A Compact-Reconstruction WENO Scheme with Semi-Implicit Time Integration

Debojyoti Ghosh **Emil M. Constantinescu**

Mathematics & Computer Science
Argonne National Laboratory

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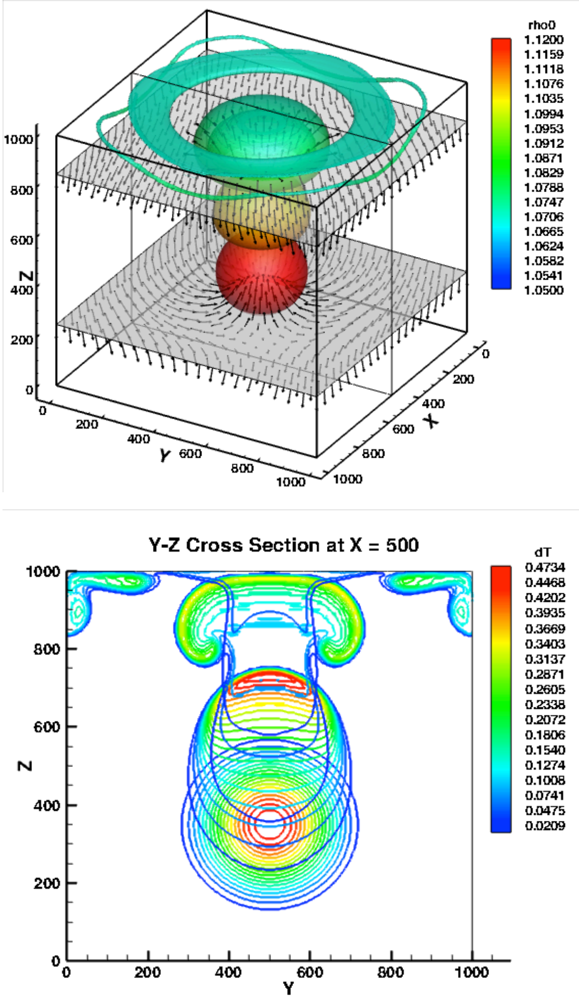
Background and Motivation

Numerical Solution of Atmospheric Flows

- Characterized by **large range of length** and **time scales**
- Compressibility → **High gradients**
- Various **forms of the governing equations**
    - **Exner pressure** and **potential temperature** → Mass, momentum, energy **not conserved** – Examples: **COAMPS** (US Navy), **NMM** (NCEP), **MM5** (NCAR/PSU) .
    - Conservation of mass and momentum; energy equation expressed as **conservation of potential temperature** (adiabatic assumption) – Examples: **WRF** (NCAR), **NUMA** (NPS).

High order accurate, conservative finite-difference solver

- **Conservation of mass, momentum and energy**
    - Conserve energy to machine precision
    - Specification of true viscous terms, if required.
- Spatial discretization (**high order**, **high spectral resolution**, **non-oscillatory**) – 5th order **WENO** and **CRWENO** schemes
- Time integration (**stable** – linear/non-linear, **optimal**, **efficient**)
    - **Multi-stage implicit-explicit (IMEX)** methods



Rising Thermal Bubble in Hydrostatically Balanced Atmosphere Solution obtained with NUMA (http://faculty.nps.edu/fxgirald/projects/NUMA/

WENO and CRWENO Schemes – Brief Overview

Weighted Essentially Non-Oscillatory (WENO) Schemes

- Weighted combination of ***r*** **interpolation schemes** of ***r*-th order accuracy**
- **Weights ← local smoothness of the solution**
- Optimal weights in smooth regions allow ***(2r-1)*th order accuracy**
- Near-zero weights for stencils with discontinuities → **non-oscillatory behavior**

$$f^{(2r-1)}_{j+1/2} = \sum_{k=1}^{r} c_k f^{(r)}_{k,j+1/2}$$

$$f^{(\mathrm{WENO})}_{j+1/2} = \sum_{k=1}^{r} \omega_k f^{(r)}_{k,j+1/2}$$

$\omega_k = \omega\left(IS_k\right)$ **Smoothness indicator**

Compact-Reconstruction WENO

$$\mathcal{A}\left(f^{(r)}_{j+1/2-m}, \cdots, f^{(r)}_{j+1/2+m}\right) = \mathcal{B}\left(f_{j-n}, \cdots, f_{j+n}\right)$$

Example: CRWENO5 (*r* = 3)

$$\frac{2}{3}\hat{f}^{(3)}_{1,j-1/2} + \frac{1}{3}\hat{f}^{(3)}_{1,j+1/2} = \frac{1}{6}\left(f_{j-1} + 5f_j\right);\ c_1 = \frac{2}{10}$$

$$\frac{1}{3}\hat{f}^{(3)}_{2,j-1/2} + \frac{2}{3}\hat{f}^{(3)}_{2,j+1/2} = \frac{1}{6}\left(5f_j + f_{j+1}\right);\ c_2 = \frac{5}{10}$$

$$\frac{2}{3}\hat{f}^{(3)}_{3,j+1/2} + \frac{1}{3}\hat{f}^{(3)}_{3,j+3/2} = \frac{1}{6}\left(f_j + 5f_{j+1}\right);\ c_3 = \frac{3}{10}$$

$$\frac{3}{10}\hat{f}^{(5)}_{j-1/2} + \frac{6}{10}\hat{f}^{(5)}_{j+1/2} + \frac{1}{10}\hat{f}^{(5)}_{j+3/2} = \frac{1}{30}f_{j-1} + \frac{19}{30}f_j + \frac{1}{3}f_{j+1}$$

