\Delta\mu_{i,j}$ denote the error of $\mu_{i,j}$ induced by the presence of $\Delta\phi_i$ and $\Delta\phi_j$, respectively.

Then,

$$-\Delta\mu_{j,i} = \Delta\mu_{i,j} = \frac{\Delta\phi_j - \Delta\phi_i}{s_{i,j}}$$

$$l_3 \cdot \Delta\mu_{1,2} + l_1 \cdot \Delta\mu_{2,3} + l_2 \cdot \Delta\mu_{3,1} = 0$$

and

$$\Delta\mu_{2,1} + \Delta\mu_{1,2} = \Delta\mu_{3,2} + \Delta\mu_{2,3} = \Delta\mu_{1,3} + \Delta\mu_{3,1} = 0$$

Gradient Vector and Directional Derivatives (VI)

Let,

$$\epsilon_1 \overset{\text{def}}{=} \Delta\mu_{2,3},\ \epsilon_2 \overset{\text{def}}{=} \Delta\mu_{3,1} \text{ and } \epsilon_3 \overset{\text{def}}{=} \Delta\mu_{1,2}$$

Then, it can be shown that:

(i) $l_1 \cdot \epsilon_1 + l_2 \cdot \epsilon_2 + l_3 \cdot \epsilon_3 = 0$

and

(ii) For any pair of i and j with $i \neq j$ and $i, j = 1, 2, 3$, $\Delta\mu_{i,j}$ can be uniquely determined in terms of any two of $\epsilon_1, \epsilon_2, \epsilon_3$ assuming (x_k, y_k), $k = 1, 2, 3$ are given.

Moreover, with the use of law of sines,

$(\sin\alpha_1)\,\epsilon_1 + (\sin\alpha_2)\,\epsilon_2 + (\sin\alpha_3)\,\epsilon_3 = 0$

The above equation links the errors ϵ_1, ϵ_2 and ϵ_3 of the directional derivatives evaluated along the three sides of $\Delta P_1 P_2 P_3$

Error Amplification Factor (I)

Let

$$R \stackrel{\text{def}}{=} \sqrt{\frac{[(\Delta\nu_x)^2 + (\Delta\nu_y)^2]/2}{[(\epsilon_1)^2 + (\epsilon_2)^2 + (\epsilon_3)^2]/3}} \geq 0 \qquad [(\epsilon_1)^2 + (\epsilon_2)^2 + (\epsilon_3)^2 \neq 0]$$

(i) By definition, R is square root of the ratio of the two simple averages, i.e., the simple average of $(\Delta\nu_x)^2$ and $(\Delta\nu_y)^2$, and that of $(\epsilon_1)^2, (\epsilon_2)^2$ and $(\epsilon_3)^2$

(ii) $\sqrt{[(\Delta\nu_x)^2 + (\Delta\nu_y)^2]/2}$ = error norm associated with evaluation of $\vec{\nabla}\phi$

(iii) $\sqrt{[(\epsilon_1)^2 + (\epsilon_2)^2 + (\epsilon_3)^2]/3}$ = error norm associated with evaluation of directional derivatives along the three sides of $\Delta P_1 P_2 P_3$

(iv)**As such R is an error amplification factor, measuring how large the error norm for evaluating the gradient vector $\vec{\nabla}\phi$ is amplified from that for evaluating the directional derivatives along the three sides of $\Delta P_1 P_2 P_3$**

Error Amplification Factor (II)

(i) The value of R is a function of any two chosen independent parameters (say ϵ_1 and ϵ_2) among ϵ_1, ϵ_2 and ϵ_3.

(ii) $\sqrt{\sigma_-(\gamma)} \leq R \leq \sqrt{\sigma_+(\gamma)}, 0 < \gamma \leq 9/4$

where,

$\sigma_\pm(\gamma) \stackrel{\text{def}}{=} \frac{3}{4\gamma}\left[3 \pm 2\sqrt{(9/4) - \gamma}\right], 0 < \gamma \leq 9/4$

and (iii) **Each of the two bounds $\sqrt{\sigma_-(\gamma)}$ and $\sqrt{\sigma_+(\gamma)}$ can be attained by R with some special ratio between ϵ_1 and ϵ_2.**

Thus $\sqrt{\sigma_-(\gamma)}$ and $\sqrt{\sigma_+(\gamma)}$ are the greatest lower bound and the least upper bound of R, respectively.

