Energy Stability Analysis of Multi-Step Methods on Unstructured Meshes

by

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Contents

1 Introduction

In an effort to avoid the geometric limitations of structured, logically rectangular meshes, much work is now being done using unstructured meshes for flow calculations around complex geometries. In particular, triangular meshes are becoming popular for two-dimensional problems with multiple components [1] or grid adaptation [2], and tetrahedral cells are being used for three-dimensional aircraft calculations [3]. It is clear that these unstructured meshes will be of increasing importance in computational methods.

During this period of rapid development the development of methods for numerical analysis has lagged behind. Questions about the maximum stable time step for explicit methods have been resolved by ad hoc procedures which are based upon the results for structured meshes and a clear understanding of the physical domain of dependence restrictions which are the underlying origin of these limits. The lack of rigorous analysis tools however leads to concerns that current methods may be overly conservative in order to ensure stability in all possible cases. As more three-dimensional calculations are being performed for engineering design and analysis, larger time steps and faster convergence rates can lead to significant savings in time and money. Thus it is important to develop new methods of analyzing numerical methods on unstructured meshes.

The standard approach for analyzing methods on structured grids is to use Fourier analysis, by considering a general solution to be a sum of Fourier modes, and then separately analyze each one [4]. The key point is that on a regular infinite grid the eigenmodes are always Fourier modes. On irregular unstructured grids this is clearly not the case and so a different approach is needed. The answer is to turn to another classic analysis method, the energy method [4]. This technique defines an energy associated with a solution and then proves stability by showing that the energy is non-increasing. For structured meshes this approach can be much more cumbersome than Fourier analysis, particularly for systems of equations where it can be difficult to pick the correct energy definition, but it is very suitable for unstructured meshes.

In this paper we demonstrate the use of the energy method to analyze multi-stage methods for solving the model convective equation on unstructured meshes, using cell-based and node-based spatial differencing, both of which were developed by Jameson [5, 3]. Cell-based differencing (in which the variable is assumed to be constant within each cell) was the first developed, but is only first-order accurate in an integral sense on irregular meshes. In node-based methods the variable is defined at each node, and in general the solution is second order accurate. In performing the energy stability analysis we will assume that all functions (and their derivatives where necessary) are zero on the boundaries, to avoid the complications introduced by boundary contributions. The inclusion of the boundary terms in the analysis would bring us into the subject of the stability analysis of numerical boundary conditions which is an additional subject in its own right and is beyond the scope of this present paper. Here we are simply concerned with finding the requirements for the interior numerical scheme to be stable.

A few comments are appropriate on the organization of this paper, since it may seem strange that unstructured grids and spatial differencing are not discussed until the fifth section. Section 2 presents the use of the energy method to prove stability for the analytic convective equation and introduces the ideas and formalism which will be used for the discrete methods. Section 3 analyzes semi-discrete methods (spatially discrete but continuous in time) in a very general form and section 4 extends this to fully discrete equations. These two sections assume that the spatial discretization has certain properties, and then the next two sections prove that the cell-based differencing and the triangular/tetrahedral node-based differencing do in fact have these properties. The reason for this approach is to emphasize the importance of these properties, in that any scheme satisfying these conditions will be stable. Finally, the last section extends the analysis to systems of equations and analyzes the Euler equations in particular.

2 Energy Analysis of Convection Equation

The model convection equation is

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0. \tag{1}$$

The ‘energy’ of $u(\vec{x}, t)$ in a three-dimensional volume V is defined by

$$E(t) = \int_V u^2(\vec{x}, t)\, dV. \tag{2}$$

The rate of change of energy is given by

$$\begin{aligned} \frac{dE}{dt} &= 2\int_V u\frac{\partial u}{\partial t}\, dV \\ &= -2\int_V u\frac{\partial u}{\partial x}\, dV \\ &= -\int_V \frac{\partial}{\partial x}(u^2)\, dV \\ &= -\int_{\partial V} u^2 n_x\, dS. \end{aligned} \tag{3}$$

The last integral is over the surface of the volume with n_x being the x-component of the outward pointing normal. If $u = 0$ on ∂V then the boundary contribution disappears and we are left with

$$\frac{dE}{dt} = 0, \tag{4}$$

proving that the convection equation is energy-preserving and thus stable.

We now repeat this analysis using the formalism which will simplify our later analyses. We begin by defining a <u>scalar product</u>, which is a generalized dot product of two functions, and a <u>norm</u>, which is a generalized magnitude of a function [6].

$$(u, v) = \int_V uv \;\; dV \tag{5}$$

$$\|u\| = \sqrt{(u, u)} \tag{6}$$

A scalar product and norm have a number of basic properties.

$$
\begin{array}{cl}
\text{linearity} & (u, v+w) = (u,v) + (u,w) \\
\text{symmetry} & (u,v) = (v,u) \\
\text{zero norm} & u = 0 \implies \|u\| = 0 \\
\text{positive norm} & u \neq 0 \implies \|u\| > 0 \\
\text{triangle inequality} & \|u+v\| \leq \|u\| + \|v\|
\end{array} \tag{7}
$$

In addition this particular scalar product also has the following property.

Property 1 $\left(u, \frac{\partial v}{\partial x}\right) + \left(\frac{\partial u}{\partial x}, v\right) = 0$

This comes from the divergence theorem with an assumption that u and/or v is zero on ∂V so that we can ignore the boundary contributions as discussed in the introduction.