Standard WENO Schemes:

$$f^{(r)}_{j+1/2} = \mathcal{B}\left(f_{j-n}, \cdots, f_{j+n}\right)$$

Example: WENO5 (*r* = 3)

$$\hat{f}^{(3)}_{1,j+1/2} = \frac{1}{3}f_{j-2} - \frac{7}{6}f_{j-1} + \frac{11}{6}f_j,\ c_1 = \frac{1}{10}$$

$$\hat{f}^{(3)}_{1,j+1/2} = -\frac{1}{6}f_{j-1} + \frac{5}{6}f_j + \frac{1}{3}f_{j+1},\ c_2 = \frac{6}{10}$$

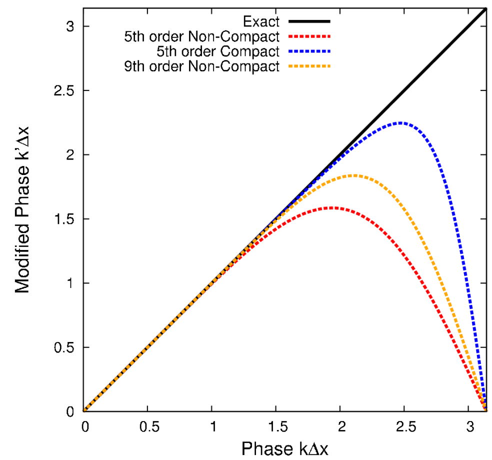
$$\hat{f}^{(3)}_{1,j+1/2} = \frac{1}{3}f_j + \frac{5}{6}f_{j+1} - \frac{1}{6}f_{j+2},\ c_3 = \frac{3}{10}$$

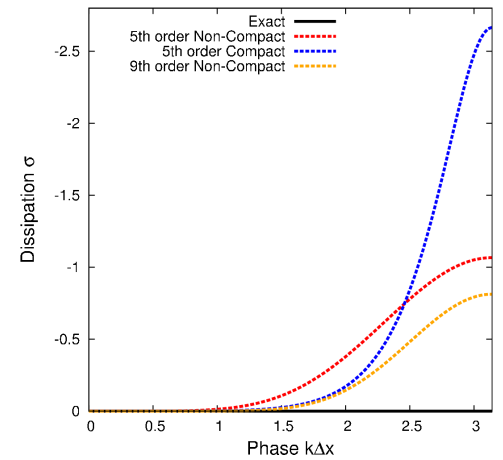
$$\hat{f}^{(5)}_{j+1/2} = \frac{1}{30}f_{j-2} - \frac{13}{60}f_{j-1} + \frac{47}{60}f_j + \frac{27}{60}f_{j+1} - \frac{1}{20}f_{j+2}$$

Why CRWENO? (Accuracy, Resolution)

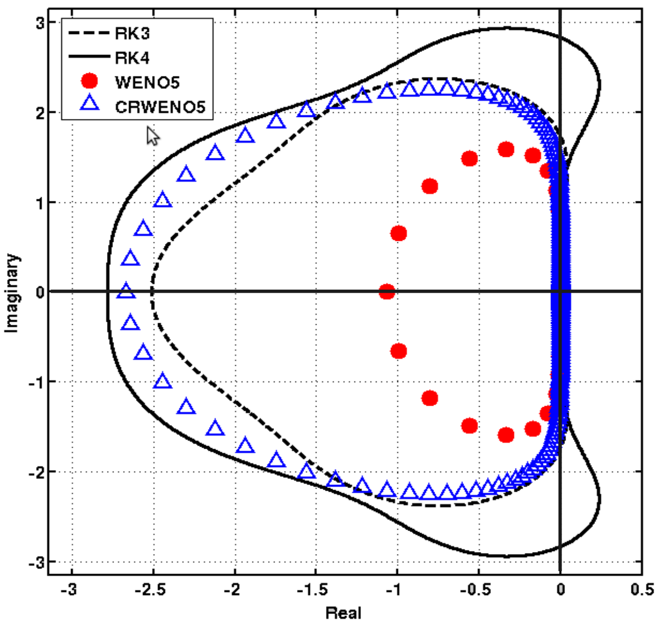
Taylor series analysis:

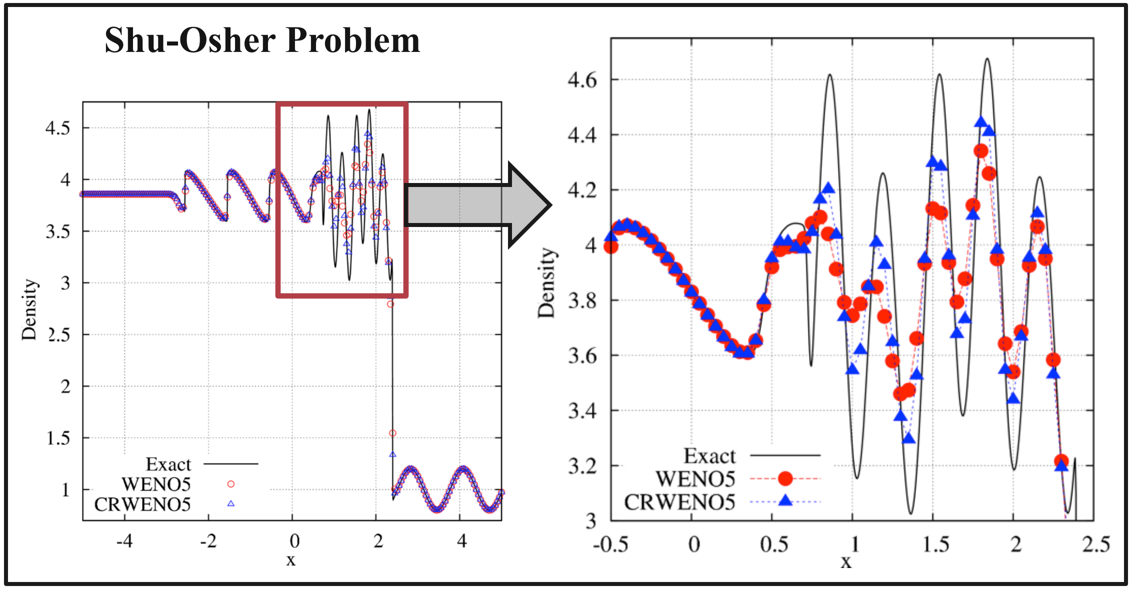
	Dissipation	Dispersion
WENO5	$\frac{1}{60}\left.\frac{\partial^6 f}{\partial x^6}\right\vert_j \Delta x^5$	$\frac{1}{140}\left.\frac{\partial^7 f}{\partial x^7}\right\vert_j \Delta x^6$
CRWENO5	$\frac{1}{600}\left.\frac{\partial^6 f}{\partial x^6}\right\vert_j \Delta x^5$	$\frac{1}{2100}\left.\frac{\partial^7 f}{\partial x^7}\right\vert_j \Delta x^6$





Fourier Analysis: Higher spectral resolution than the 5th (WENO5) and 9th order (WENO9) non-compact schemes.





➔ WENO5 requires **~ 1.5 times more grid points per dimension** to yield a solution of comparable accuracy as the CRWENO5 scheme, and time step size limit is **~ 1.6 times smaller** for CRWENO than WENO5.

Implicit-Explicit Time Integration

Implicit-Explicit time integration for atmospheric flows: Giraldo, Restelli, Laeuter (2010): **Non-hydrostatic Unified Model of the Atmosphere (NUMA)** – Spectral-element solver, operational weather prediction code used by U.S. Navy.

Governing equations expressed in **perturbation form**

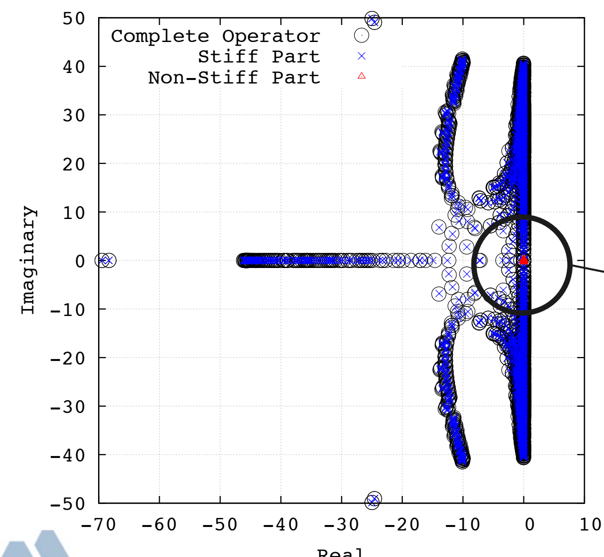
$$\frac{\partial}{\partial t}\begin{bmatrix}\rho' \\ \rho\mathbf{u} \\ \Theta'\end{bmatrix} + \begin{bmatrix}\nabla\cdot(\rho\mathbf{u}) \\ \nabla(\rho\mathbf{u}\otimes\mathbf{u} - P') - \rho g\hat{\mathbf{k}} \\ \nabla\cdot(\Theta\mathbf{u})\end{bmatrix} = 0$$

IMEX splitting based on the **order of perturbation**

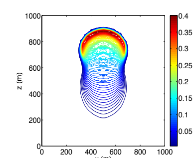
$$\frac{\partial}{\partial t}\begin{bmatrix}\rho' \\ \rho\mathbf{u} \\ \Theta'\end{bmatrix} = \begin{bmatrix}0 \\ -\nabla\rho\mathbf{u}\otimes\mathbf{u} \\ -\nabla\cdot(\Theta'\mathbf{u})\end{bmatrix} + \begin{bmatrix}-\nabla\cdot(\rho\mathbf{u}) \\ \nabla P' + \rho g\hat{\mathbf{k}} \\ -\nabla\cdot(\Theta_0\mathbf{u})\end{bmatrix}$$