Note: γ is the shape factor of $\Delta P_1 P_2 P_3$

Properties of $\sigma_-(\gamma)$ and $\sigma_+(\gamma)$ and Their Implications

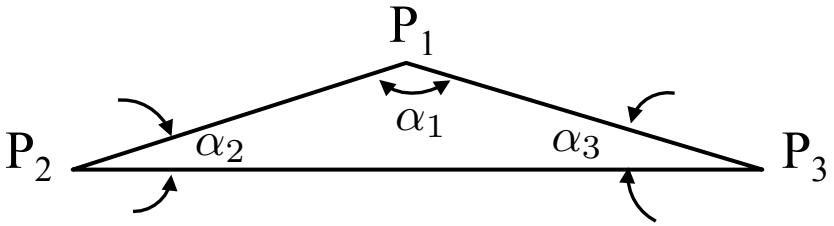
As the value of γ decreases from its maximal value $9/4$ to its minimal limit 0^+,

(i) the value of $\sigma_+(\gamma)$ increases monotonically from 1 to $+\infty$,
and
(ii) the value of $\sigma_-(\gamma)$ decreases monotonically from 1 to $(\frac{1}{2})^+$.

As such one can show that :

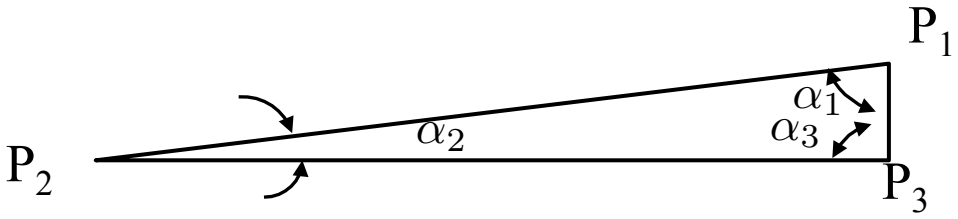
(i) $\sigma_-(\gamma) = 1 \Leftrightarrow \sigma_+(\gamma) = 1 \Leftrightarrow \gamma = \frac{9}{4} \Leftrightarrow \Delta P_1 P_2 P_3$ is equilateral
(ii) $\frac{1}{2} < \sigma_-(\gamma) < 1 < \sigma_+(\gamma), \quad$ if $0 < \gamma < \frac{9}{4}$
(iii) $\sigma_-(\gamma) \to (\frac{1}{2})^+ \Leftrightarrow \sigma_+(\gamma) \to +\infty \Leftrightarrow \gamma \to 0^+ \Leftrightarrow max\{\alpha_1, \alpha_2, \alpha_3\} \to \pi^-$
and
(iv) $\max\{\alpha_1, \alpha_2, \alpha_3\} = \frac{\pi}{2} \Rightarrow \gamma = 2 \Rightarrow \sqrt{\sigma_+(\gamma)} = \sqrt{\frac{3}{2}} \approx 1.225$

Properties of $\sigma_-(\gamma)$ and $\sigma_+(\gamma)$ and Their Implications



$0 < \pi - \alpha_1 \ll 1$ and $0 < \alpha_2, \alpha_3 \ll 1$

(a) $\Delta P_1P_2P_3$ is highly obtuse with $\eta \gg 1$ and $\gamma \ll 1$



$\alpha_1 \approx \alpha_3 \approx \pi/2$ and $0 < \alpha_2 \ll 1$

(b) $\Delta P_1P_2P_3$ is not obtuse with $\eta \gg 1$ and $\gamma \approx 2$

(i) $R = 1$ for any $(\epsilon_1, \epsilon_2, \epsilon_3)$, i.e., no amplification error for gradient computation, if and only if $\Delta P_1P_2P_3$ is equilateral

(ii) A very large error amplification for evaluating $\vec{\nabla}\phi$ could occur if $\Delta P_1P_2P_3$ is highly obtuse

(iii) Only minor error amplification for evaluating $\vec{\nabla}\phi$ would occur if $\Delta P_1P_2P_3$ is nearly a right-angled triangle

Extension to 3D (for tetrahedrons)

- Mathematical framework presented here for triangles can be extended in a straightforward manner for tetrahedral elements.
  - Algebra becomes complicated

- For a regular tetrahedron (i.e., one with all four of its faces being equilateral triangles), it can be shown that $R = 1$ for all possible combinations of the numerical errors associated with the directional derivatives evaluated along all six edge-directions of the tetrahedron
  - No accuracy deterioration in gradient evaluation for a regular tetrahedron

