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A Posteriori Stability Analysis of Finite-Volume Methods on Unstructured Meshes

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Abstract: The new approach proposed here, improves the stability of unstructured mesh finite-volume CFD calculations by moving vertices in the mesh as a posteriori process. In this process, we exploit the gradients of eigenvalues with respect to the local changes in the mesh to find directions and magnitudes of mesh perturbations that will make the Jacobian of a semi-discrete system of equations negative semi-definite. This will ensure the energy stability of the system; consequently resulting in convergence. Our numerical results have shown that the proposed method was able to locate the problematic parts of the mesh responsible for instabilities as well as to modify the glitches for several physical problems. It is conjectured that the failure of our method for some specific problems is probably due to the insensitivity of these problems to local changes in the mesh. In these cases, the effects of boundary conditions and modes of the physical features are dominant.

Keywords: Spectral stability analysis, Computational Fluid Dynamics, Energy stability, Eigen-analysis.

1 Introduction

As the capabilities of computational fluid dynamics software has grown, so too have the size and complexity of the problems to which industrial users apply CFD. Even for expert users — who understand how to generate meshes and choose flow solver options to get good solutions for routine problems in their area of expertise — new large scale problems are challenging: trial and error are required to identify and resolve important flow features and find a stable solution. Historically the main tool for increasing the solution accuracy has been either employing grid refinement or high order schemes. However, for real world application problems, the baseline simulation often pushes the limits of available computing resources. Such studies are often prohibitive due to instability issues. This problem is particularly challenging since commercial CFD software typically handles complex problem geometries using unstructured meshes, for which accuracy and stability issues are not as well understood as for structured meshes. Thereby, with this rapid development of high order numerical methods comes the need for stability analysis. However, these studies are lagging behind to fully understand and predict unstable features on general unstructured meshes; hence to remedy them. The lack of rigorous analysis tools to fix the instabilities along with the larger time steps and more complicated geometries for engineering purposes calls for a thorough stability analysis.

The stability of numerical discretization methods depends not only on the methodology but also on the mesh: bad features in a mesh far from any flow features of interest can still have a deleterious effect on the stability or convergence of a CFD solver. A thorough understanding of this connection can provide guidance in the design of numerical methods or mesh generation that would improve solver performance and robustness. In this paper, we use eigen-analysis to study and improve the mathematical stability of the semi-discrete system of equations arising from unstructured mesh space discretization. This analysis will hopefully enable us to predict instabilities and help to remedy them prior to solving the problem. To the best of our knowledge, eigenvalue analysis has always been used to find some upper bound and thresholds of stability such as energy stability analysis which is attractive in both Finite element (e.g. [1]) and finite volume (e.g. [2, 3]) communities; and it has never been applied to modify mesh or flow features as a controlling feedback tool to stabilize an unstable case. With the aid of entropy and the notion that entropy should always increase, many other stability schemes have also been developed. These methods (e.g. see [4, 5, 6] and the references therein) utilize entropy variables to devise entropy stable schemes for nonlinear partial differential equations. However, all these various works have failed to provide an interactive practical tool to automatically stabilize a discretized linear or nonlinear PDE on a general unstructured mesh.

In this paper, we use eigen-analysis to study and improve the mathematical stability of the semi-discrete system of equations arising from unstructured mesh finite volume space discretization. This approach has its roots in energy analysis (e.g. [3, 7]). Energy stability for semi-discrete systems requires that all eigenvalues have negative real part. Our goal is to stabilize a (linearized) PDE by perturbing the mesh vertices locally. To do this, we must predict the stability prior to the mesh modification and find the size and direction of mesh perturbation that improves stability. The rest of this paper lays out as follows: in Section 2 we describe how the gradients of the spatial semi-discrete Jacobian with respect to mesh vertices are calculated; in Section 3, the direct and optimization approaches for finding the perturbation vector are explained; after specifying which vertices to perturb in Section 4, the local mesh modification is applied to stabilize the unstable problems in Section 5. Moreover in Section 6, in an alternative way to perturb the mesh we can change the discretization by increasing the reconstruction stencil size of a collection of control volumes to stabilize an originally unstable problem.