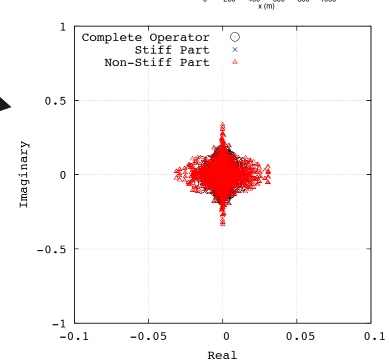
Non-Stiff (Explicit)

Stiff (Implicit)



Rising Thermal Bubble





- Non-stiff eigenvalues orders of magnitude smaller.
- **Time step size restricted by the smaller, non-stiff eigenvalues**

Characteristic-based Flux Splitting (1)

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

1D Euler equations

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

Spatial discretization

Semi-discrete ODE in time

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

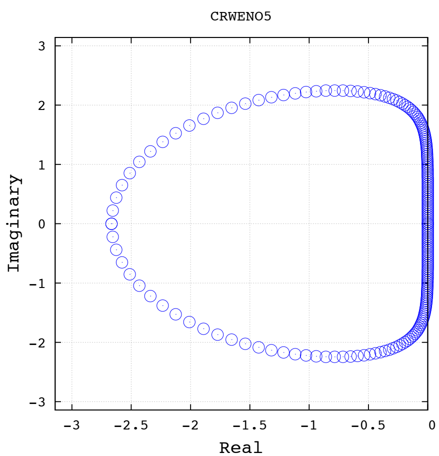
Discretization operator (e.g.:WENO5, CRWENO5)

Flux Jacobian

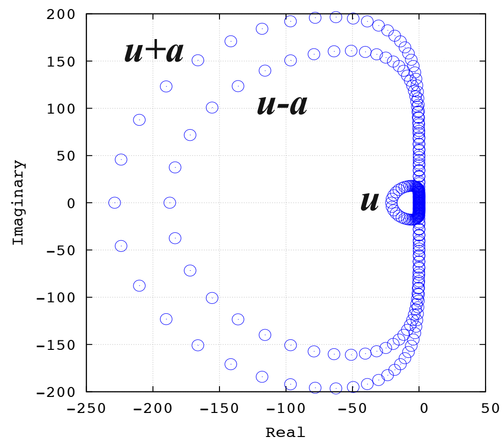
Example: Periodic density sine wave on a unit domain discretized by N=80 points.

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

Time step size limit for linear stability



Eigenvalues of the CRWENO5 discretization



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

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)

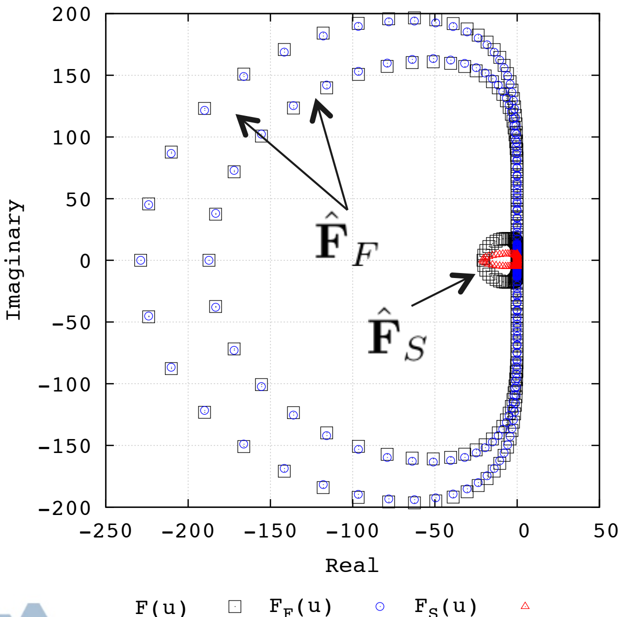
Splitting of the **flux Jacobian** based on its eigenvalues

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

"Slow" flux **"Fast" Flux**

$$\mathcal{A}(\mathbf{u}) = \mathcal{R}\Lambda\mathcal{L} = \mathcal{R}\Lambda_S\mathcal{L} + \mathcal{R}\Lambda_F\mathcal{L} = \mathcal{A}_\mathcal{S}(\mathbf{u}) + \mathcal{A}_\mathcal{F}(\mathbf{u})$$

$$\Lambda_S = \begin{bmatrix} u & & \\ & 0 & \\ & & 0 \end{bmatrix} \quad \Lambda_F = \begin{bmatrix} 0 & & \\ & u+a & \\ & & u-a \end{bmatrix}$$



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

$$\frac{\partial \mathbf{F}_{S,F}(\mathbf{u})}{\partial \mathbf{u}} \neq [\mathcal{A}_{S,F}]$$