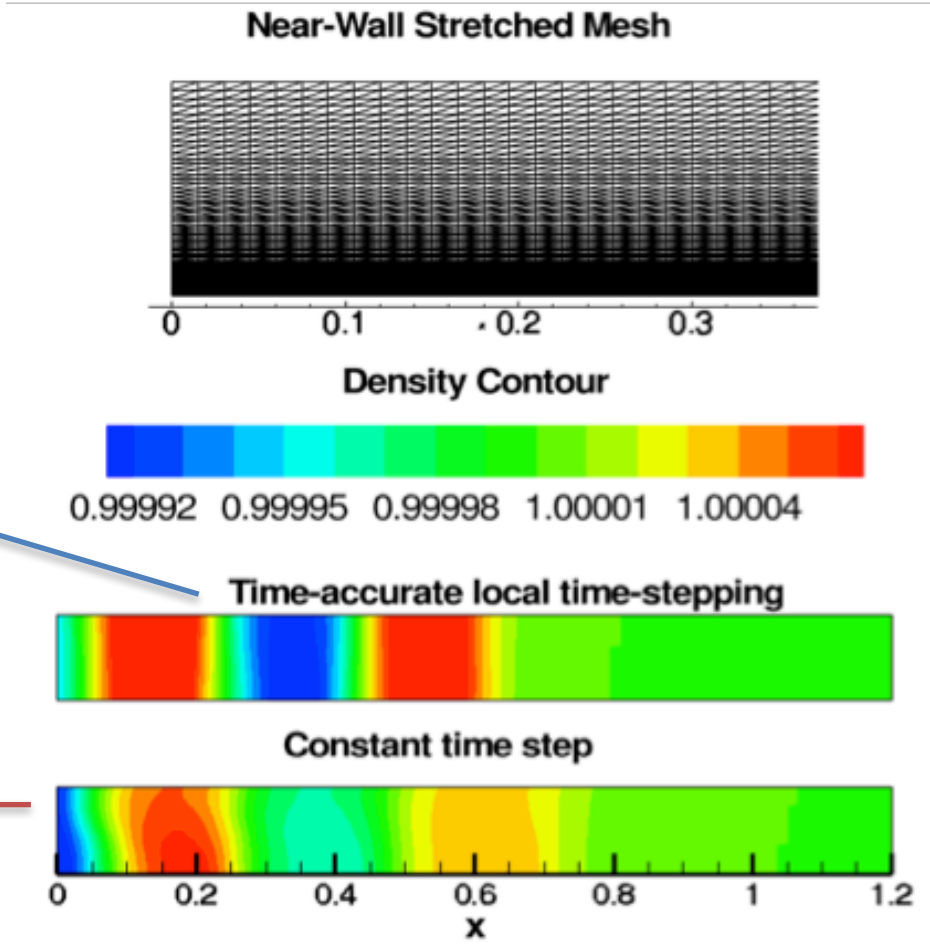
- For a tetrahedron in which three right internal angles share a common vertex, it can be shown that the least upper bound of R is $\sqrt{2}$, a number slightly larger than 1.
  - Mild accuracy deterioration in gradient evaluation

Numerical Results from CESE

Propagation of plane acoustic wave

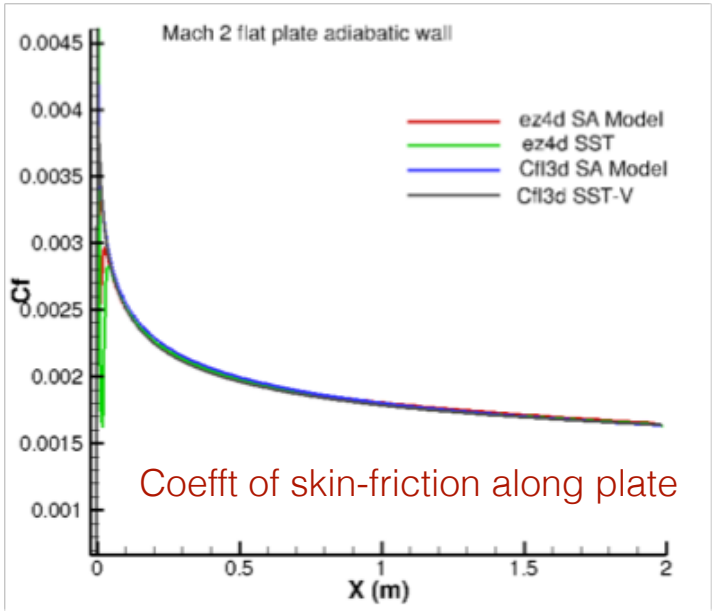
- Acoustic wave sent through a viscous-type mesh with non-uniform spacing
  - Preserving the phase and amplitude of the wave without damping on a non-uniform mesh is challenging
- Largest Aspect-ratio location: bottom of the domain =225
- The time-accurate local time stepping procedures, along with ability to minimize dissipation in CESE helps with this.