An immediate deduction from Property 1 is that

$$
\left(u, \frac{\partial u}{\partial x}\right) = \frac{1}{2}\left[\left(u, \frac{\partial u}{\partial x}\right) + \left(\frac{\partial u}{\partial x}, u\right)\right] = 0. \tag{8}
$$

With the energy defined by $E = \|u\|^2$, the energy analysis is now almost trivial.

$$
\begin{aligned}
\frac{dE}{dt} &= \left(u, \frac{\partial u}{\partial t}\right) + \left(\frac{\partial u}{\partial t}, u\right) \\
&= 2\left(u, \frac{\partial u}{\partial t}\right) \\
&= -2\left(u, \frac{\partial u}{\partial x}\right) \\
&= 0
\end{aligned} \tag{9}
$$

3 Semi-discrete Analysis

In this section we consider a function $u_i(t)$ which is spatially discrete but continuous in time. We assume that we have some discrete spatial differencing operator ∂_x so that $\partial_x u$ is a discrete approximation to $\frac{\partial u}{\partial x}$. The semi-discrete approximation to the convection equation is then given by

$$\frac{\partial u_i}{dt} + (\partial_x u)_i = 0 \tag{10}$$

To perform the energy stability analysis we <u>assume</u> that we also have a scalar product (u, v) which has the property

Property 1 $\quad (u, \partial_x v) + (\partial_x u, v) = 0$

As with the analytic version of Property 1, an immediate corollary is

$$(u, \partial_x u) = 0 \tag{11}$$

The stability proof is now exactly the same as for the analytic equation.

$$\begin{aligned}
\frac{dE}{dt} &= \frac{d}{dt}\|u\|^2 \\
&= \left(u, \frac{du}{dt}\right) + \left(\frac{du}{dt}, u\right) \\
&= 2\left(u, \frac{du}{dt}\right) \\
&= -2\,(u, \partial_x u) \\
&= 0
\end{aligned} \tag{12}$$

The proof is so simple because all of the hard work is hidden in determining the properties of the differencing scheme, which is particularly involved on irregular grids.

4 Fully Discrete Analysis

4.1 Two-stage time discretization

The two-step predictor/corrector method is given by

$$u_i^* = u_i^n - \Delta t \partial_x u_i^n \tag{13}$$

$$\begin{aligned} u_i^{n+1} &= u_i^n - \Delta t \partial_x u_i^* \\ &= u_i^n - \Delta t \partial_x u_i^n + \Delta t \partial_x \Delta t \partial_x u_i^n \end{aligned} \tag{14}$$

The reason that the ordering of Δt and ∂_x is kept as it is in the last equation, is because a very useful technique for accelerating convergence to steady state solutions is to use 'local time steps' in which Δt varies over the domain. In order to analyze this possibility Δt and ∂_x cannot be interchanged because the ordering produces different results.

Because of the variable time steps we define a new generalized energy

$$E^n = \|\Delta t^m u^n\|^2 \tag{15}$$

Note: m is an exponent whereas n is a superscript denoting an iteration time level. We also need to assume an additional property.

Property 2 *$(e_i, e_j) = 0$ if $i \neq j$, where e_i is a function which has value 1 at node i (or in cell i) and value 0 elsewhere.*

There are two important corollaries that arise from this assumption. If s is a scalar function then using the linearity of the scalar product it follows that

$$\begin{aligned} (su, v) &= \sum_{i,j} s_i u_i \, v_j \, (e_i, e_j) \\ &= \sum_i s_i u_i \, v_i \, (e_i, e_i) \\ &= \sum_i u_i \, s_i v_i \, (e_i, e_i) \\ &= \sum_{i,j} u_i \, s_j v_j \, (e_i, e_j) \\ &= (u, sv). \end{aligned} \tag{16}$$

The reason that this refers to s_i being scalar is that we are leaving open for the future the possibility that u_i and v_i are vectors, in order to analyze systems of equations.

The second corollary is similar to the first. If s and t and two scalar functions, and $|s_i| < |t_i|$ for each i, then

$$
\begin{aligned}
\|su\| &= \sum_{i,j} s_i u_i \, s_j u_j \, (e_i, e_j) \\
&= \sum_i s_i^2 u_i^2 \, (e_i, e_i) \\
&\leq \sum_i t_i^2 u_i^2 \, (e_i, e_i) \\
&= \sum_{i,j} t_i u_i \, t_j u_j \, (e_i, e_j) \\
&= \|tu\|. \qquad (17)
\end{aligned}
$$

We now proceed with the stability analysis as before.

$$
\begin{aligned}
&\left\|\Delta t^m u^{n+1}\right\|^2 - \|\Delta t^m u^n\|^2 \\
&= \left(\Delta t^m \left(u^n - \Delta t \partial_x u^n + \Delta t \partial_x \Delta t \partial_x u^n\right), \Delta t^m \left(u^n - \Delta t \partial_x u^n + \Delta t \partial_x \Delta t \partial_x u^n\right)\right) \\
&\quad - \left(\Delta t^m u^n, \Delta t^m u^n\right) \\
&= \left\|\Delta t^{m+1} \partial_x u^n\right\|^2 + \left\|\Delta t^{m+1} \partial_x \Delta t \partial_x u^n\right\|^2 + 2\left(\Delta t^m u^n, \Delta t^{1+m} \partial_x \Delta t \partial_x u^n\right) \\
&\quad -2\left(\Delta t^m u^n, \Delta t^{1+m} \partial_x u^n\right) - 2\left(\Delta t^{1+m} \partial_x u^n, \Delta t^{1+m} \partial_x \Delta t \partial_x u^n\right) \\
&= \left\|\Delta t^{m+1} \partial_x u^n\right\|^2 + \left\|\Delta t^{m+1} \partial_x \Delta t \partial_x u^n\right\|^2 + 2\left(\Delta t^{1+2m} u^n, \partial_x \Delta t \partial_x u^n\right) \\
&\quad -2\left(\Delta t^{1+2m} u^n, \partial_x u^n\right) - 2\left(\Delta t^{1+2m}\left(\Delta t \partial_x u^n\right), \partial_x \left(\Delta t \partial_x u^n\right)\right) \qquad (18)
\end{aligned}
$$

The first corollary was used in the above equation to 'switch' the time step terms from one side of the scalar product to the other. In order to eliminate the last two terms using Corollary 1, we now choose $m = -\frac{1}{2}$. The third term can be rearranged using Property 1 to obtain

$$
\left\|u^{n+1}/\sqrt{\Delta t}\right\|^2 - \left\|u^n/\sqrt{\Delta t}\right\|^2 = -\left\|\sqrt{\Delta t}\, \partial_x u^n\right\|^2 + \left\|\sqrt{\Delta t}\, \partial_x \Delta t \partial_x u^n\right\|^2 \qquad (19)
$$

Thus the method is stable provided

$$
\left\|\sqrt{\Delta t}\, \partial_x \sqrt{\Delta t}\, v\right\| \leq \|v\| \qquad (20)
$$

for all v. We now introduce the last assumed property for the spatial discretization.