2 Gradients of the eigenvalues

From the energy stability analysis and the method of lines, we know that a (linear) PDE, discretized in space, produces a coupled set of ODE's such as:

$$\frac{\partial u}{\partial t} = R(u) \tag{1}$$

$$\frac{du}{dt} = \frac{\partial R}{\partial u} u = Au \tag{2}$$

is stable if and only if the Jacobian matrix $A = \frac{\partial R}{\partial u}$ is negative semi-definite whereas we assume the transient growth is negligible and remains zero. To obtain the semi-discrete Jacobian matrix, A, for non-linear problems we use a lower order solution at the steady state to linearize the Jacobian matrix.

In preliminary unpublished work, we realized that eigen-analysis of semi-discrete systems for realistic finite volume discretization can accurately predict the convergence rate for an implicit solver. This revelation motivated us to use eigen-analysis to show stability and gradients of eigenvalues to predict how spectral stability will change upon changes in the mesh. In other words, the key to our work is the ability to predict changes in the eigenvalues with changes in the mesh. The derivatives of eigenvalues and eigenvectors of general matrices dependent on multiple variables have been studied by many (e.g. see [8, 9] and references therein). If the matrix eigenvalue problem of interest is

$$A(\overrightarrow{\xi})x_i(\overrightarrow{\xi}) = \lambda_i x_i(\overrightarrow{\xi}) \tag{3}$$

where x_i is the i^{th} right eigenvector associated with the i_{th} eigenvalue λ_i, then the eigenvalue derivatives with respect to some parameter ξ (which in our case is the mesh coordinates vector) are obtained as follows:

$$\frac{\partial}{\partial \xi_i}(Ax_i = \lambda_i x_i) \tag{4}$$

$$y_i(\frac{\partial A}{\partial \xi}x_i + A\frac{\partial x_i}{\partial \xi} = \frac{\partial \lambda_i}{\partial \xi}x_i + \lambda_i \frac{\partial x_i}{\partial \xi}) \tag{5}$$

$$\frac{\partial \lambda_i}{\partial \xi} = y_i \frac{\partial A}{\partial \xi} x_i \qquad with \ \text{condition}: \ y_i \cdot x_i = 1 \tag{6}$$

Notice that we left-multiplied the equation 5 by the left (row) eigenvector y_i and normalized so that $y_i \cdot x_i = 1$. Amongst the ways to approximate the gradients of the eigenvalues such as doing the finite difference on eigenvalues or reverse differentiation, we choose to do finite differences on the Jacobian matrix instead, since the former is expensive owing to the difficulty of eigen-problem and the latter is simply much harder to do. The derivative of the A matrix with respect to the mesh entities is approximated using finite differences:

$$\frac{\partial A}{\partial \xi} = \frac{A(\overrightarrow{\xi} + \delta\overrightarrow{\xi}) - A(\overrightarrow{\xi})}{\left\|\delta\overrightarrow{\xi}\right\|} \tag{7}$$

Hence, using equation 6, we are able to predict changes induced in eigenvalues by the mesh perturbations. Fig. 1 shows that for a good range of ξ parameter, the gradient of the Jacobian more or less does not change for a specific mesh location. The horizontal axis in Fig. 1 is the size of the ξ parameter in Eq. 7 where the length scale is the smallest edge incident on each vertex. This analysis validates as well as further substantiates the use of finite differences to calculate the gradients of the Jacobian matrix.