No attempt to control dissipation/CFL variation

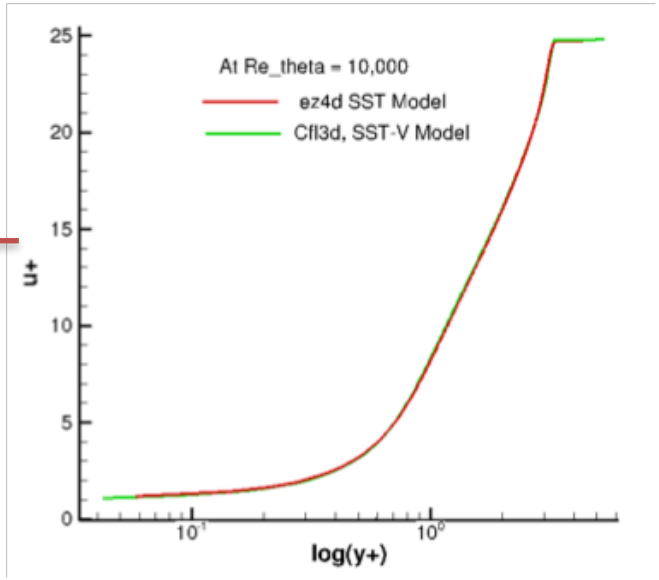


RANS computations of Mach 2 flow over adiabatic flat plate

- Mach 2 freestream, Re =15x10^6, Adiabatic Wall
- Reynolds-Averaged Navier-Stokes (RANS) computations
- Spalart-Allmaras (SA) and Mentor's Shear-stress transport (SST) models
- Triangular Mesh (105,000 elements) with highest aspect ratio of 3000.
- Mesh (the structured mesh was sliced into triangles) and comparison data obtained from NASA Langley turbulence modeling resource website



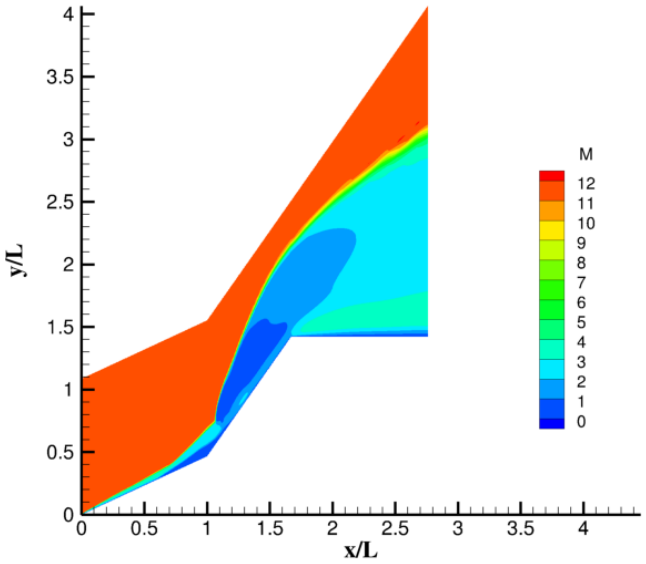
Velocity profile comparison at a location where Re (based on momentum thickness) =10,000

