SPAM Numerical Discretizations

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1 Model Equations

The equations of motion used in this model are:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x}+\frac{\partial \rho v}{\partial y}+\frac{\partial \rho w}{\partial z}=0$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}+\frac{1}{\rho}\frac{\partial p}{\partial x}=0$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}+\frac{1}{\rho}\frac{\partial p}{\partial y}=0$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}+\frac{1}{\rho}\frac{\partial p}{\partial z}=-g$$

$$\frac{\partial \rho\theta}{\partial t}+\frac{\partial \rho u\theta}{\partial x}+\frac{\partial \rho v\theta}{\partial y}+\frac{\partial \rho w\theta}{\partial z}=0$$

where ρ is density, u, v, and w are winds in the x-, y-, and z-directions, respectively, θ is potential temperature related to temperature, T, by $\theta = T\left(P_0/P\right)^{R_d/c_p}$, $P_0 = 10^5\,\mathrm{Pa}$, $g = 9.8\ \mathrm{m\,s^{-2}}$ is acceleration due to gravity, $p = C_0\left(\rho\theta\right)^{\gamma}$ is pressure, $C_0 = R_d^{\gamma} p_0^{-R_d/c_v}$, $R_d = 287\,\mathrm{J\,kg^{-1}\,K^{-1}}$, $\gamma = c_p/c_v$, $c_p = 1004\,\mathrm{J\,kg^{-1}\,K^{-1}}$, $c_v = 717\,\mathrm{J\,kg^{-1}\,K^{-1}}$, and $p_0 = 10^5\,\mathrm{Pa}$. Transforming these into a more convenient Jabocian form, we have:

$$\frac{\partial \mathbf{q}}{\partial t}+\frac{\partial \mathbf{f}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial x}+\frac{\partial \mathbf{g}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial x}+\frac{\partial \mathbf{h}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial x}=\mathbf{s}$$

$$\mathbf{q}=\left[\begin{array}{c}\rho\\ u\\ v\\ w\\ \rho\theta\end{array}\right]$$

$$\frac{\partial \mathbf{f}}{\partial \mathbf{q}}=A_x=\left[\begin{array}{ccccc}u & \rho & 0 & 0 & 0\\ 0 & u & 0 & 0 & \frac{c_s^2}{\rho\theta}\\ 0 & 0 & u & 0 & 0\\ 0 & 0 & 0 & u & 0\\ 0 & \rho\theta & 0 & 0 & u\end{array}\right]$$

$$\frac{\partial \mathbf{g}}{\partial \mathbf{q}}=A_y=\left[\begin{array}{ccccc}v & 0 & \rho & 0 & 0\\ 0 & v & 0 & 0 & 0\\ 0 & 0 & v & 0 & \frac{c_s^2}{\rho\theta}\\ 0 & 0 & 0 & v & 0\\ 0 & 0 & \rho\theta & 0 & v\end{array}\right]$$

$$
\frac{\partial \mathbf{h}}{\partial \mathbf{q}} = A_z = \begin{bmatrix} w & 0 & 0 & \rho & 0 \\ 0 & w & 0 & 0 & 0 \\ 0 & 0 & w & 0 & 0 \\ 0 & 0 & 0 & w & \frac{c_s^2}{\rho\theta} \\ 0 & 0 & 0 & \rho\theta & w \end{bmatrix}
$$

$$
\mathbf{s} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -g \\ 0 \end{bmatrix}
$$

Note that the mass continuity equation and the thermodynamic equation are in conservative (flux) form while the motion equations are in non-conservative form. There are ways to treat the entire equation set in non-conservative form that will still conserve ρ and $\rho\theta$.

1.1 Characteristics

Diagonalizing each of the flux Jacobians, $A = R\Lambda R^{-1}$, in the x, y, and z directions, respectively:

$$
\begin{bmatrix} u & \rho & 0 & 0 & 0 \\ 0 & u & 0 & 0 & \frac{c_s^2}{\rho\theta} \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & \rho\theta & 0 & 0 & u \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ -\frac{c_s}{\rho} & \frac{c_s}{\rho} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ \theta & \theta & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -c_s+u & 0 & 0 & 0 & 0 \\ 0 & c_s+u & 0 & 0 & 0 \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{bmatrix} \begin{bmatrix} 0 & -\frac{\rho}{2\,c_s} & 0 & 0 & \frac{1}{2\,\theta} \\ 0 & \frac{\rho}{2\,c_s} & 0 & 0 & \frac{1}{2\,\theta} \\ 1 & 0 & 0 & 0 & -\frac{1}{\theta} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}
$$