Property 3 *There exists a function* $(\Delta t_{\max})_i$ *such that* $\|\sqrt{\Delta t_{\max}}\, \partial_x \sqrt{\Delta t_{\max}}\, v\| \leq \|v\|$ *for all* v.

Given this property, then provided $\Delta t_i \leq (\Delta t_{\max})_i$ it follows that

$$\begin{aligned}
\left\| \sqrt{\Delta t}\, \partial_x \sqrt{\Delta t}\, v \right\| &\leq \left\| \sqrt{\Delta t_{\max}}\, \partial_x \sqrt{\Delta t}\, v \right\| \\
&= \left\| \sqrt{\Delta t_{\max}}\, \partial_x \sqrt{\Delta t_{\max}} \left(\sqrt{\frac{\Delta t}{\Delta t_{\max}}}\, v \right) \right\| \\
&\leq \left\| \sqrt{\frac{\Delta t}{\Delta t_{\max}}}\, v \right\| \\
&\leq \| v \| \qquad (21)
\end{aligned}$$

and so the two-step method is stable. The second corollary of Property 2 was used to obtain two of the inequalities in the above equation.

To obtain steady state solutions as quickly as possible one would use $\Delta t_i = (\Delta t_{\max})_i$ but for time accurate calculations requiring a uniform time step one would have to use $\Delta t = \min_i (\Delta t_{\max})_i$.

4.2 Jameson's four-step method

Jameson's four-step method is

$$\begin{aligned}
u^{(1)} &= u^n - \tfrac{1}{4} \Delta t \partial_x u^n \\
u^{(2)} &= u^n - \tfrac{1}{3} \Delta t \partial_x u^{(1)} \\
u^{(3)} &= u^n - \tfrac{1}{2} \Delta t \partial_x u^{(2)} \\
u^{n+1} &= u^n - \Delta t \partial_x u^{(3)} \qquad (22)
\end{aligned}$$

$$\begin{aligned}
\Longrightarrow \quad u^{n+1} &= u^n - \Delta t \partial_x u^n + \tfrac{1}{2} \Delta t \partial_x \Delta t \partial_x u^n \\
&\quad - \tfrac{1}{6} \Delta t \partial_x \Delta t \partial_x \Delta t \partial_x u^n + \tfrac{1}{24} \Delta t \partial_x \Delta t \partial_x \Delta t \partial_x \Delta t \partial_x u^n \qquad (23)
\end{aligned}$$

Substitution of this into the energy norm, and using the usual methods to eliminate and reduce terms, leads to

$$\begin{aligned}
\left\| u^{n+1} / \sqrt{\Delta t} \right\|^2 - \left\| u^n / \sqrt{\Delta t} \right\|^2 &= -\tfrac{1}{72} \left\| \sqrt{\Delta t}\, \partial_x \Delta t \partial_x \Delta t \partial_x u^n \right\|^2 \\
&\quad + \tfrac{1}{576} \left\| \sqrt{\Delta t}\, \partial_x \Delta t \partial_x \Delta t \partial_x \Delta t \partial_x u^n \right\|^2 \\
&= -\tfrac{1}{576} \left\{ 8 \| v \|^2 - \left\| \sqrt{\Delta t}\, \partial_x \sqrt{\Delta t}\, v \right\|^2 \right\} \qquad (24)
\end{aligned}$$

where $v = \sqrt{\Delta t}\, \partial_x \Delta t \partial_x \Delta t \partial_x u^n$. Thus it is stable provided $\Delta t \leq 2\sqrt{2}\, \Delta t_{\max}$. The same procedure can be used to analyze other multi-stage schemes.

5 Cell-based Differencing

5.1 Basic definitions

Consider a two-dimensional, infinite, irregular grid which is composed of polygonal cells C_i. Variables are defined to be constant in each cell, so u_i is the value of a function u in C_i. On the cell face separating cells C_i and C_j, $\overline{u}$ is defined to be the average of the values on either side, $\frac{1}{2}(u_i+u_j)$ and $\vec{n}_{ij}$ is the unit vector normal to the face pointing outwards from C_i, so $\vec{n}_{ji}=-\vec{n}_{ij}$. Figure 1 illustrates all of these definitions.

If $u(x,y)$ is a continuous differentiable function, then the mean value of $\frac{\partial u}{\partial x}$ in a cell C_i is given by

$$\begin{aligned}\left(\overline{\frac{\partial u}{\partial x}}\right)_i &= \frac{1}{A_i}\int_{C_i}\frac{\partial u}{\partial x}dA \\ &= \frac{1}{A_i}\int_{\partial C_i} u n_x \, dl \end{aligned} \tag{25}$$

where A_i is the area of the cell, and the latter integral is around the boundary of C_i with n_x being the x-component of the outward normal. Hence we define the discrete differential operator ∂_x to be

$$(\partial_x u)_i = \frac{1}{A_i}\sum_{\partial C_i}\overline{u} n_x \Delta l \tag{26}$$

The integral has been replaced by a summation over the faces forming ∂C_i with Δl being the length of the face. This definition is equivalent to that used by Jameson *et al* [5].

The scalar product for this spatial discretization is defined by

$$(u,v) \equiv \sum_i A_i u_i v_i \tag{27}$$

It is obvious that this definition satisfies the basic requirements for a scalar product and Property 2. The hard part is to demonstrate that it satisfies Properties 1 and 3.

5.2 Property 1

By linearity,

$$(u, \partial_x v) + (\partial_x u, v) = \sum_{i,j} u_i v_j \left[(e_i, \partial_x e_j) + (\partial_x e_i, e_j) \right] \tag{28}$$

where e_i is again the function which is 1 in cell i and 0 elsewhere. Thus it is necessary and sufficient to prove that

$$(e_i, \partial_x e_j) + (\partial_x e_i, e_j) = 0 \tag{29}$$

for all i, j.