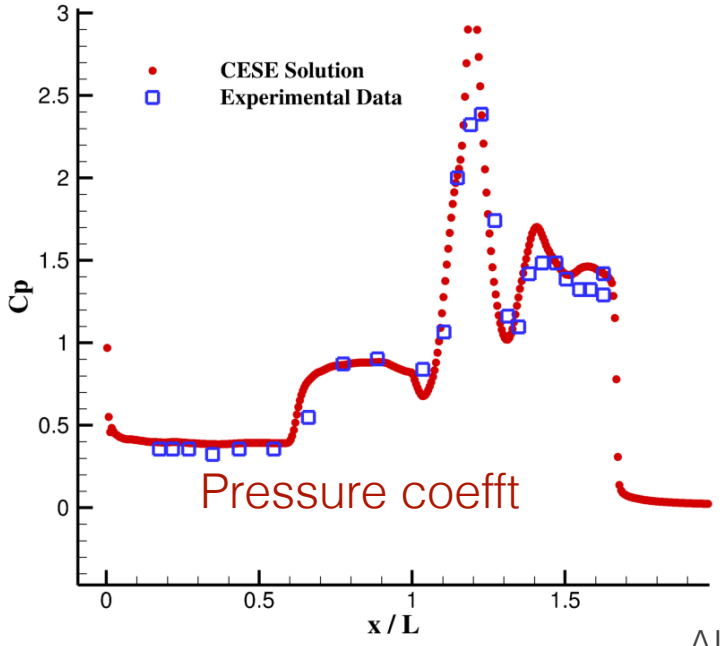


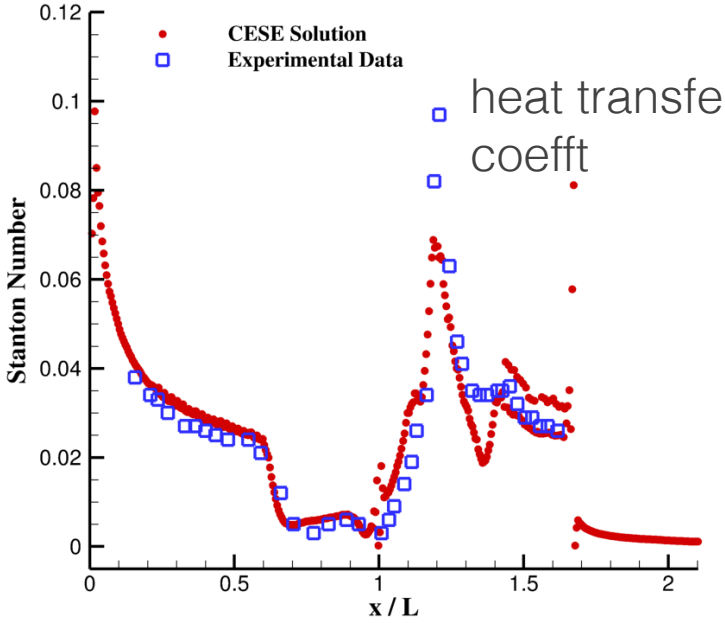
y+ = normalized wall distance = y * u_tau / kinematic viscosity
u + = normalized velocity = u/ u_tau
u_tau = friction velocity = sqrt(Shear stress at wall/density)

Hypersonic flow over a 15° – 25° double cone

- Mach 11.3 Laminar flow
  - CUBRC experiment (Run 35)
- 313,000 Triangular elements, Max aspect ratio: 1400
- Triangular/tetrahedral elements traditionally avoided in hypersonic computations (carbuncle, poor heat-transfer prediction)
- Separation bubbles around the two corners and heat transfer coefft predicted well.
- Small discrepancy in heat transfer peak levels being investigated upon through grid refinement







Summary

- Discussion on fundamental accuracy issues when a mesh with large-aspect -ratio triangular/tetrahedral elements are used in CFD simulations, especially inside the boundary layer.

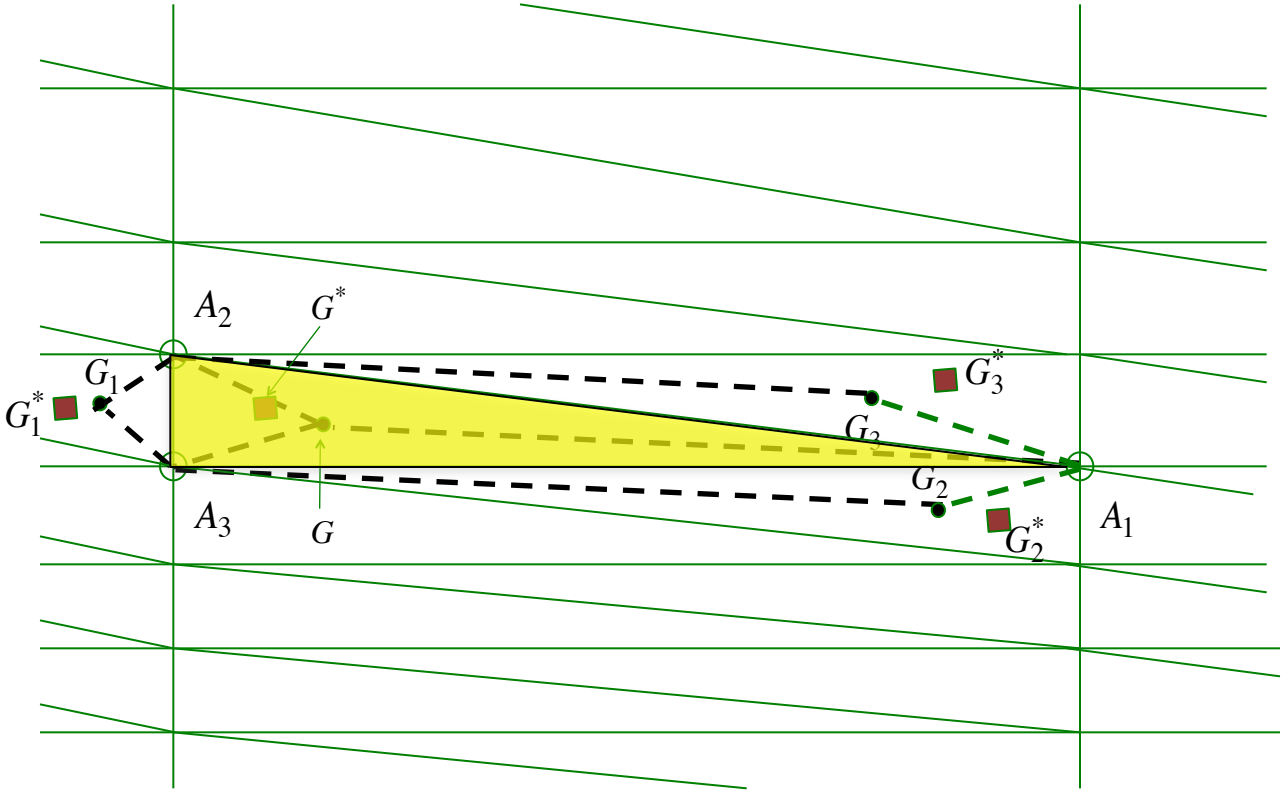
- Sources of inaccuracy related to triangular grids was identified theoretically
  - closely related to the elements shape factor (and not simply aspect ratio)
  - deterioration in accuracy of gradient evaluation can be mitigated by use of right-angle / equilateral triangles for gradient evaluation