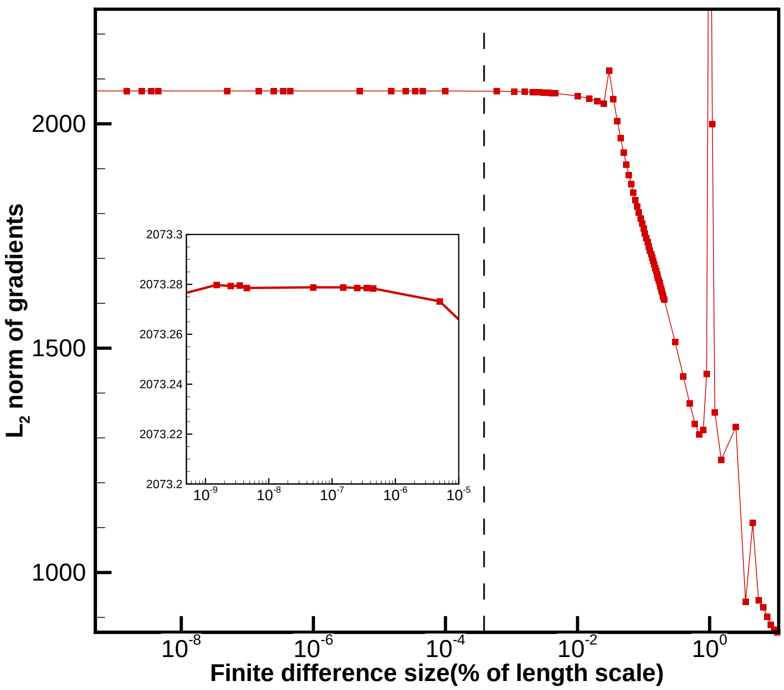


Figure 1: Sensitivity map of the gradient of the Jacobian matrix with respect to perturbation parameters for an inviscid Burgers' problem

3 How to find the perturbation vector?

All in all, using energy stability results along with the knowledge of eigenvalue derivatives upon any mesh perturbation, we can tune the perturbations in a way such that the real parts of eigenvalues (specially the unstable ones) decrease. However, this is not an easy task, as naively perturbing the mesh to improve one eigenvalue may lead to destabilizing the other (stable) eigenvalues.

One intuitive way to perturb the mesh is to consider all (right-most) eigenvalues separately. Surely, the fastest route to stabilizing a single eigenvalue regardless of the other eigenvalues is to perturb the mesh in the exactly opposite direction of the gradient of the eigenvalue (steepest descent method) which means that the following inequality should hold:

$$\Re\left\{\lambda_{orig}\right\} + \triangle\overrightarrow{\xi}\cdot\frac{\partial\lambda}{\partial\xi} \leq 0 \tag{8}$$

This results in a perturbation vector with the direction and size of:

$$\triangle\xi = -|k|\Re\left\{\frac{\partial\lambda}{\partial\xi}\right\} \text{ With } k \geqslant \frac{\Re\left\{\lambda\left(\xi_{org}\right)\right\}}{\left(\frac{\partial\lambda}{\partial\xi}\right)^2} \tag{9}$$

A complication arises when there are multiple unstable or nearly unstable eigenvalues due to there being multiple perturbation vectors which could partly or completely contradict each other. One way to solve this is to take a weighted average of these multiple perturbation vectors with weights proportional to how positive (unstable) the corresponding eigenvalues are to gain a single perturbation vector. Another more sophisticated approach is to reform the problem to stabilize all the unstable eigenvalues collectively. To do so, we minimize (negate) the real part of the right-most eigenvalues directly. The single perturbation vector $\overrightarrow{d} = \triangle\xi$, should satisfy all the linear inequalities (Eq. 10) required to stabilize the problem:

$$\Re\left\{\lambda_j\right\} + \overrightarrow{d} \cdot \frac{\partial\lambda_j}{\partial\xi} \leq 0 \qquad 1 \leq j \leq M \tag{10}$$

where M is the number of unstable eigenvalues. With choosing the optimization variables as the entities of the perturbation vector, the linear optimization problem is defined as:

$$\min\left\{\sum_j^M s_j\right\} \qquad \text{where} \qquad s_j = \left(\Re\left\{\lambda_j\right\} + \overrightarrow{d} \cdot \frac{\partial\lambda_j}{\partial\xi}\right) \tag{11}$$