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

(Not an error)

$$\text{eig}\left[\frac{\partial \hat{\mathbf{F}}_S}{\partial \mathbf{u}}\right] \approx u \times \text{eig}\,[\mathcal{D}] \qquad \text{eig}\left[\frac{\partial \hat{\mathbf{F}}_F}{\partial \mathbf{u}}\right] \approx \{u \pm a\} \times \text{eig}\,[\mathcal{D}]$$

IMEX Time Integration with Characteristic-based Flux Splitting (1)

Apply **Additive Runge-Kutta (ARK)** (PETSc) time-integrators to the split form

$$\mathbf{U}^{(i)} = \mathbf{u}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} \hat{\mathbf{F}}_S \left(\mathbf{U}^{(j)} \right) + \Delta t \sum_{j=1}^{i} \tilde{a}_{ij} \hat{\mathbf{F}}_F \left(\mathbf{U}^{(j)} \right)$$

Stage values

(s stages)

$$i = 1, \cdots, s$$

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t \sum_{i=1}^{s} b_i \hat{\mathbf{F}}_S \left(\mathbf{U}^{(i)} \right) + \Delta t \sum_{i=1}^{s} \tilde{b}_i \hat{\mathbf{F}}_F \left(\mathbf{U}^{(i)} \right)$$

Step completion

⇨ **Non-linear system of equations**

$$\hat{\mathbf{F}}_F \left(\mathbf{u} \right) = \left[\mathcal{D} \left(\omega \right) \otimes \mathcal{A}_F \left(\mathbf{u} \right) \right] \mathbf{u}$$

$$\uparrow$$

$$\omega = \omega \left[\mathbf{F} \left(\mathbf{u} \right) \right]$$

Solution-dependent weights for the WENO5/CRWENO5 scheme

Linearized Formulation

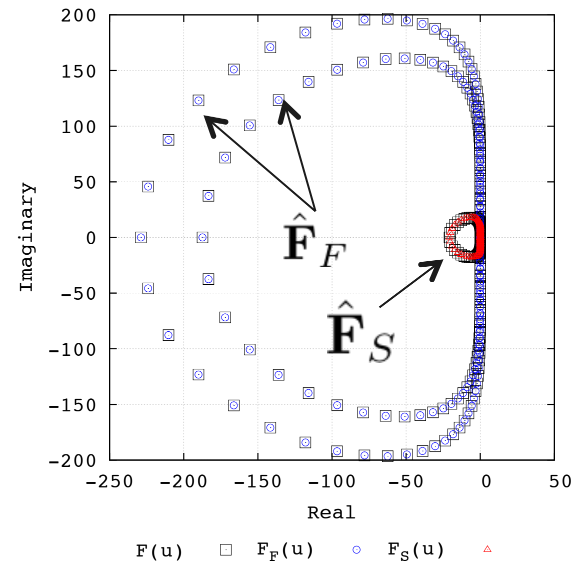
Redefine the splitting as

$$\mathbf{F}_F \left(\mathbf{u} \right) = \left[\mathcal{A}_F \left(\mathbf{u}_n \right) \right] \mathbf{u}$$
$$\mathbf{F}_S \left(\mathbf{u} \right) = \mathbf{F} \left(\mathbf{u} \right) - \mathbf{F}_F \left(\mathbf{u} \right)$$

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

At the beginning of a time step:-

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



Is F_F a good approximation at each stage?

IMEX Time Integration with Characteristic-based Flux Splitting (2)

Linearization of the WENO/CRWENO discretization:

Within a stage, the non-linear weights are kept fixed.

Example: 2-stage ARK method

$\omega\left[\mathbf{F}\left(\mathbf{u}_n\right)\right]$

$$\mathbf{U}^{(1)} = \mathbf{u}^n$$

$\omega\left[\mathbf{F}\left(\mathbf{U}^{(1)}\right)\right]$

$$\mathbf{U}^{(2)} = \mathbf{u}^n + \Delta t \tilde{a}_{21} \hat{\mathbf{F}}_F\left(\mathbf{U}^{(1)}\right) + \Delta t \tilde{a}_{22} \hat{\mathbf{F}}_F\left(\mathbf{U}^{(2)}\right) + \Delta t a_{21} \hat{\mathbf{F}}_S\left(\mathbf{U}^{(1)}\right)$$

$\omega\left[\mathbf{F}\left(\mathbf{U}^{(2)}\right)\right]$

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \tilde{b}_1 \hat{\mathbf{F}}_F\left(\mathbf{U}^{(1)}\right) + \Delta t \tilde{b}_2 \hat{\mathbf{F}}_F\left(\mathbf{U}^{(2)}\right) + \Delta t b_1 \hat{\mathbf{F}}_S\left(\mathbf{U}^{(1)}\right) + \Delta t b_2 \hat{\mathbf{F}}_S\left(\mathbf{U}^{(2)}\right)$$

Linear system of equations for implicit stages:

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

$$i = 1, \cdots, s$$

ARK Methods (PETSc)

ARKIMEX 2c

- 2nd order accurate
- 3 stage (1 explicit, 2 implicit)
- L-Stable implicit part
- Large real stability of the explicit part