There are three cases to consider, depending whether i is equal to j, and if not whether i belongs to the set N_j of nodes which are neighbors to j (meaning that C_i and C_j share a common face).

a) $i = j$

$$\begin{aligned}(\partial_x e_i, e_i) = (e_i, \partial_x e_i) &= \tfrac{1}{2} \sum_{\partial C_i} n_x \Delta l \\ &= \tfrac{1}{2} \int_{\partial C_i} n_x dl \\ &= \tfrac{1}{2} \int_{C_i} \frac{\partial}{\partial x}(1)\, dA \\ &= 0 \end{aligned} \tag{30}$$

The fact that $\sum_{\partial C_i} n_x \Delta l = 0$ will be used several times later on in other proofs.

b) $i \neq j, \quad i \notin N_j$

$$(\partial_x e_i, e_j) = (e_i, \partial_x e_j) = 0 \tag{31}$$

since $\partial_x e_j$ is only non-zero on the cells neighboring C_j.

c) $i \neq j, \quad i \epsilon N_j$

$$(e_i, \partial_x e_j) + (\partial_x e_i, e_j) = \tfrac{1}{2} n_{x_{ij}} + \tfrac{1}{2} n_{x_{ji}} = 0 \tag{32}$$

since the outward normals to each cell are in opposite directions.

This completes the proof that cell-based differencing satisfies Property 1.

5.3 Property 3

We need to prove that there exists a function Δt such that

$$\left\| \sqrt{\Delta t}\, \partial_x \sqrt{\Delta t}\, v \right\| \le \|v\| \tag{33}$$

for all v.

Let

$$(\Delta t)_i = 2A_i / \sum_{\partial C_i} |n_x| \Delta l \tag{34}$$

Then

$$\begin{aligned} \left\| \sqrt{\Delta t}\, \partial_x \sqrt{\Delta t}\, v \right\|^2 &= \sum_i \Delta t_i A_i \left(\partial_x \sqrt{\Delta t}\, v \right)^2 \\ &= \sum_i \frac{\Delta t_i}{A_i} \left(\sum_{\partial C_i} \overline{\sqrt{\Delta t}\, v}\, n_x \Delta l \right)^2 \end{aligned} \tag{35}$$

On the face shared by cells C_i and C_j, $\overline{\sqrt{\Delta t}\, v} = \frac{1}{2}\left[\left(\sqrt{\Delta t}\, v\right)_i + \left(\sqrt{\Delta t}\, v\right)_j \right]$. Hence

$$\sum_{\partial C_i} \overline{\sqrt{\Delta t}\, v} n_x \Delta l = \tfrac{1}{2} \left(\sqrt{\Delta t}\, v\right)_i \sum_{\partial C_i} n_x \Delta l + \tfrac{1}{2} \sum_{j \epsilon N_i} \left(\sqrt{\Delta t}\, v\right)_j (n_x \Delta l)_{ij} \tag{36}$$

The first sum is zero because $\sum_{\partial C_i} n_x \Delta l = 0$. Substituting this equation into Equation (35) we find that the contribution due to cell C_i is

$$\begin{aligned} \frac{\Delta t_i}{A_i} \left(\sum_{\partial C_i} \overline{\sqrt{\Delta t}\, v} n_x \Delta l \right)^2 &= \tfrac{1}{4} \frac{\Delta t_i}{A_i} \sum_{j_1} \sum_{j_2} \left(\sqrt{\Delta t}\, v\right)_{j_1} \left(\sqrt{\Delta t}\, v\right)_{j_2} (n_x \Delta l)_{ij_1} (n_x \Delta l)_{ij_2} \\ &\le \tfrac{1}{4} \frac{\Delta t_i}{A_i} \sum_{j_1} \sum_{j_2} \left|\sqrt{\Delta t}\, v\right|_{j_1} \left|\sqrt{\Delta t}\, v\right|_{j_2} |n_x \Delta l|_{ij_1} |n_x \Delta l|_{ij_2} \\ &\le \tfrac{1}{4} \frac{\Delta t_i}{A_i} \sum_{j_1} \sum_{j_2} \tfrac{1}{2} \left[\left(\sqrt{\Delta t}\, v\right)^2_{j_1} + \left(\sqrt{\Delta t}\, v\right)^2_{j_2} \right] |n_x \Delta l|_{ij_1} |n_x \Delta l|_{ij_2} \\ &= \tfrac{1}{4} \frac{\Delta t_i}{A_i} \left[\sum_{j_2} |n_x \Delta l|_{ij_2} \right] \left[\sum_{j_1} \left(\Delta t\, v^2\right)_{j_1} |n_x \Delta l|_{ij_1} \right] \\ &= \tfrac{1}{2} \sum_{j \epsilon N_i} \left(\Delta t\, v^2\right)_j |n_x \Delta l|_{ij} \end{aligned} \tag{37}$$

The key result which is used in establishing the inequality in the above equation, is that for any pair of real numbers f and g, $(f \pm g)^2 > 0 \Longrightarrow |f||g| < \frac{1}{2}(f^2 + g^2)$. Summing over all of the cells we finally get

$$
\begin{aligned}
\left\| \sqrt{\Delta t} \partial_x \sqrt{\Delta t}\, v \right\|^2 &\leq \tfrac{1}{2} \sum_i \sum_{j \epsilon N_i} \left(\Delta t\, v^2 \right)_j |n_x \Delta l|_{ij} \\
&= \tfrac{1}{2} \sum_j \left(\Delta t\, v^2 \right)_j \sum_{i \epsilon N_j} |n_x \Delta l|_{ij} \\
&= \sum_j A_j v_j^2 \\
&= \|v\|^2
\end{aligned} \tag{38}
$$

This completes the proof that the cell-based differencing satisfies Property 3, with

$$
(\Delta t_{\max})_i = 2A_i / \sum_{\partial C_i} |n_x| \Delta l \tag{39}
$$

Not only does this give a sufficient condition for stability (when combined with the theory of the last section); it also gives the necessary condition for regular quadrilateral. Using Fourier analysis it can be shown that for a uniform grid of parallelograms the stability limit is

$$
\Delta t \leq \lambda \Delta t_{\max} \tag{40}
$$

where

$$
\lambda = \begin{cases} 1 & \text{two-step method} \\ 2\sqrt{2} & \text{four-step method} \end{cases}
$$

and $\Delta t_{\max} = A/\Delta y$ where A is the area of the cells and Δy is defined in Figure 2. This equation for $\Delta t_{\max}$ is exactly the same as is given by the present theory.

