Characteristic-Based Flux Splitting for Implicit-Explicit Time Integration of Low-Mach Number Flows

Debojyoti Ghosh  Emil M. Constantinescu

Mathematics & Computer Science
Argonne National Laboratory

13th U. S. National Congress on Computational Mechanics (USNCCM13)
San Diego, CA, July 26 – 30, 2015
Motivation & Objectives

Numerical simulation of atmospheric flows

Governing equations: 2D Euler equations with gravitational forces (conservation of mass, momentum and energy)

\[
\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} \rho u^2 + p \\ \rho u v \\ \rho v^2 + p \\ (e + p)u \end{bmatrix} + \frac{\partial}{\partial y}\begin{bmatrix} \rho u v \\ \rho v^2 + p \\ (e + p)v \end{bmatrix} = \begin{bmatrix} 0 \\ \rho g \cdot \hat{i} \\ \rho g \cdot \hat{j} \\ \rho u g \cdot \hat{i} + \rho v g \cdot \hat{j} \end{bmatrix}
\]

Time scales: \(\text{entropy} \quad (u) \ll \text{acoustic} \quad (u \pm a)\)

Time integration

- **Explicit time-integration** \(\Rightarrow\) time step size restricted by acoustic waves; but acoustic waves do not significantly impact any atmospheric phenomenon.
- **Implicit time-integration** \(\Rightarrow\) Unconditionally stable; but requires solutions to non-linear system or linearized approximation.
- **Implicit-Explicit (IMEX) time-integration** \(\Rightarrow\) Integrate “fast” waves implicitly, “slow” waves explicitly.
  - **Characteristic-based partitioning of the hyperbolic flux** (Acoustic waves integrated implicitly, entropy waves integrated explicitly)

Other (more popular) forms of the governing equations

- **Exner pressure, velocity, potential temperature:**
  - COAMPS (US Navy), NMM (NCEP), MM5 (NCAR/PSU).
- **Mass, momentum, potential temperature:**
  - WRF (NCAR), NUMA (NPS).

**Selective preconditioning of acoustic modes**

- Implicit Continuous Eulerian (ICE) technique ([Harlow, Amsden, 1971](#))
- Preconditioning applied to stiff modes ([Reynolds, Samtaney, Woodward, 2010](#))
Spatial Discretization

Conservative finite-difference discretization of a hyperbolic conservation law

\[ u_t + f(u)_x = 0; \quad f'(u) \in \mathbb{R} \]

\[
\frac{du_j}{dt} + \frac{1}{\Delta x} \left[ f(x_{j+1/2}, t) - f(x_{j-1/2}, t) \right] = 0
\]

**Weighted Essentially Non-Oscillatory (WENO) Schemes**

- Weights depend on the local smoothness of the solution
- Optimal weights in smooth regions allow \((2r-1)th\) order accuracy
- Near-zero weights for stencils with discontinuities \(\rightarrow\) non-oscillatory behavior
- Compact-Reconstruction WENO (CRWENO) \(\rightarrow\) Higher spectral resolution and lower absolute errors for same order of convergence

\[
f_{j+1/2}^{(WENO)}(r) = \sum_{k=1}^{r} \omega_k f_{k,j+1/2}^{(r)}
\]

\[
\omega_k = \omega(IS_k)
\]

**WENO5**

\[
\hat{f}_{j+1/2}^{(5)} = \frac{1}{30} f_{j-2} - \frac{13}{60} f_{j-1} + \frac{47}{60} f_j + \frac{27}{60} f_{j+1} - \frac{1}{20} f_{j+2}
\]

**CRWENO5** (Compact finite difference scheme)

\[
\frac{3}{10} \hat{f}_{j-1/2}^{(5)} + \frac{6}{10} \hat{f}_{j+1/2}^{(5)} + \frac{1}{10} \hat{f}_{j+3/2}^{(5)} = \frac{1}{30} f_{j-1} + \frac{19}{30} f_j + \frac{1}{3} f_{j+1}
\]
Characteristic-based Flux Splitting (1)