$$
\begin{bmatrix} v & 0 & \rho & 0 & 0 \\ 0 & v & 0 & 0 & 0 \\ 0 & 0 & v & 0 & \frac{c_s^2}{\rho\theta} \\ 0 & 0 & 0 & v & 0 \\ 0 & 0 & \rho\theta & 0 & v \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -\frac{c_s}{\rho} & \frac{c_s}{\rho} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ \theta & \theta & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -c_s+v & 0 & 0 & 0 & 0 \\ 0 & c_s+v & 0 & 0 & 0 \\ 0 & 0 & v & 0 & 0 \\ 0 & 0 & 0 & v & 0 \\ 0 & 0 & 0 & 0 & v \end{bmatrix} \begin{bmatrix} 0 & 0 & -\frac{\rho}{2\,c_s} & 0 & \frac{1}{2\,\theta} \\ 0 & 0 & \frac{\rho}{2\,c_s} & 0 & \frac{1}{2\,\theta} \\ 1 & 0 & 0 & 0 & -\frac{1}{\theta} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}
$$

$$
\begin{bmatrix} w & 0 & 0 & \rho & 0 \\ 0 & w & 0 & 0 & 0 \\ 0 & 0 & w & 0 & 0 \\ 0 & 0 & 0 & w & \frac{c_s^2}{\rho\theta} \\ 0 & 0 & 0 & \rho\theta & w \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ -\frac{c_s}{\rho} & \frac{c_s}{\rho} & 0 & 0 & 0 \\ \theta & \theta & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -c_s+w & 0 & 0 & 0 & 0 \\ 0 & c_s+w & 0 & 0 & 0 \\ 0 & 0 & w & 0 & 0 \\ 0 & 0 & 0 & w & 0 \\ 0 & 0 & 0 & 0 & w \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & -\frac{\rho}{2\,c_s} & \frac{1}{2\,\theta} \\ 0 & 0 & 0 & \frac{\rho}{2\,c_s} & \frac{1}{2\,\theta} \\ 1 & 0 & 0 & 0 & -\frac{1}{\theta} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}
$$

where R is the matrix whose columns are right eigenvectors, Λ is the matrix whose diagonal components are eigenvalues, $R^{-1} \equiv L$ is the matrix whose rows are left eigenvectors, and $c_s = \sqrt{\gamma p/\rho}$ is the speed of sound. The eigenvectors create "characteristic" variables that travel at velocities denoted by the eigenvalues:

$$
\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial x} = \mathbf{0} \implies \frac{\partial \mathbf{q}}{\partial t} + R\Lambda L\frac{\partial \mathbf{q}}{\partial x} = \mathbf{0} \implies L\frac{\partial \mathbf{q}}{\partial t} + \Lambda L\frac{\partial \mathbf{q}}{\partial x} = \mathbf{0}
$$

If you assume the flux Jacobian is locally constant with respect to space and time (the so-called "locally frozen" approximation), you get:

$$
\frac{\partial L\mathbf{q}}{\partial t} + \Lambda\frac{\partial L\mathbf{q}}{\partial x} = \mathbf{0} \implies \frac{\partial}{\partial t}\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{bmatrix} + \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 \\ 0 & 0 & 0 & \lambda_4 & 0 \\ 0 & 0 & 0 & 0 & \lambda_5 \end{bmatrix} \frac{\partial}{\partial x}\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{bmatrix} = \mathbf{0}
$$

This is a decoupled set of simple transport equations, showing characteristic variables, $w_p = \ell_p \cdot \mathbf{q}$, travelling at finite and non-zero speed, λ_p, where ℓ_p is the p-th row of L, and λ_p is the pth diagonal component of Λ.

1.2 Acoustic Stiffness

The two wave speeds in play in this hyperbolic equation set are wind velocity u, v, and w, and the acoustic speed, $c_s = \sqrt{\gamma p/\rho}$. Acoustics travel the fastest at the Earth's surface with a speed of roughly $c_s \approx \sqrt{1.4 \cdot 10^5 \cdot 1.1^{-1}} \approx 360$ m/s. In the global atmosphere, winds in jet streak maxima and in the stratosphere can reach up to 80 m/s, which is only 4.5× smaller than the speed of sound. Therefore, the global atmosphere cannot really be described as "stiff" – certainly not enough to warrant a numerical method with global data dependence (e.g., time implicit, anelastic, or spectral). At the throughputs climate must reach, the per-node workloads on compute nodes in a parallel computer are quite small, and the cost of data transfers across a large machine are prohibitively large. Four cycles of nearest neighbor communication is faster than multiple iterations of MPI_AllReduce() calls for implicit methods, or a single set of MPI_AllToAll() for spectral at scale on the largest computers available today.

However, there is significant acoustic stiffness in two different contexts: (1) the vertical direction, and (2) limited area models.

In the vertical direction, the grid spacing is significantly smaller than in the horizontal directions. Making this situation more extreme is the fact that the vertical grid is stretched to give more levels near the Earth's surface, and the level nearest the Earth's surface often has a grid spacing in several meters to tens of meters. If we also consider that vertical velocity in that cell is often very close to zero, we suddenly have an acoustic speed that is usually more than 100× larger than wind speed. This is something we would consider very stiff, and this is the reason for Horizontally Explicit, Vertically Implicit (HEVI) methods. Regardless, handling vertical stiffness separately is often necessary in non-hydrostatic models, which admit acoustics in the vertical direction.