ARKIMEX 2e

- 2nd order accurate
- 3 stage (1 explicit, 2 implicit)
- L-Stable implicit part

ARKIMEX 3

- 3rd order accurate
- 4 stage (1 explicit, 3 implicit)
- L-Stable implicit part

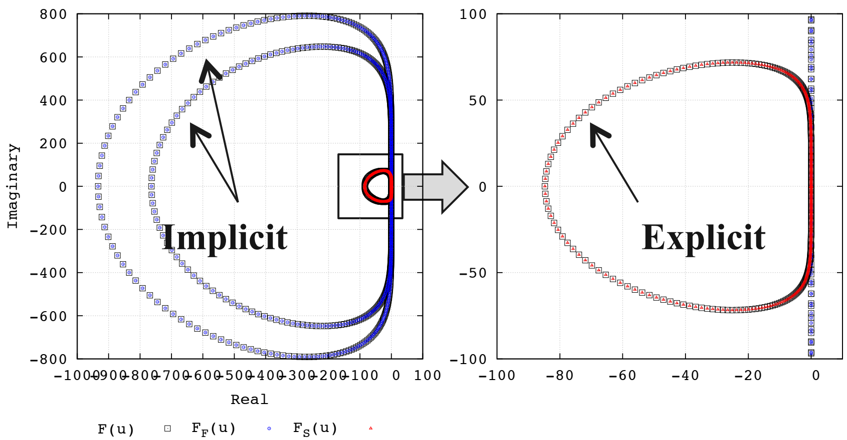
ARKIMEX 4

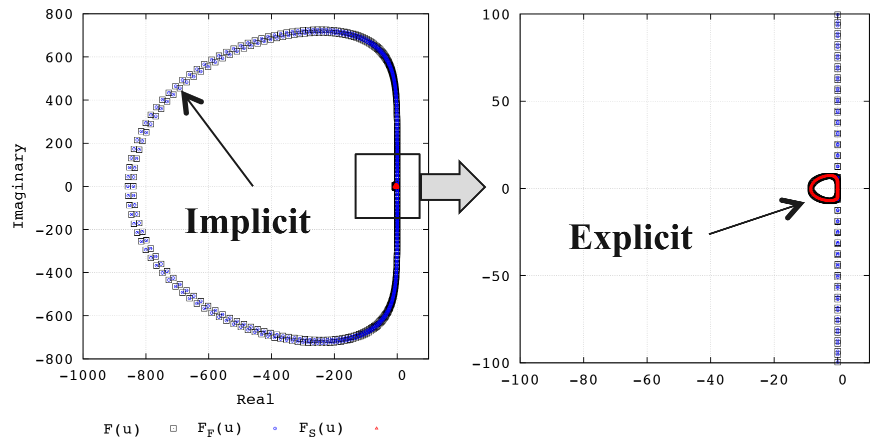
- 4th order accurate
- 5 stage (1 explicit, 4 implicit)
- L-Stable implicit part

Example: 1D Density Wave Advection

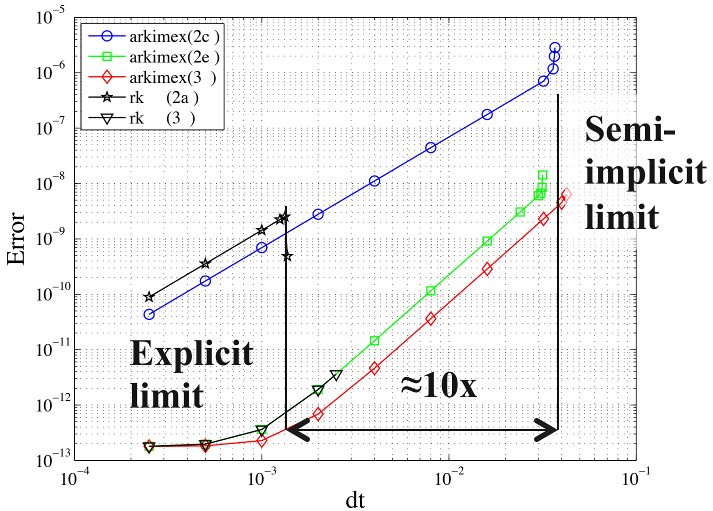
Initial solution $\rho = \rho_\infty + \hat{\rho}\sin\left(2\pi x\right), u = u_\infty, p = p_\infty;\ 0 \le x \le 1$

$M_\infty = 0.1$ **Eigenvalues** $M_\infty = 0.01$

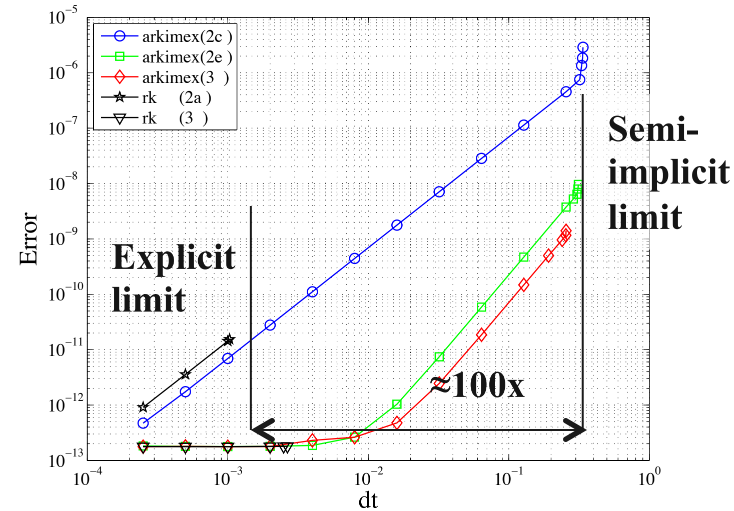




CRWENO5, 320 grid points



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



Example: Low Mach Isentropic Vortex Convection

Freestream flow

$$\left.\begin{array}{r} \rho_\infty = 1 \\ p_\infty = 1 \\ u_\infty = 0.1 \\ v_\infty = 0 \end{array}\right\} M_\infty \approx 0.08$$