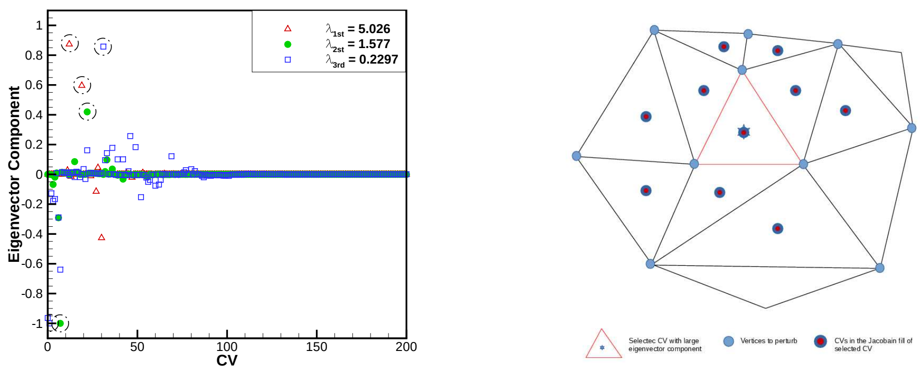
where s_j are the negative of the slack variables (positivity of each inequality), subject to the linear constraints $s_j \leq 0$. The upper bound for the optimization variables are based on the local length scale to avoid any non-conformality or irregularity in the mesh after the modification. In this case, each perturbation size at each vertex is kept less that 10% of the length of the longest incident edge. Since we have a linear optimization problem, the optimum solution to the summation of the objective functions is equivalent to the solution of the multi-objective minimization of each eigenvalue. In other words, instead of minimizing the slack variable for each eigenvalue separately, we can minimize the summation of the slack variables.

4 Which vertices to perturb?

The key to our analysis is to approximate $\frac{\partial\lambda_j}{\partial\xi_i}$. However we do not need to calculate this for the whole mesh as only part of the mesh is responsible for instabilities most of the time. We know that the right eigenvector is a mode of the solution. Therefore if a Jacobian matrix tends to have an unstable solution, the right eigenvectors of the unstable modes will specify the parts of the mesh where things have gone wrong. Moreover, there is no need for the exact calculation of the gradient of the eigenvalues, as any approximate one is able to guide the mesh modification in the right direction for better stability properties. Hence to approximate $\frac{\partial\lambda_j}{\partial\xi_i}$:

1. Span the right eigenvector (e.g., see Fig. 2a)
2. Pick up the largest components of the eigenvector
3. List all CVs corresponding to these components as well as the ones in their Jacobian fill (e.g., see Fig. 2b)

4. Perturb vertices located on these CVs



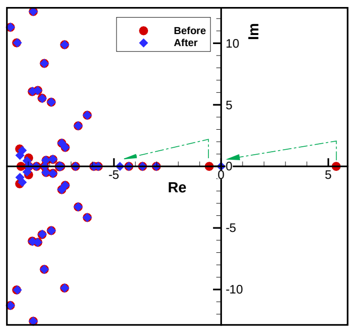
(a) Span of the right eigenvectors for an inviscid burgers problem

(b) Vertices on the control volumes of the Jacobian fill of the control volume with the largest eigenvector component

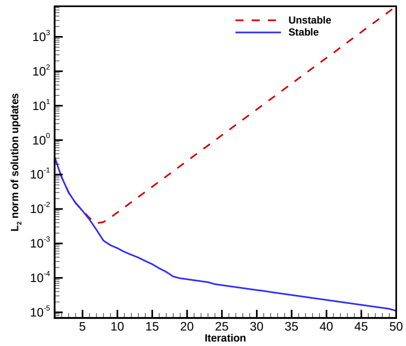
Figure 2: How to choose vertices for perturbation

5 Mesh improvement

A preliminary test case has been done to showcase the applicability of our approach in stabilizing an initially unstable problem. In this case, a 3D MUSCL Advection problem has been stabilized by pushing its single unstable eigenvalue to the left half complex plane (see Fig. 3a). As is obvious from Fig. 4, by perturbing only four vertices the problem has transfered to a stable region. The stability can also be observed from the plot of residual over the iterations (as is seen from Fig. 3b)



(a) Spectral map



(b) Residual history

Figure 3: Spectral map before and after the mesh perturbation for a 3D 2^{nd} order MUSCL advection. Time stepping is done by backward Euler.