The other context in which acoustics can be stiff in the atmosphere is in limited area models. Jet streaks and large stratospheric winds comprise a relatively small surface area of the sphere, so most limited area models, especially over a small snapshot of time will have wind speeds significantly smaller, and in these cases, acoustics can be $> 10\times$ more than the speed of wind. While less stiff than the vertical direction, it is still advantageous to be able to use a time step larger than that determined by acoustics.

2 Spatial Discretization

SPAM uses the Finite-Volume approach to integarting the Euler equations. This allows upwind fluxes between cells to add dissipation to the model, enough that the model is stable without any additional limiting. Also, this allows treating each Degree of Freedom (DOF) individually, which is advantageous when sharp discontinuities need to be resolved. Finally, Finite-Volume allows a large maximum stable CFL value of one when paried with a fully discrete time discretization, and this large CFL value remains fixed no matter how high-order-accurate the numerics are. This is in contrast with Galerkin element-based methods, which have time steps that decrease superlinearly with increasing order of accuracy and must limit DOFs together in blocks rather than individually.

For simplicity, consider the 1-D generic Jacobian-form equation:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial x} = \mathbf{0}$$

If we partition assume the domain is fully and uniquely spanned by non-overlapping cells, we can integrate over a single cell domain, $\Omega_i \in \left[x_{i-1/2}, x_{i+1/2}\right]$, where $x_{i\pm1/2} = x_i \pm \Delta x_i$:

$$\int_{\Omega_i} \frac{\partial \mathbf{q}}{\partial t} dx + \int_{\Omega_i} \frac{\partial \mathbf{f}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial x} dx = \mathbf{0}$$

$$\frac{\partial \overline{\mathbf{q}}_i}{\partial t}\Delta x_i + \int_{\Omega_i} A\frac{\partial \mathbf{q}}{\partial x} dx = \mathbf{0}$$

where the overbar decorator denotes a cell average over the domain Ω_i. If we split the Jacobian into characteristics, then the update for each cell is split into three components: (1) rightward fluctuations propagating in from the left cell interface ($A^+_{i-1/2}\delta\mathbf{q}_{i-1/2}$), (2) leftward fluctuations propagating in from the right cell interface ($A^-_{i+1/2}\delta\mathbf{q}_{i+1/2}$), and (3) The integral computed over the cell domain ($\int_{\Omega_i} A\frac{\partial \mathbf{q}}{\partial x}dx$):

$$\frac{\partial \overline{\mathbf{q}}_i}{\partial t}\Delta x_i + A^+_{i-1/2}\delta\mathbf{q}_{i-1/2} + A^-_{i+1/2}\delta\mathbf{q}_{i+1/2} + \int_{\Omega_i} A\frac{\partial \mathbf{q}}{\partial x}dx = \mathbf{0}$$

The last term can be computed via quadrature for terms cast in non-conservation form. However, for terms for which the flux vector actually exists, it can be exactly computed via:

$$\int_{\Omega_i} A\frac{\partial \mathbf{q}}{\partial x}dx = \mathbf{f}^-_{i+1/2} - \mathbf{f}^+_{i-1/2}$$

Further, when the flux vector exists, this formulation renders the overall scheme conservative for those terms. However, for terms for which the flux vector does not exist (thus the need for quadrature to evaluate this integral), in general, those quantities are not conserved.

The fluctuation matrices A^+ and A^-, are created by reconstituting the flux Jacobian using only the rightward and leftward propagating eigenvalues, respectively:

$$A^-_{i-1/2} = \sum_{p:\lambda_p<0} \left(\ell_p \cdot \delta\mathbf{q}_{i-1/2}\right)\mathbf{r}_p$$

$$A^+_{i-1/2} = \sum_{p:\lambda_p>0} \left(\ell_p \cdot \delta\mathbf{q}_{i-1/2}\right)\mathbf{r}_p$$

In our case, however, we do not compute the fluctuations as $A^{\pm}\delta\mathbf{q}$. Rather, we create characteristics based on $A\delta\mathbf{q}$ as opposed to $\mathbf{q}$ itself. Mathematically, this is equivalent to left-multiplying the equation by the flux Jacobian before we split the flux difference into propagating characteristics, which further implies:

$$\mathcal{Z}^-_{i-1/2} = A^-_{i-1/2}\delta\mathbf{q}_{i-1/2} = \sum_{p:\lambda_p<0} \left(\ell_p \cdot \left(A_{i-1/2}\delta\mathbf{q}_{i-1/2}\right)\right)\mathbf{r}_p$$

$$\mathcal{Z}^+_{i-1/2} = A^+_{i-1/2}\delta\mathbf{q}_{i-1/2} = \sum_{p:\lambda_p>0} \left(\ell_p \cdot \left(A_{i-1/2}\delta\mathbf{q}_{i-1/2}\right)\right)\mathbf{r}_p$$

The advantage of this form is that for variables for which the flux vector exists, this scheme is conservative with any linearization of the locally frozen flux Jacobian. Without this treatment, we would have to create an analog of the Roe averaging to achieve conservation of ρ and $\rho\theta$, which may or may not exist for this particular equation set.