- Effectiveness of CESE in handling high-aspect ratio triangular meshes demonstrated through a few viscous flow computations
  - Gradient evaluation procedure take advantage of the analysis shown and utilize triangles with good shape factors for gradient evaluation

- Extension of mathematical framework to tetrahedral elements is in progress.

Backup Slides

Original approach of evaluating derivatives in CESE



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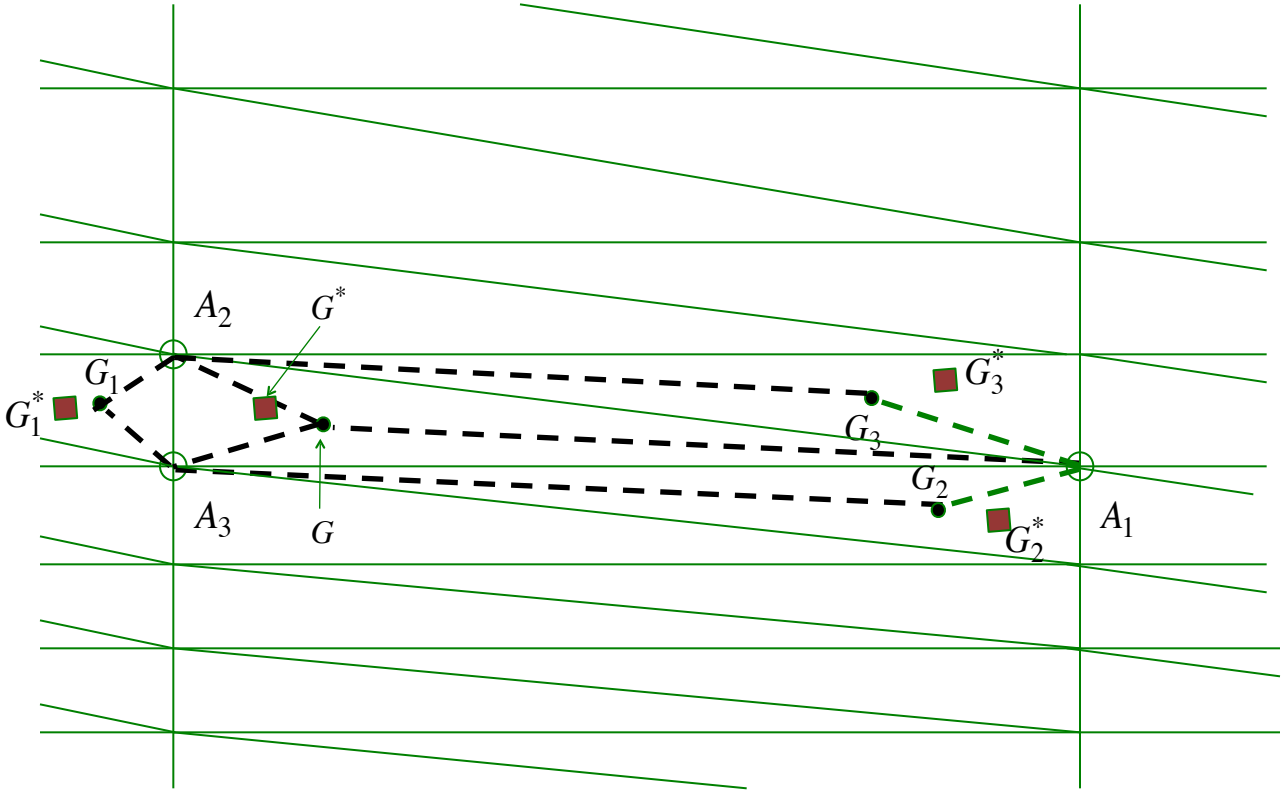
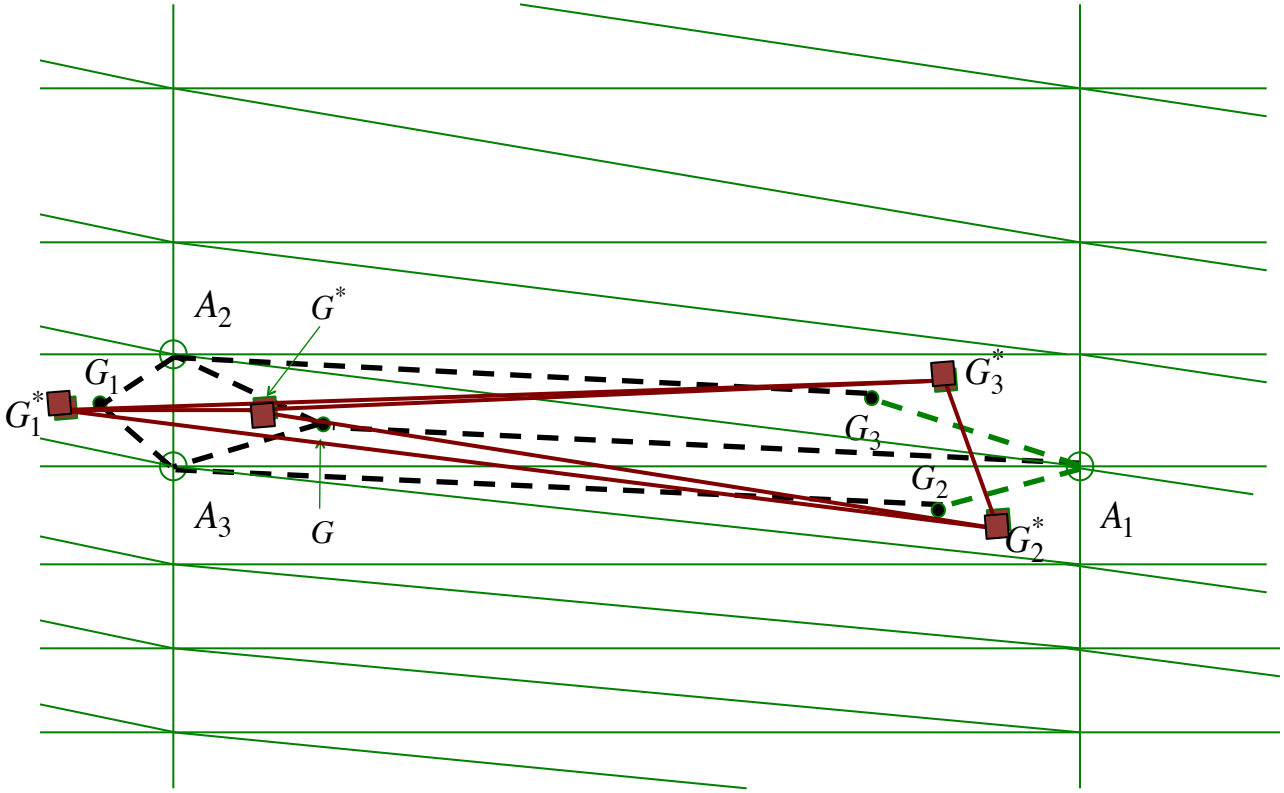
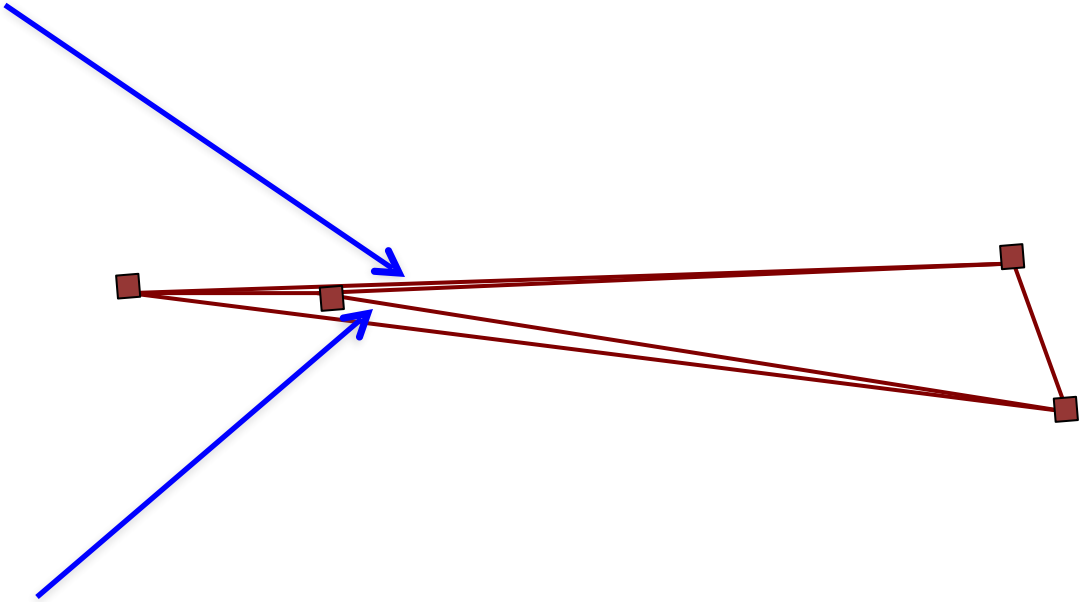