Vortex (Strength *b = 0.5*)

$$\rho = \left[1.0 - \frac{(\gamma-1)\,b^2}{8\gamma\pi^2}\exp\left(1-r^2\right)\right]^{\frac{1}{\gamma-1}}$$

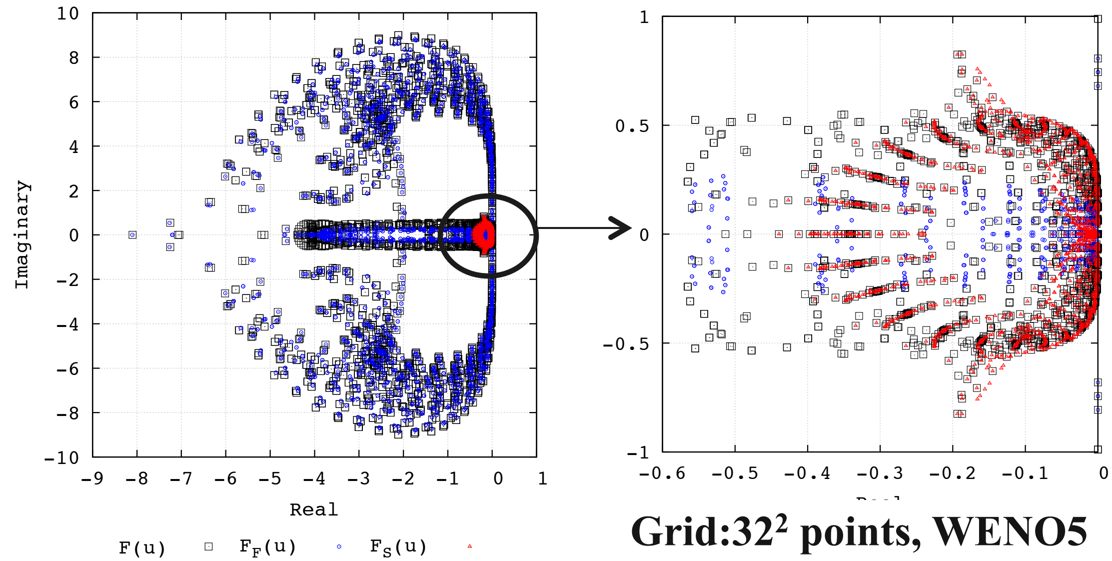
$$p = \left[1.0 - \frac{(\gamma-1)\,b^2}{8\gamma\pi^2}\exp\left(1-r^2\right)\right]^{\frac{\gamma}{\gamma-1}}$$

$$u = u_\infty - \frac{b}{2\pi}\exp\left(\frac{1-r^2}{2}\right)(y-y_c)$$

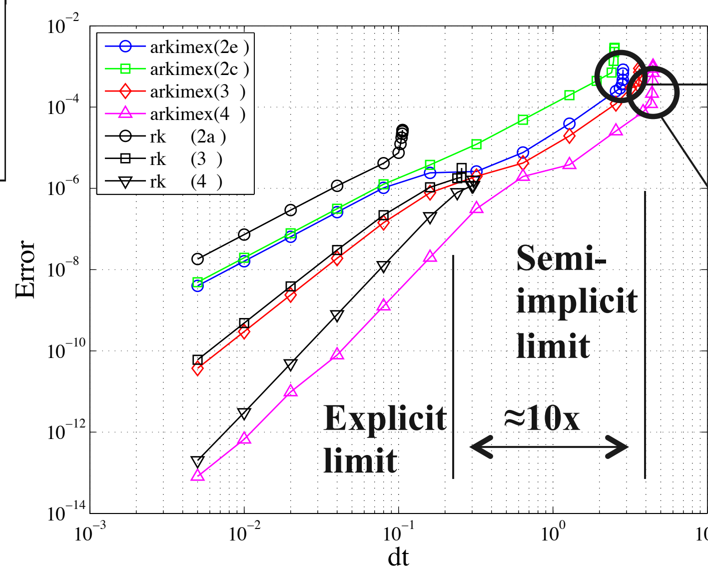
$$v = v_\infty + \frac{b}{2\pi}\exp\left(\frac{1-r^2}{2}\right)(x-x_c)$$