Separation of **acoustic** and **entropy** modes in the flux for implicit-explicit time integration

**1D Euler equations**

\[
\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{u})}{\partial x} = 0
\]

**Semi-discrete ODE in time**

\[
\frac{\partial \mathbf{u}}{\partial t} = \hat{\mathbf{F}}(\mathbf{u}) = \left[ \mathcal{D} \otimes \mathcal{A}(\mathbf{u}) \right] \mathbf{u}
\]

**Example:** Periodic density sine wave on a unit domain discretized by \( N=80 \) points.

**Eigenvalues of the CRWENO5 discretization**

**Eigenvalues of the right-hand-side operator** \((u=0.1, a=1.0, dx=0.0125)\)

**Discretization operator** (e.g.: WENO5, CRWENO5)

**Flux Jacobian**

\[
\text{eig} \left[ \frac{\partial \hat{\mathbf{F}}}{\partial \mathbf{u}} \right] = \text{eig} [\mathcal{D}] \times \text{eig} [\mathcal{A}(\mathbf{u})]
\]

**Time step size limit for linear stability**

**Eigenvalues of the right-hand-side of the ODE** are the **eigenvalues of the discretization operator** times the **characteristic speeds** of the physical system.
Characteristic-based Flux Splitting (2)

Splitting of the flux Jacobian based on its eigenvalues

\[
\frac{\partial \mathbf{u}}{\partial t} = \hat{\mathbf{F}}(\mathbf{u}) = \left[ \mathcal{D} \otimes \mathcal{A}(u) \right] \mathbf{u} \\
= \left[ \mathcal{D} \otimes \mathcal{A}_S(u) + \mathcal{D} \otimes \mathcal{A}_F(u) \right] \mathbf{u} \\
= \hat{\mathbf{F}}_S(\mathbf{u}) + \hat{\mathbf{F}}_F(\mathbf{u})
\]

“Slow” flux  “Fast” flux

\[
\mathcal{A}(\mathbf{u}) = \mathcal{R} \Lambda \mathcal{L} \\
\Lambda_S = \begin{bmatrix} u & 0 \\ 0 & 0 \end{bmatrix} \\
\Lambda_F = \begin{bmatrix} 0 & u + a \\ u - a & 0 \end{bmatrix}
\]

Example: Periodic density sine wave on a unit domain discretized by \( N=80 \) points (CRWENO5).

Small difference between the eigenvalues of the complete operator and the split operator.

(Not an error)

\[
\text{eig} \left[ \frac{\partial \hat{\mathbf{F}}_S(\mathbf{u})}{\partial \mathbf{u}} \right] \approx u \times \text{eig} [\mathcal{D}] \\
\text{eig} \left[ \frac{\partial \hat{\mathbf{F}}_F(\mathbf{u})}{\partial \mathbf{u}} \right] \approx \{u \pm a\} \times \text{eig} [\mathcal{D}] 
\]
IMEX Time Integration with Characteristic-based Flux Splitting (1)

Apply **Implicit-Explicit Runge-Kutta** (PETSc - **TSARKIMEX**) time-integrators

\[
U^{(i)} = u_n + \Delta t \sum_{j=1}^{i-1} a_{ij} \hat{F}_S \left( U^{(j)} \right) + \Delta t \sum_{j=1}^{i} \tilde{a}_{ij} \hat{F}_F \left( U^{(j)} \right)
\]

**Stage values**

\( (s \text{ stages}) \)

\[
u_{n+1} = u_n + \Delta t \sum_{i=1}^{s} b_i \hat{F}_S \left( U^{(i)} \right) + \Delta t \sum_{i=1}^{s} \tilde{b}_i \hat{F}_F \left( U^{(i)} \right)
\]

**Step completion**

**Non-linear system of equations**

\[
\hat{F}_F \left( u \right) = \left[ D \left( \omega \right) \otimes A_F \left( u \right) \right] u
\]

\( \omega = \omega \left[ F \left( u \right) \right] \)

**Solution-dependent** weights for the WENO5/CRWENO5 scheme

**Linearized Formulation**

Redefine the splitting as

\[
F_F \left( u \right) = \left[ A_F \left( u_n \right) \right] u
\]

\[
F_S \left( u \right) = F \left( u \right) - F_F \left( u \right)
\]

Note: Introduces **no error** in the governing equation.

