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Gradient and Grid Perturbation

1. Finite Difference Method
2. Complex-Step Method
3. Grid Perturbation

Gradient and Grid Perturbation

Finite Difference Method

- Traditionally finite-difference methods have been used to calculate sensitivities of aerodynamic cost functions.
- The computational cost of the finite-difference method for problems involving large numbers of design variables is both unaffordable and prone to subtractive cancellation error.
- In order to produce an accurate finite-difference gradient, a range of step sizes must be used, and thus the ultimate cost of producing, $\mathcal{N}$ gradient evaluations with the finite-difference method is the product $m\mathcal{N}$, where m is the number of different step sizes used to obtain a converged finite-difference gradient.

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Finite Difference Method

- An estimate of the first derivative of a cost function I using a first order forward difference approximation is as follows:

$$\frac{\partial I}{\partial \alpha_i} = \frac{1}{\partial \alpha_i}\left[I(.....,\alpha_i + \delta\alpha_i, ...) - I(.....,\alpha_i, ...)\right]$$

- $$= \frac{I(\alpha_i + \delta\alpha_i) - I(\alpha_i)}{\delta\alpha_i} + \mathcal{O}(\delta\alpha_i)$$

  where $\delta\alpha_i$ is the perturbation in the design variable.

- A small step size is desired to reduce the truncation error $\mathcal{O}(\delta\alpha_i)$ but a very small step size would also increase subtractive cancellation errors.

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Complex-Step Method

- Lyness and Moler introduced the use of the complex-step in calculating the derivative of an analytical function.
- Instead of using a real step $\delta\alpha_i$ the step size $\delta\alpha_i$ is added to the imaginary part of the cost function. $\delta\alpha_i$ will be represented as h in the following equations.
- A Taylor series expansion of the cost function I yields:

$$I(x+ih) = I(x) + ihI^{'}(x) - h^2 \frac{I^{''}(x)}{2!} - ih^3 \frac{I^{'''}(x)}{3!} + \cdots .$$

- Take the imaginary parts of the above equation and divide by the step size h to produce a second order complex-step approximation to the first derivative:

$$I^{'}(x) = \frac{\mathrm{Im}[\mathrm{I}(\mathrm{x}+ih)]}{h} + h^2 \frac{I^{'''}(x)}{3!} + \cdots .$$

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Complex-Step Method

- The complex step formula does not require any subtraction to yield the approximate derivative.
- The following figure illustrates the complex-step versus the finite-difference gradient errors for the inverse design case for decreasing step sizes.
- At a step size of 10^{-4} the finite-difference and complex-step approximations to the first derivative of the cost function are very similar.
- As the step size is reduced, the finite-difference gradient error starts to increase because of subtractive cancellation errors; however, the complex-step continues to produce more accurate results.
- Therefore, the complex-step is more robust and does not require repeated calculations in order to produce an accurate gradient.
- If a very small step size is chosen, the gradient is calculated only once per design variable. Due to the use of double precision complex numbers, the code requires three times the wall clock time when compared to the finite-difference method.
- But the benefits of using the complex-step to acquire accurate gradients outweighs its disadvantages.

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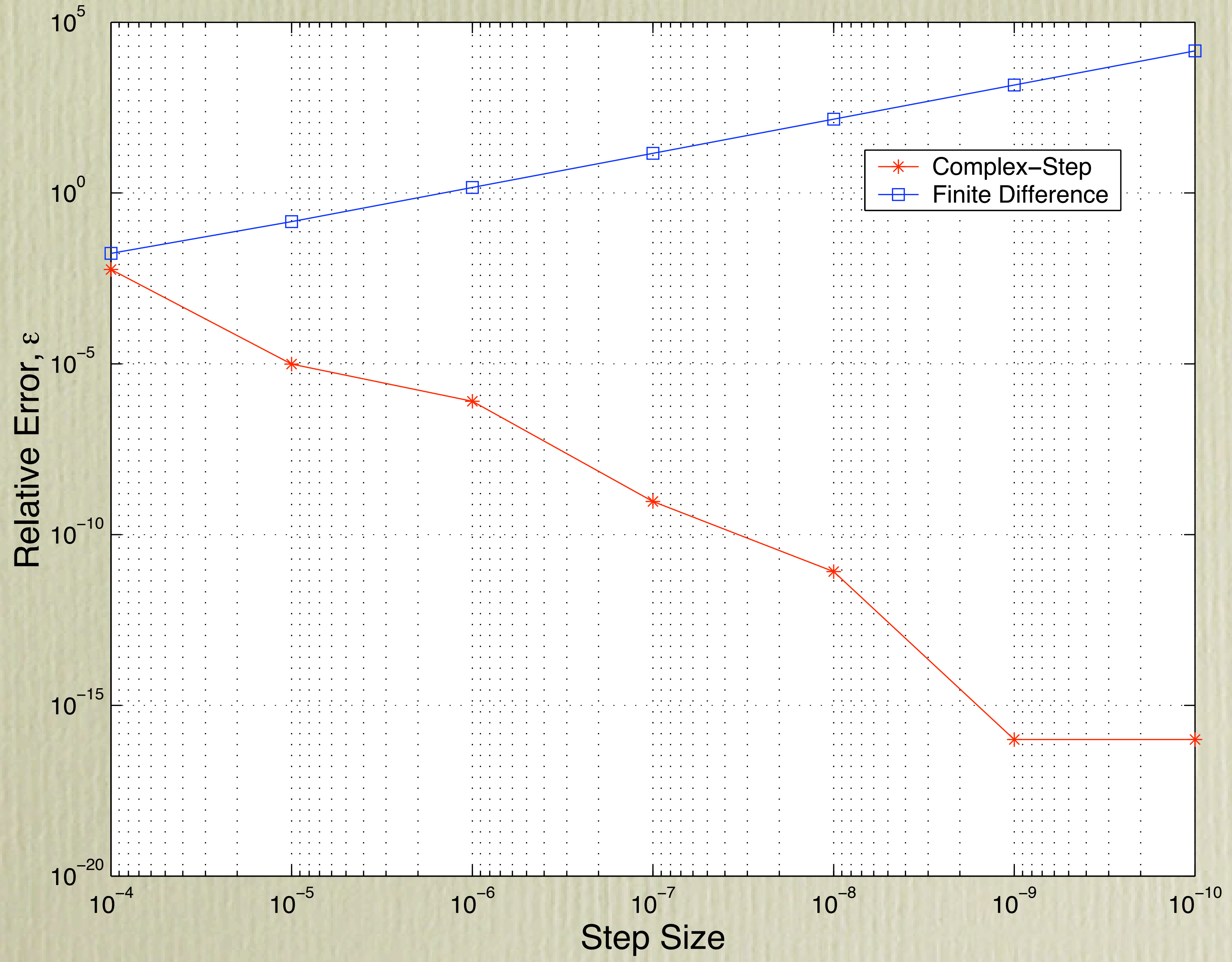
Complex-Step Method

