0.1 Introduction and Background

0.1.1 Understanding and Mitigating Numerical Error in Scientific Computing

Numerical errors are a common issue in scientific computing, where mathematical calculations are performed using digital computers with finite precision. Two main types of numerical errors are floating-point error and truncation error. Floating-point error occurs due to the limited number of digits that can be represented in floating-point arithmetic. Calculations involving very large or small numbers or those requiring a large number of decimal places may result in inaccuracies due to rounding or truncation of digits. Truncation error arises when an approximation is made in place of an exact mathematical operation, such as an infinite sum or an integral. For instance, when using numerical methods to solve differential equations, the equations are usually approximated in discrete time steps, leading to a truncation error that can accumulate over time.

Truncation error can lead to numerical dispersion and dissipation in some methods such as finite difference methods. Numerical dispersion is the amplification of high-frequency content in a signal, while numerical dissipation is the damping of low-frequency components. These errors can lead to inaccurate results and may limit the applicability of the method. One approach to mitigating truncation error is to impose artificial dissipation. This technique is used in finite differences to suppress numerical oscillations and instabilities that can arise due to truncation error. In some cases, the truncation error can result in oscillations or spurious high-frequency modes that are not present in the original problem. Artificial dissipation is designed to mitigate these oscillations by introducing additional dissipation into the numerical method. The dissipation can be added in various ways, such as numerical filters, artificial viscosity, or upwind differencing. The additional dissipation has the effect of damping out the spurious oscillations, leading to more accurate and stable numerical solutions.

In many cases, a small amount of artificial dissipation can greatly improve the accuracy and stability of a finite difference method. However, excessive dissipation can lead to loss of accuracy and numerical "smearing" of the solution. Thus, the amount of artificial dissipation added to the numerical method must be carefully chosen to balance stability and accuracy. It is important to note that while artificial dissipation can help mitigate truncation error, it cannot completely eliminate it. Therefore, researchers must carefully consider the limitations and assumptions of their numerical methods, and validate their results through comparison with exact solutions or experimental data.

0.1.2 Numerical Error from Boundary Conditions

Imposing boundary conditions on a numerical problem can sometimes cause high frequency oscillations in the solution, especially if the boundary conditions are not well-suited to the problem or if the numerical method used to solve the problem is not well-designed.

Boundary conditions are essential in many numerical problems because they provide information about the solution at the boundaries of the computational domain. This information is used by the numerical method to compute the solution throughout the domain. However, if the boundary conditions are not well-chosen, they can introduce artificial oscillations in the solution that are not present in the physical problem.

For example, if a boundary condition specifies a fixed value of the solution at a boundary, and the numerical method used to solve the problem is not stable or accurate enough, it can lead to high frequency oscillations in the solution near the boundary. This is because the numerical method may be unable to accurately represent the sharp gradients or discontinuities that can occur in the solution near the boundary.

In some cases, imposing boundary conditions that are too restrictive can also lead to high frequency oscillations in the solution. For example, if a boundary condition specifies that the derivative of the solution is zero at a boundary, it can create oscillations in the solution near the boundary because the numerical method may have difficulty accurately representing the steep gradients that can occur at the boundary.

To avoid these types of issues, it's important to choose boundary conditions that are appropriate for the problem and to use numerical methods that are well-suited to the problem and can accurately represent the gradients and discontinuities in the solution near the boundaries. Techniques such as the second order central finite difference dissipation operator can be used to add numerical dissipation and stabilize the solution near the boundaries.

0.1.3 Dissipation Schemes

The second order central finite difference approximation to the first derivative:

$$f'(r) \approx \frac{f(r+\Delta r) - f(r-\Delta r)}{2\Delta r} \tag{1}$$

where $f'(r)$ is the first derivative of $f(r)$ with respect to r, Δr is the spacing between the grid points, and $f(r+\Delta r)$ and $f(r-\Delta r)$ are the function values at the neighboring grid points.

To introduce some dissipation, a second order term is added to the approximation that includes the second derivative:

$$f''(r) \approx \frac{f(r+\Delta r) - 2f(r) + f(r-\Delta r)}{(\Delta r)^2} \tag{2}$$

where $f''(r)$ is the second derivative of $f(r)$ with respect to r.

By combining these two approximations , a second order central finite difference dissipation operator is defined,

$$D(f(r)) = \frac{f(r+\Delta r) - f(r-\Delta r)}{(2\Delta r)} - \chi \frac{f(r+\Delta r) - 2f(r) + f(r-\Delta r)}{(\Delta r)^2} \tag{3}$$

where χ is a parameter that controls the amount of dissipation. A larger value of χ results in more dissipation.

This operator can be used to add some numerical dissipation to a computational method, which can help to stabilize the solution and reduce the impact of high frequency oscillations. However, it's worth noting that adding too much dissipation can also lead to loss of accuracy in the solution.

For a second order filter with first-order boundary points ,

$$D_2 = \frac{1}{4} \begin{bmatrix} -1 & +1 & 0 & 0 & 0 & 0 \\ +1 & -2 & +1 & 0 & 0 & 0 \\ 0 & +1 & -2 & +1 & 0 & 0 \\ 0 & 0 & +1 & -2 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 \end{bmatrix} \tag{4}$$

] Second order boundary points can be represented with a matrix,

$$\begin{bmatrix} +1 & -1 \\ -1 & +2 \end{bmatrix} \tag{5}$$

The lower row and right column element belongs to the interior operator. The full dissipation matrix for a fourth-order filter can be constructed using the interior matrix,

$$\begin{bmatrix} -1 & +2 & -1 \\ +2 & -5 & +4 \\ -1 & +4 & -6 \end{bmatrix} \tag{6}$$

Combining equations (5) and (6)

$$D_4 = \frac{1}{16} \begin{bmatrix} -1 & +2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ +2 & -5 & +4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & +4 & -6 & +4 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +4 & -6 & +4 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +4 & -6 & +4 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & +2 & -5 & +4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & +2 & -1 \end{bmatrix} \tag{7}$$

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Bibliography

[1] Christopher A Kennedy. *Comparison of several numerical methods for simulation of compressible shear layers*, volume 3484. NASA, Langley Research Center, 1997.