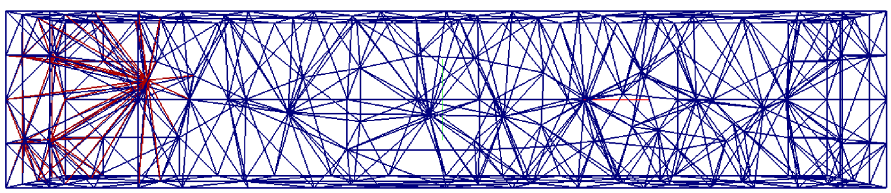
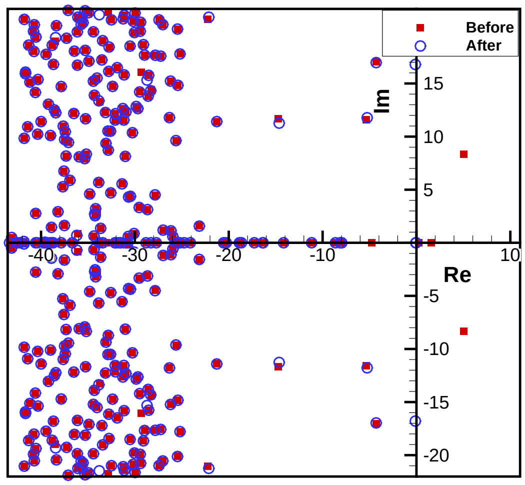


Figure 4: Mesh modification to stabilize the problem for a 3D 2^{nd} order MUSCL advection

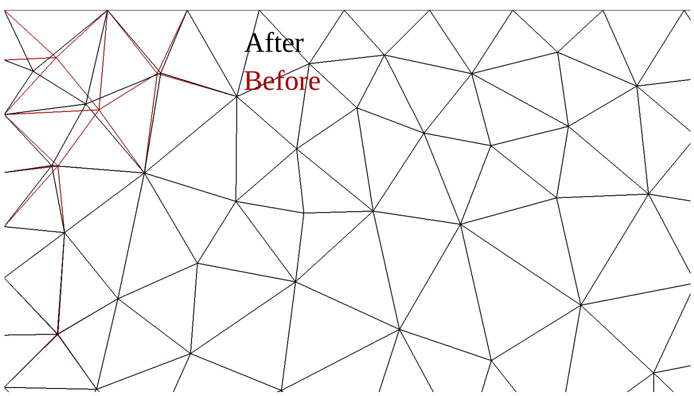
Note that the Jacobian in the linear advection problem is only a function of mesh coordinates and constant wave speeds and is completely independent of the solution. This in turn asserts that perturbing the mesh in a direction predicted by the gradients of the eigenvalues is indeed a proper approach to gain stability. However, for more complicated nonlinear problems, more care and thoughts need to be put into consideration as the Jacobian is also a function of the solution.

Another complication arises when there are multiple unstable or near instability eigenvalues; thereby there are multiple perturbation vectors which could partly or completely contradict each other. To mitigate this problem we opted to put more emphasis on the rightmost eigenvalues, so as to disregard an eigenvalue in calculating the perturbation vector, in case it was contradicting the resultant perturbation vector calculated solely from the rightest-most ones.

The first trial for non-linear problems is done using inviscid Burgers' problem where the Jacobian of the semi-discrete system is no longer independent of the solution. To linearize the Jacobian, we uses a first order solution to approximate the second order Jacobian. By doing so, we will specify the unstable eigenvalues as well as parts of the mesh responsible for these instabilities. Fig. 5b shows how modifying the mesh locally has changed the unstable eigenvalues in Fig. 5a to the left half of the complex plane.