Complex-Step Versus Finite Difference Gradient Errors for an Inverse Design Case



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Grid Perturbation

- The variation of the cost function written as a function of the variation of the state vector, δw, grid point location, $\delta \mathcal{X}$, and surface, $\delta \mathcal{F}$, can be expressed as:

$$\delta I = \frac{\partial I^T}{\partial w}\delta w + \frac{\partial I^T}{\partial \mathcal{X}}\delta \mathcal{X} + \frac{\partial I^T}{\partial \mathcal{F}}\delta \mathcal{F}$$

- The solution of the adjoint equation removes the dependence of the gradient on the flow solution, so that only the variations of the grid point locations and the variation of the surface shape remain.
- The variation of the surface shape, $\delta \mathcal{F}$, only introduces surface integrals into the equation that computes the gradient.
- Therefore, the computational cost is negligible even for complex three-dimensional geometries.
- However, the variations of the grid point locations, $\delta \mathcal{X}$, introduce volume integrals into the gradient computation.

Grid Perturbation

- In order to compute this contribution, regeneration of the grid is required based on perturbations on the surface.
- The grid regeneration is needed for every surface perturbation.
- This procedure can be costly if the geometry is three-dimensional and complex, and would have to be repeated a number of times proportional to the number of design variables.
- Jameson} introduced a grid perturbation method that modifies the current location of the grid points based on perturbations at the geometry surface.
- The approach is not dependent on the type of structured grid generation used.
- The method modifies, the grid points along each grid index line projecting from the surface.
- The arc length between the surface point and the far-field point along the grid line is first computed.

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Grid Perturbation

- Then the grid points at each location along the grid line is attenuated proportional to its arc length distance from the surface point and the total arc length between the surface and the far-field.
- The algorithm can be described as:

$$x_{i,j}^{new} = x_{i,j}^{old} + C_j \left(x_{i,1}^{new} - x_{i,1}^{old}\right)$$

$$y_{i,j}^{new} = y_{i,j}^{old} + C_j \left(y_{i,1}^{new} - y_{i,1}^{old}\right) \qquad \text{,for } \; i = I, j = 2, \ldots.., j_{max}$$

,where I is the current grid index.

- The vector C_j can be defined as follows

$$C_j = 1 - (3 - 2\mathcal{N}_j)\,\mathcal{N}_j^2,$$

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Grid Perturbation

- $\mathcal{N}$ is the ratio of the arc length from the surface to the current grid point and the total arc length from the surface to the far-field along the grid line as
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- $$\mathcal{N}_j = \frac{\sum_{l=2}^{j} \sqrt{\left(x_{i,l} - x_{i,l-1}\right)^2 + \left(y_{i,l} - y_{i,l-1}\right)^2}}{\sum_{l=2}^{j_{max}} \sqrt{\left(x_{i,l} - x_{i,l-1}\right)^2 + \left(y_{i,l} - y_{i,l-1}\right)^2}}.$$
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- From equation to update the grid point location from the previous slide the variation of the grid point location can be expressed as a function of the variation of the surface points as

$$\delta\mathcal{X} = C_j \delta\mathcal{F}.$$

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- This allows the variation of the grid point location in the equation for gradient evaluation, to be substituted with the variation of the surface points.
- The variations, $\delta\mathcal{X}$, and, $\delta\mathcal{F}$, are both absorbed into the metric variations, δS_{ij}

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Grid Perturbation

- This simple grid perturbation scheme has been found to be very robust.
- The grid perturbation method is successful in producing smooth meshes without grid point cross-overs, even in regions of high nonlinearity with large surface perturbations.
- The grid perturbation method described in this section is ideal for structured meshes, however, the complexity increases with unstructured meshes.
- The simplicity in the method is in the effortlessness in producing new grid point locations along the grid line.
- In the unstructured case, the lack of a continuous grid line extending from the surface to the far-field, removes the efficient property of the grid perturbation method.
- An alternative, would be not to dampen the grid modification along the grid line but to dampen the changes within a specified bubble around the surface node.

Grid Perturbation

- The nodes in the unstructured mesh can be shifted based upon their distance from the surface point.
- Possible alternatives to the grid perturbation scheme have yet to be researched and would be an ideal future work topic.