5.4 Extension to 3-D

The extension to three-dimensional grids is actually very straightforward. All that changes is that cell areas A_i become cell volumes V_i, and face lengths Δl become face areas A. With these minor changes all of the theory and the proofs carry over directly (although it becomes much harder to visualize some of the steps involved). The discrete differential operator and maximum time step are

$$
(\partial_x u)_i = \frac{1}{V_i} \sum_{\partial C_i} \overline{u}\, n_x\, A \tag{41}
$$

$$
(\Delta t_{\max})_i = 2V_i \,/ \sum_{\partial C_i} |n_x| A \tag{42}
$$

6 Node-based Differencing with Triangular/Tetrahedral Cells

6.1 Basic definitions

In node-based schemes the variables are defined at the nodes of the computational cells, and because of a critical step in the proofs to be presented we only consider triangular cells. Associated with each node i is the 'supercell' C_i' formed by the union of the triangles with node i, as shown in Figure 3.

The discrete differential operator ∂_x is defined by

$$(\partial_x u)_i = \frac{1}{A_i'} \sum_{\partial C_i'} \overline{u}' n_x' \Delta l' \tag{43}$$

with $\overline{u}'$ on a face defined as the average of the values at the two nodes at either end.

The scalar product is defined by associating $\frac{1}{3}$ of the area of each triangular cell with each of its nodes.

$$(u, v) \equiv \sum_i \tfrac{1}{3} A_i u_i v_i \tag{44}$$

Again it is obvious that this definition satisfies the basic requirements for a scalar product and Property 2.

6.2 Equivalence to cell-centered differencing

To prove that the node-based differencing satisfies properties 1 and 3, we will show that the node-based differencing is equivalent to a cell-based differencing on an alternative cell with a modified area, and hence the proofs of the last section are equally applicable to node-based differencing.

Figure 3 shows the alternative cell C_i for the cell-based differencing, which is formed by joining the centroids of the triangles surrounding node i.

The important geometric relation is that

$$\vec{x}_a = \tfrac{1}{3}(\vec{x}_i + \vec{x}_j + \vec{x}_k), \qquad \vec{x}_b = \tfrac{1}{3}(\vec{x}_i + \vec{x}_j + \vec{x}_l) \tag{45}$$

$$\Longrightarrow \quad (\Delta l \vec{n})_{ij} = \tfrac{1}{3}\left[(\Delta l \vec{n}')_{kj} + (\Delta l \vec{n}')_{jl} \right] \tag{46}$$

Thus the contribution of node j to $(\partial_x u)_i$ is

$$\frac{1}{A_i'} \tfrac{1}{2} \left[(\Delta l \vec{n}')_{kj} + (\Delta l \vec{n}')_{jl} \right] u_j \quad = \quad \frac{1}{A_i'/3} \left(\Delta l n_x \right)_{ij} \tfrac{1}{2} u_j \tag{47}$$

$$
\begin{aligned}
\Longrightarrow \qquad (\partial_x u)_i &= \frac{1}{A'_i/3} \sum_{j\epsilon N_i} \tfrac{1}{2} u_j \, (n_x \Delta l)_{ij} \\
&= \frac{1}{A'_i/3} \sum_{j\epsilon N_i} \tfrac{1}{2} \, (u_i + u_j) \, (n_x \Delta l)_{ij} \\
&= \frac{1}{A'_i/3} \sum_{\partial C_i} \overline{u} \, n_x \Delta l
\end{aligned} \tag{48}
$$

since

$$
\sum_{j\epsilon N_i} u_i \, (n_x \Delta l)_{ij} = u_i \sum_{\partial C_i} n_x \Delta l = 0 \tag{49}
$$

Thus the definition of $\partial_x u$ for node-based differencing on C'_i is identical to the definition of $\partial_x u$ for cell-based differencing on C_i, except that it uses $\frac{1}{3} A'_i$ instead of A_i. For regular grids these two are equal but in general for irregular grids they will not be equal.

Examining all of the proofs in the last section on cell-based differencing, the fact that A_i is the area of the computational cell is not required in any of the proofs, and so any value for A_i can be used provided that value is consistently used in the definition of ∂_x, the scalar product and $\Delta t_{\max}$.

Also interesting is that when using local time-steps the important expressions are $\| \sqrt{\Delta t_{\max}} \, u \|^2$ and $\Delta t_{\max} \partial_x u$, and in both cases the area terms cancel out leaving only $\sum\limits_i u_i^2 \sum\limits_{\partial C_i} |n_x| \Delta l$ and $2 \sum\limits_{\partial C_i} \overline{u} \, n_x \Delta l / \sum\limits_{\partial C_i} |n_x| \Delta l$ respectively. Thus the cell area plays a very minor role and the important terms are due to the faces.

Returning to the node-based differencing, all of the proofs for properties 1 and 3 apply directly with

$$
\Delta t_{\max} = 2 \left(\tfrac{1}{3} A'_i \right) / \sum_{\partial C_i} |n_x| \Delta l \tag{50}
$$

It is interesting that the maximum time step depends on the faces for the equivalent cell-based algorithm. It suggests that in some sense the cell-based differencing is more natural or more basic.