At the beginning of a time step:-

\[
\text{eig} \left[ \frac{\partial \hat{F}_S}{\partial u} \right] = u \times \text{eig} \left[ D \right], \quad \text{eig} \left[ \frac{\partial \hat{F}_F}{\partial u} \right] = \{ u \pm a \} \times \text{eig} \left[ D \right]
\]

**Is \( F_F \) a good approximation at each stage?**
**Linearization of the WENO/CRWENO discretization:** Within a stage, the non-linear coefficients are kept fixed.

**Linear system of equations for implicit stages:**

\[ [I - \Delta t\tilde{a}_{ii} D \otimes A_F (u_n)] U^{(i)} = u_n + \Delta t \sum_{j=1}^{i-1} a_{ij} \hat{F}_S \left( U^{(j)} \right) + \Delta t \left[ D \otimes A_F (u_n) \right] \sum_{j=1}^{i-1} \tilde{a}_{ij} U^{(j)}, \]

\[ i = 1, \ldots, s \]

**Preconditioning** (Preliminary attempts)

\[ P = [I - \Delta t\tilde{a}_{ii} D^{(1)} \otimes A_F (u_n)] \approx [I - \Delta t\tilde{a}_{ii} D \otimes A_F (u_n)] \]

**First order upwind discretization**

- Periodic boundaries ignored

- **Jacobian-free approach** \(\rightarrow\) Linear Jacobian defined as a function describing its action on a vector (MatShell)

- **Preconditioning matrix** \(\rightarrow\) Stored as a sparse matrix (MatAIJ)

**ARK Methods** (PETSc)

**ARKIMEX 2c**
- 2\(^{nd}\) order accurate
- 3 stage (1 explicit, 2 implicit)
- L-Stable implicit part
- Large real stability of explicit part

**ARKIMEX 2e**
- 2\(^{nd}\) order accurate
- 3 stage (1 explicit, 2 implicit)
- L-Stable implicit part

**ARKIMEX 3**
- 3\(^{rd}\) order accurate
- 4 stage (1 explicit, 3 implicit)
- L-Stable implicit part

**ARKIMEX 4**
- 4\(^{th}\) order accurate
- 5 stage (1 explicit, 4 implicit)
- L-Stable implicit part
Example: 1D Density Wave Advection

Initial solution \( \rho = \rho_\infty + \hat{\rho} \sin (2\pi x), u = u_\infty, p = p_\infty; \ 0 \leq x \leq 1 \)

\[ M_\infty = 0.1 \]

Eigenvalues \( M_\infty = 0.01 \)

C R W E N O 5, 320 grid points

Semi-implicit time step size limit determined by the flow velocity

\( \approx 10x \)

\( \approx 100x \)
Example: 1D Density Wave Advection (Computational Cost)

\[ M_\infty = 0.1 \]

\[ M_\infty = 0.01 \]

**Number of function calls**

- ARK2c - No preconditioner
- ARK2c - Block Jacobi
- ARK2c - ILU(0)
- RK2a

**Error (L₂)**

\[ \approx 5x \]

**Wall time**

\[ \approx 4x \]

**Error (L₂)**

\[ \approx 60x \]

**Wall time**

\[ \approx 45x \]
Example: Low Mach Isentropic Vortex Convection

Freestream flow
\[
\begin{align*}
\rho_\infty &= 1 \\
p_\infty &= 1 \\
u_\infty &= 0.1 \\
v_\infty &= 0
\end{align*}
\]
\[M_\infty \approx 0.08\]