(a) Spectral map



(b) Mesh modification

Figure 5: Before and after mesh perturbation for an inviscid Burgers' problem

6 Selective increase of the stencil size

Haider et al. [2, 10] showed that for a linear advection problem increasing the stencil size of the solution reconstruction (see [11, 12, 13] and the references therein on how to do the reconstruction) have a positive effect on stabilizing the problem. To do this, they introduced a special norm of part of the reconstruction matrix called reconstruction map, and showed a relative correlation between the value of this parameter and the stability of the reconstruction. The main takeaway point was that adding another layer of control volumes to the solution reconstruction in spacial discretization will make the problem more stable. Therefore in a parallel attempt to mesh modifications, we will change the discretization. We have observed that by using the right eigenvector of the unstable mode, we can cherry-pick a small number of control volumes (instead of the whole mesh) with large values in the eigenvector to increase their stencil size. Fig. 6 shows how increasing the stencil size of only 6 control volumes out of the 1382 control volumes for an inviscid burgers problem stabilizes the four existing unstable eigenvalues. In this way, without any changes in the mesh, we were able to stabilize the problem by changing the spatial discretization locally.

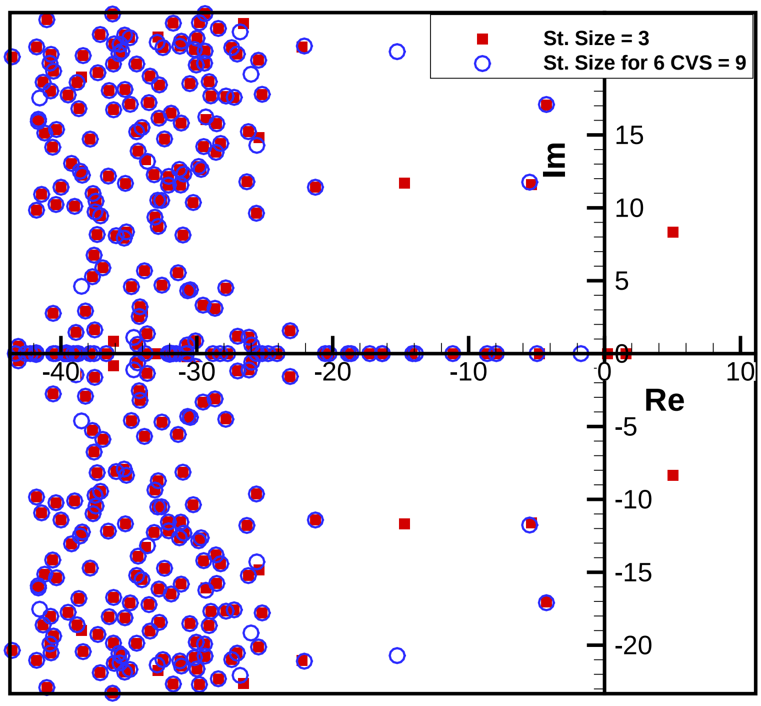


Figure 6: Inviscid Burgers in a channel with 1382 CVs

7 Conclusion

In this work, we studied stability and more specifically a new approach to stabilize PDE's governing computational fluid dynamics problems. In the proposed approach, which to the best of our knowledge, is the first of its kind perturbs the mesh vertices locally so that the new mesh is more suitable for the PDE of interest. In our quest to improve stability, we exploit the gradients of eigenvalues as feedback tools to determine in which direction and how much the mesh vertices should be perturbed so that the Jacobian of the semi-discretized set of equations have more amiable eigenvalues. The less positive these eigenvalues are, the more stable the semi-discrete system of equations are. Our linear Advection results along with nonlinear inviscid Burgers' problem showcase a proof of concept and paves the way for stabilizing more complicated and nonlinear problems. Moreover, in a parallel work to mesh modifications, we showed that changing the discretization locally, especially the reconstruction stencil, can stabilize the initially unstable problems.

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