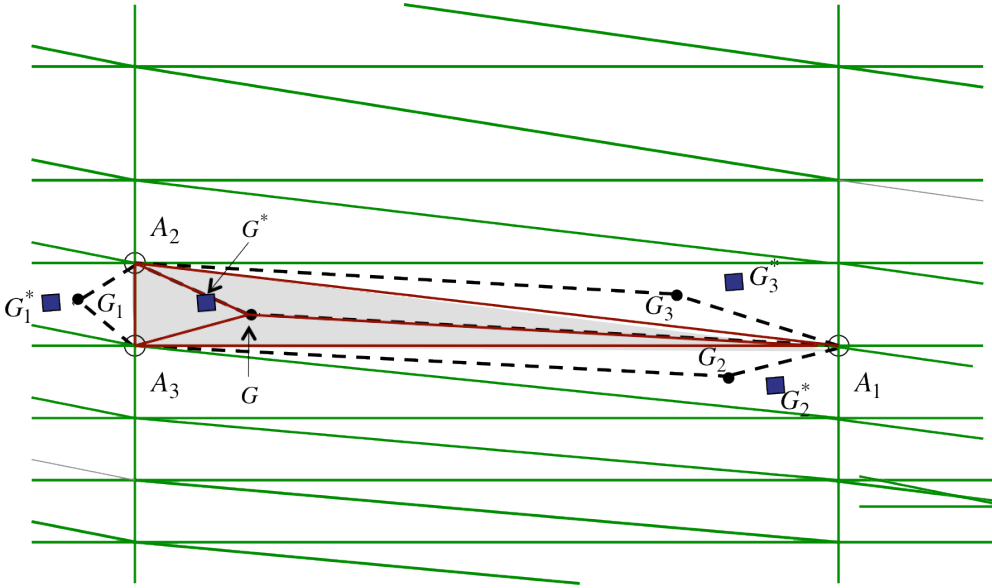
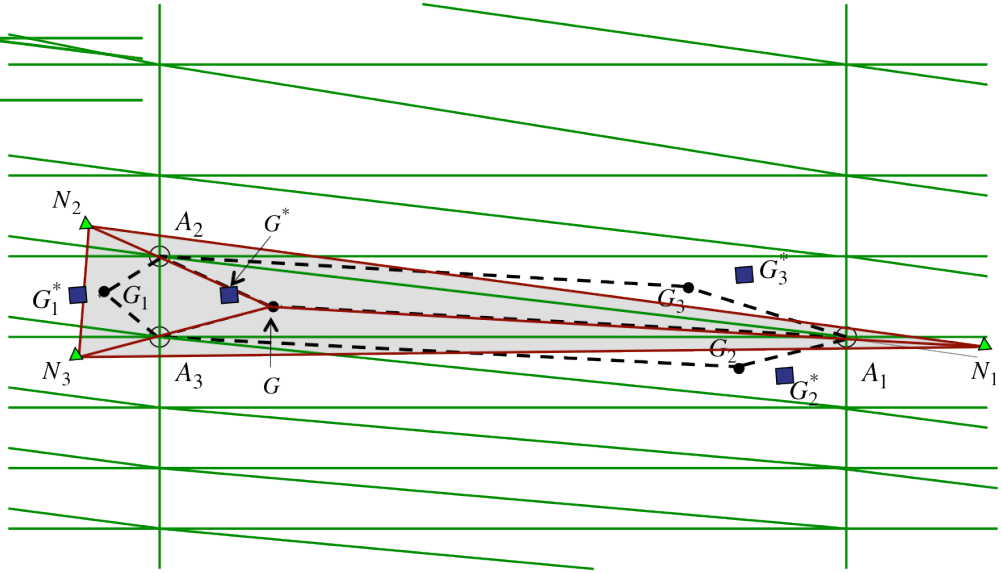
Original approach of evaluating derivatives in CESE



Original approach of evaluating derivatives in CESE

Triangles with bad shape factor that are used in gradient computations



New edge-based derivative approach

Triangles with good shape factors to be used in gradient computations, obtained by adjusting stencil (can also be used to adjust dissipation)