6.3 Extension to 3-D

The extension to 3-D is quite natural, with the cells for the equivalent cell-based algorithm being constructed by joining the centroids of the tetrahedra. ∂_x is defined by

$$
(\partial_x u)_i \quad = \quad \frac{1}{V'_i} \sum_{\partial C'_i} \overline{u}' n'_x A' \qquad \text{node-based}
$$

$$= \quad \frac{1}{\frac{1}{4}V_i'} \sum_{\partial C_i} \overline{u}\, n_x A \quad \text{cell-based} \tag{51}$$

and

$$\Delta t_{\max} = 2\left(\tfrac{1}{4}V_i'\right) / \sum_{\partial C_i} |n_x| A \tag{52}$$

7 Analysis of Systems of Equations

7.1 Analytic equations

To extend the preceding analyses to first order systems of equations we begin by considering the following vector equation.

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{A}\frac{\partial \boldsymbol{u}}{\partial x} + \boldsymbol{B}\frac{\partial \boldsymbol{u}}{\partial y} = 0 \tag{53}$$

$\boldsymbol{u}$ is now a vector of dimension m and $\boldsymbol{A}$ and $\boldsymbol{B}$ are constant $m \times m$ matrices.

The scalar product is now defined as

$$(\boldsymbol{u}, \boldsymbol{v}) = \int_V \boldsymbol{u}^T \boldsymbol{v}\, dV. \tag{54}$$

Property 1 is still satisfied since

$$\begin{aligned}\left(\boldsymbol{u}, \frac{\partial \boldsymbol{v}}{\partial x}\right) + \left(\frac{\partial \boldsymbol{u}}{\partial x}, \boldsymbol{v}\right) &= \int_V \frac{\partial}{\partial x}\left(\boldsymbol{u}^T \boldsymbol{v}\right) dV \\ &= \int_{\partial V} \boldsymbol{u}^T \boldsymbol{v}\, n_x\, dA \\ &= 0 \end{aligned} \tag{55}$$

provided we ignore boundary contributions.

Also it is clear from the definition of the scalar product that

$$(\boldsymbol{u}, \boldsymbol{A}\boldsymbol{v}) = \left(\boldsymbol{A}^T \boldsymbol{u}, \boldsymbol{v}\right). \tag{56}$$

Using these results the energy stability analysis proceeds as follows.

$$\begin{aligned}\frac{dE}{dt} &= \left(\boldsymbol{u}, \frac{\partial \boldsymbol{u}}{\partial t}\right) + \left(\frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{u}\right) \\ &= -\left(\boldsymbol{u}, \boldsymbol{A}\frac{\partial \boldsymbol{u}}{\partial x} + \boldsymbol{B}\frac{\partial \boldsymbol{u}}{\partial y}\right) - \left(\boldsymbol{A}\frac{\partial \boldsymbol{u}}{\partial x} + \boldsymbol{B}\frac{\partial \boldsymbol{u}}{\partial y}, \boldsymbol{u}\right) \\ &= -\left(\boldsymbol{u}, \boldsymbol{A}\frac{\partial \boldsymbol{u}}{\partial x}\right) - \left(\boldsymbol{u}, \boldsymbol{B}\frac{\partial \boldsymbol{u}}{\partial y}\right) - \left(\frac{\partial \boldsymbol{u}}{\partial x}, \boldsymbol{A}^T \boldsymbol{u}\right) - \left(\frac{\partial \boldsymbol{u}}{\partial y}, \boldsymbol{B}^T \boldsymbol{u}\right) \\ &= -\left(\boldsymbol{u}, \left(\boldsymbol{A} - \boldsymbol{A}^T\right)\frac{\partial \boldsymbol{u}}{\partial x}\right) - \left(\boldsymbol{u}, \left(\boldsymbol{B} - \boldsymbol{B}^T\right)\frac{\partial \boldsymbol{u}}{\partial y}\right)\end{aligned} \tag{57}$$

For $\frac{dE}{dt}$ to be zero for all possible $\boldsymbol{u}$ requires that $\boldsymbol{A}$ and $\boldsymbol{B}$ both be symmetric. For the present purposes we are only interested in hyperbolic, energy-preserving systems and so we will assume that this is the case.

7.2 Semi-discrete equations

The semi-discrete analysis assumes that for any symmetric matrix $\boldsymbol{A}$

$$(\boldsymbol{u}, \boldsymbol{A}\boldsymbol{v}) = (\boldsymbol{A}\boldsymbol{u}, \boldsymbol{v}), \tag{58}$$

in addition to the usual basid properties and Property 1. It is clear that these are all satisfied by the scalar product definitions for both cell-centered and node-centered differencing in which

$$(\boldsymbol{u}, \boldsymbol{v}) = \sum_i A_i \boldsymbol{u}_i^T \boldsymbol{v}_i \tag{59}$$

The non-bold A_i is the cell area as defined earlier. A corollary from this assumption is that

$$\begin{aligned}(\boldsymbol{u}, \boldsymbol{A}\partial_x \boldsymbol{u}) &= \tfrac{1}{2}\left[(\boldsymbol{u}, \partial_x \boldsymbol{A}\boldsymbol{u}) + (\boldsymbol{A}\boldsymbol{u}, \partial_x \boldsymbol{u})\right] = 0, &(60)\\ (\boldsymbol{u}, \boldsymbol{B}\partial_y \boldsymbol{u}) &= \tfrac{1}{2}\left[(\boldsymbol{u}, \partial_y \boldsymbol{B}\boldsymbol{u}) + (\boldsymbol{B}\boldsymbol{u}, \partial_y \boldsymbol{u})\right] = 0. &(61)\end{aligned}$$

Hence the stability analysis of the semi-discrete equation,

$$\frac{d\boldsymbol{u}}{dt} + \boldsymbol{A}\partial_x \boldsymbol{u} + \boldsymbol{B}\partial_y \boldsymbol{u} = 0, \tag{62}$$

is simply

$$\begin{aligned}\frac{dE}{dt} &= 2\left(\boldsymbol{u}, \frac{d\boldsymbol{u}}{dt}\right)\\ &= -2(\boldsymbol{u}, \boldsymbol{A}\partial_x \boldsymbol{u}) - 2(\boldsymbol{u}, \boldsymbol{B}\partial_y \boldsymbol{u})\\ &= 0. &(63)\end{aligned}$$