Vortex (Strength \(b = 0.5\))
\[
\begin{align*}
\rho &= \left[ 1.0 - \frac{(\gamma - 1) b^2}{8\gamma\pi^2} \exp \left( 1 - r^2 \right) \right]^{\frac{1}{\gamma-1}} \\
p &= \left[ 1.0 - \frac{(\gamma - 1) b^2}{8\gamma\pi^2} \exp \left( 1 - r^2 \right) \right]^{\frac{\gamma}{\gamma-1}} \\
u &= u_\infty - \frac{b}{2\pi} \exp \left( \frac{1 - r^2}{2} \right) (y - y_c) \\
v &= v_\infty + \frac{b}{2\pi} \exp \left( \frac{1 - r^2}{2} \right) (x - x_c)
\end{align*}
\]

- Optimal orders of convergence observed for all methods
- Time step size limited by the “slow” eigenvalues.
Example: Vortex Convection (Computational Cost)

**ARK 2c**

- **Number of function calls**
  - Graph showing the relationship between error ($L_2$) and number of RHS function calls.
  - Different methods: ARK2c - No preconditioner, ARK2c - Block Jacobi, ARK2c - ILU(0), ARK2c - LU, RK2a.

- **Wall time**
  - Graph showing the relationship between error ($L_2$) and wall time (seconds).
  - Different methods: ARK2c - No preconditioner, ARK2c - Block Jacobi, ARK2c - ILU(0), ARK2c - LU, RK2a.

**ARK 3**

- **Number of function calls**
  - Graph showing the relationship between error ($L_2$) and number of RHS function calls.
  - Different methods: ARK3 - No preconditioner, ARK3 - Block Jacobi, ARK3 - ILU(0), ARK3 - LU, RK3.

- **Wall time**
  - Graph showing the relationship between error ($L_2$) and wall time (seconds).
  - Different methods: ARK3 - No preconditioner, ARK3 - Block Jacobi, ARK3 - ILU(0), ARK3 - LU, RK3.
Example: Inertia – Gravity Wave

- Periodic channel – 300 km x 10 km
- No-flux boundary conditions at top and bottom boundaries
- Mean horizontal velocity of 20 m/s in a uniformly stratified atmosphere ($M_\infty \approx 0.06$)
- Initial solution – Potential temperature perturbation

Potential temperature perturbations at 3000 seconds (Solution obtained with WENO5 and ARKIMEX 2e, 1200x50 grid points)

<table>
<thead>
<tr>
<th>CFL</th>
<th>Wall time (s)</th>
<th>Function counts</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.5</td>
<td>6149</td>
<td>24800</td>
</tr>
<tr>
<td>13.6</td>
<td>4118</td>
<td>17457</td>
</tr>
<tr>
<td>17.0</td>
<td>3492</td>
<td>14820</td>
</tr>
<tr>
<td>20.4</td>
<td>2934</td>
<td>12895</td>
</tr>
</tbody>
</table>

RK4
CFL ~ 1.0
Wall time: 5400 s
Function counts: 24000

Cross-sectional potential temperature perturbations at 3000 seconds ($y = 5$ km) at various CFL numbers (0.2 – 13.6)

Grid: 300x10 points, CRWENO5
Conclusions

Characteristic-based flux splitting (Work in progress):

- Partitioning of flux separates the acoustic and entropy modes \rightarrow Allow larger time step sizes (determined by flow velocity, not speed of sound).

- Comparison to alternatives
  - Vs. explicit time integration: Larger time steps \rightarrow More efficient algorithm
  - Vs. implicit time integration: Semi-implicit solves a linear system without any approximations to the overall governing equations (as opposed to: solve non-linear system of equations or linearize governing equations in a time step).

To do:

- Improve efficiency of the linear solve
  - Better preconditioning of the linear system

- Extend to 3D flow problems
Thank you!

Acknowledgements