7.3 Discrete equations

The analysis of the fully discrete equations also proceeds almost exactly as before. Omitting the tedious algebra, the final result for the two-step method is

$$\begin{aligned}\left\|\boldsymbol{u}^{n+1}/\sqrt{\Delta t}\right\|^2 - \left\|\boldsymbol{u}^{n}/\sqrt{\Delta t}\right\|^2 &= -\left\|\sqrt{\Delta t}\,(\boldsymbol{A}\partial_x + \boldsymbol{B}\partial_y)\,\boldsymbol{u}^n\right\|^2\\ &\quad + \left\|\sqrt{\Delta t}\,(\boldsymbol{A}\partial_x + \boldsymbol{B}\partial_y)\,\Delta t\,(\boldsymbol{A}\partial_x + \boldsymbol{B}\partial_y)\,\boldsymbol{u}^n\right\|^2 &(64)\end{aligned}$$

and so it is stable provided

$$\left\|\sqrt{\Delta t}\,(\boldsymbol{A}\partial_x + \boldsymbol{B}\partial_y)\,\sqrt{\Delta t}\,\boldsymbol{v}\right\| \le \|\boldsymbol{v}\| \tag{65}$$

for all $\boldsymbol{v}$. For the cell-centered differencing, this is true if $\Delta t_i < (\Delta t_{\max})_i$ where

$$(\Delta t_{\max})_i = 2A_i / \sum_{\partial C_i} |\boldsymbol{A}n_x + \boldsymbol{B}n_y| \Delta l. \tag{66}$$

The matrix norm $|\boldsymbol{C}|$ is defined by

$$|\boldsymbol{C}| = \max_{\boldsymbol{v}} \frac{|\boldsymbol{C}\boldsymbol{v}|}{|\boldsymbol{v}|}, \tag{67}$$

so that $|\boldsymbol{C}\boldsymbol{v}| \leq |\boldsymbol{C}||\boldsymbol{v}|$. If $\boldsymbol{C}$ is symmetric then the norm is equal to the absolute magnitude of the largest eigenvalue of $\boldsymbol{C}$. The proof that the given definition of $\Delta t_{\max}$ is sufficient is again very similar to the scalar proof.

$$\begin{aligned}
&\left\| \sqrt{\Delta t}\, (\boldsymbol{A}\partial_x + \boldsymbol{B}\partial_y)\, \sqrt{\Delta t}\, \boldsymbol{v} \right\|^2 \\
&= \sum_i \frac{\Delta t_i}{A_i} \left| \sum_{\partial C_i} (\boldsymbol{A}n_x + \boldsymbol{B}n_y)\, \overline{\sqrt{\Delta t}\, \boldsymbol{v}}\, \Delta l \right|^2 \\
&= \sum_i \frac{\Delta t_i}{4A_i} \left| \sum_{j \epsilon N_i} \sqrt{\Delta t_j}\, (\boldsymbol{A}n_x + \boldsymbol{B}n_y)_{ij}\, \boldsymbol{v}_j\, \Delta l_{ij} \right|^2 \\
&= \sum_i \frac{\Delta t_i}{4A_i} \left\{ \sum_{j_1 \epsilon N_i} \sum_{j_2 \epsilon N_i} \left(\sqrt{\Delta t_{j_1}}\, (\boldsymbol{A}n_x + \boldsymbol{B}n_y)_{ij_1} \boldsymbol{v}_{j_1} \right)^T \left(\sqrt{\Delta t_{j_2}}\, (\boldsymbol{A}n_x + \boldsymbol{B}n_y)_{ij_2} \boldsymbol{v}_{j_2} \right) \Delta l_{ij_1} \Delta l_{ij_2} \right\} \\
&\leq \sum_i \frac{\Delta t_i}{4A_i} \left\{ \sum_{j_1 \epsilon N_i} \sum_{j_2 \epsilon N_i} \left| \sqrt{\Delta t_{j_1}}\, (\boldsymbol{A}n_x + \boldsymbol{B}n_y)_{ij_1} \boldsymbol{v}_{j_1} \right| \left| \sqrt{\Delta t_{j_2}}\, (\boldsymbol{A}n_x + \boldsymbol{B}n_y)_{ij_2} \boldsymbol{v}_{j_2} \right| \Delta l_{ij_1} \Delta l_{ij_2} \right\} \\
&\leq \sum_i \frac{\Delta t_i}{4A_i} \left\{ \sum_{j_1 \epsilon N_i} \sum_{j_2 \epsilon N_i} \sqrt{\Delta t_{j_1}}\, |\boldsymbol{v}_{j_1}|\, \sqrt{\Delta t_{j_2}}\, |\boldsymbol{v}_{j_2}|\; |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij_1}\, |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij_2}\, \Delta l_{ij_1} \Delta l_{ij_2} \right\} \\
&\leq \sum_i \frac{\Delta t_i}{4A_i} \left\{ \sum_{j_1 \epsilon N_i} \sum_{j_2 \epsilon N_i} \tfrac{1}{2} \left(\Delta t_{j_1} |\boldsymbol{v}_{j_1}|^2 + \Delta t_{j_2} |\boldsymbol{v}_{j_2}|^2 \right) |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij_1}\, |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij_2}\, \Delta l_{ij_1} \Delta l_{ij_2} \right\} \\
&= \sum_i \frac{\Delta t_i}{4A_i} \left\{ \sum_{j_1 \epsilon N_i} |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij_1}\, \Delta l_{ij_1} \right\} \left\{ \sum_{j_2 \epsilon N_i} \Delta t_{j_2} |\boldsymbol{v}_{j_2}|^2\, |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij_2}\, \Delta l_{ij_2} \right\} \\
&= \tfrac{1}{2} \sum_i \sum_{j \epsilon N_i} \Delta t_j |\boldsymbol{v}_j|^2 |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij} \Delta l_{ij} \\
&= \tfrac{1}{2} \sum_j \Delta t_j |\boldsymbol{v}_j|^2 \sum_{i \epsilon N_j} |\boldsymbol{A}n_x + \boldsymbol{B}n_y|_{ij}\, \Delta l_{ij} \\
&= \sum_j A_i |\boldsymbol{v}_j|^2 \\
&= \|\boldsymbol{v}\|^2
\end{aligned} \tag{68}$$

7.4 Euler equations

Abarbanel and Gottlieb [7] have shown that with an appropriate choice of variables the linearized Euler equations can be written in the above first-order form with symmetric matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ equal to

$$\boldsymbol{A} = \begin{pmatrix} u & \sqrt{\frac{1}{\gamma}}c & 0 & 0 \\ \sqrt{\frac{1}{\gamma}}c & u & 0 & \sqrt{\frac{\gamma-1}{\gamma}}c \\ 0 & 0 & u & 0 \\ 0 & \sqrt{\frac{\gamma-1}{\gamma}}c & 0 & u \end{pmatrix}, \quad \boldsymbol{B} = \begin{pmatrix} v & 0 & \sqrt{\frac{1}{\gamma}}c & 0 \\ 0 & v & 0 & 0 \\ \sqrt{\frac{1}{\gamma}}c & 0 & v & \sqrt{\frac{\gamma-1}{\gamma}}c \\ 0 & 0 & \sqrt{\frac{\gamma-1}{\gamma}}c & v \end{pmatrix} \tag{69}$$

With these definitions it is a straightforward exercise to show that the eigenvalues of $\boldsymbol{A}n_x+\boldsymbol{B}n_y$ are $\vec{u}.\vec{n}$, $\vec{u}.\vec{n}$, $\vec{u}.\vec{n}-c$ and $\vec{u}.\vec{n}+c$, where $\vec{u}.\vec{n}$ is the normal flow velocity and c is the speed of sound. Thus it follows that for the cell-based differencing the time step limit is given by

$$(\Delta t_{\max})_i = 2A_i / \sum_{\partial C_i} (|\vec{u}.\vec{n}|+c)\, \Delta l \tag{70}$$

It can be shown that for low Mach number flow over a regular square mesh this 'maximum time step' is a factor $\frac{1}{\sqrt{2}}$ smaller than the value obtained by Fourier analysis, but they are equal in the limit of high Mach number <u>or</u> high cell aspect ratio <u>or</u> high cell skewing. Thus for practical purposes it is a sufficient and almost necessary condition for numerical stability.

As before the theory extends easily to three dimensions, and for the Euler equations the resultant time step limit for cell-based differencing is

$$(\Delta t_{\max})_i = 2V_i / \sum_{\partial C_i} (|\vec{u}.\vec{n}|+c)\, A \tag{71}$$

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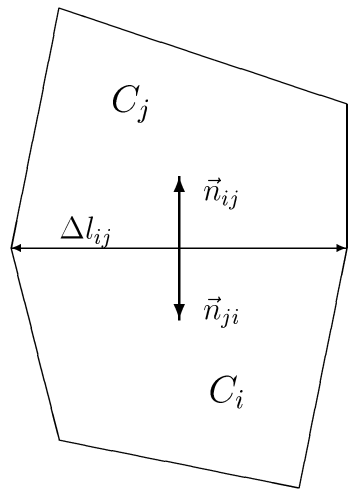

Figure 1: Geometric definitions for cell-based differencing

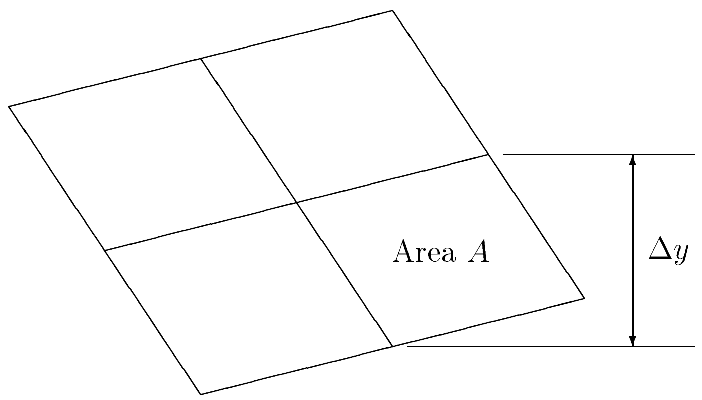

Figure 2: Definition of Δy for regular skewed mesh

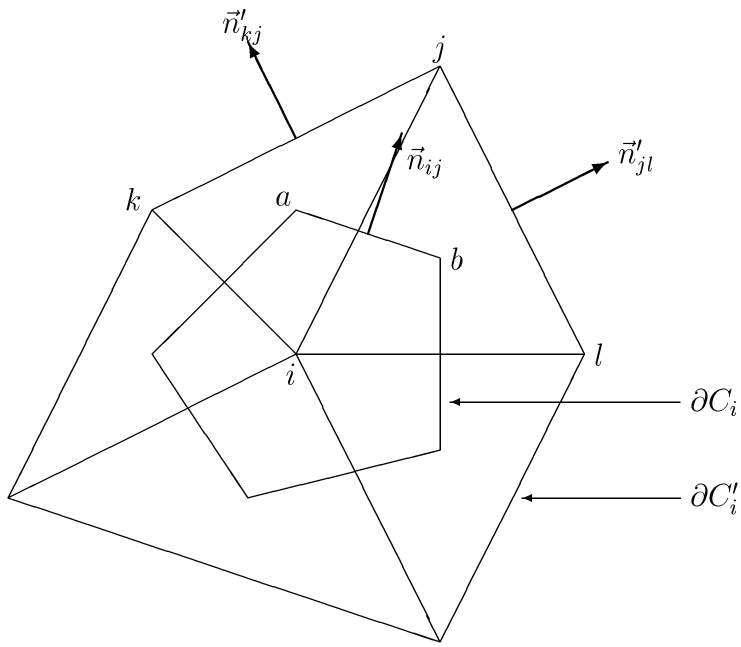

Figure 3: Geometric definitions for node-based differencing