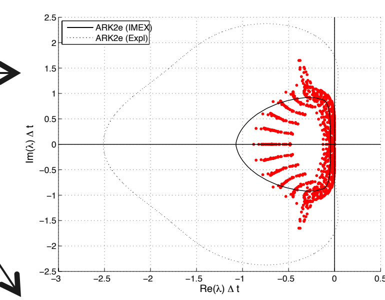
- **Optimal orders** of convergence observed for all methods
- **Time step size limited by the "slow" eigenvalues.**

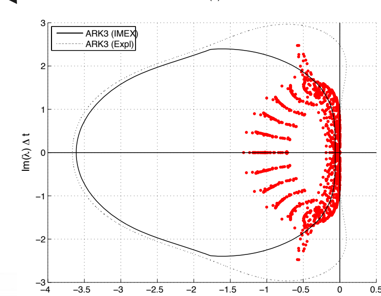
Eigenvalues of the right-hand-side operators



Grid:32^2 points, WENO5



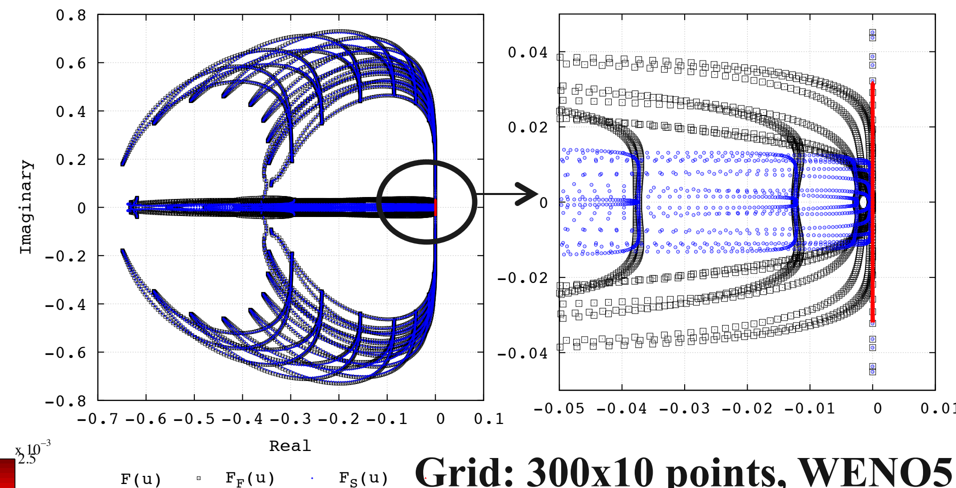




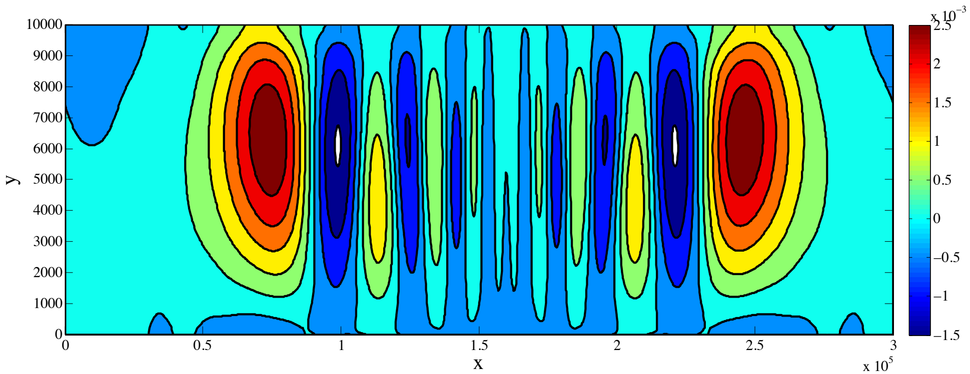
Example: Inertia – Gravity Wave

- **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**

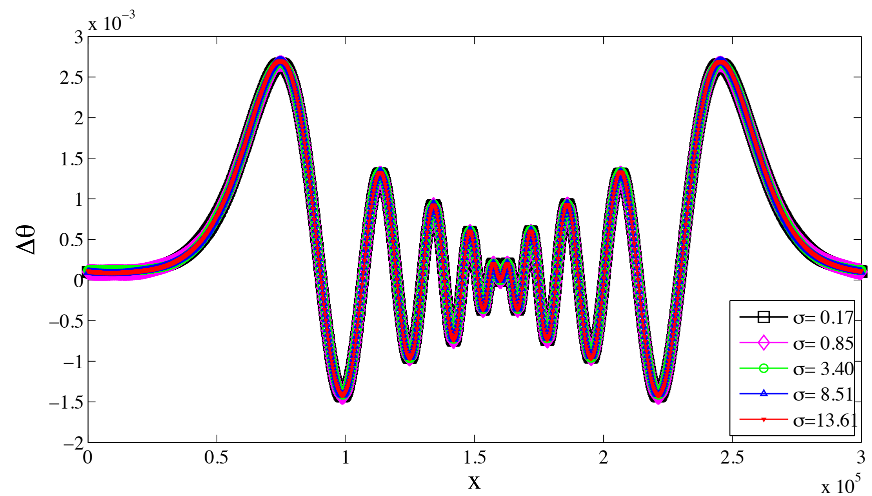
Eigenvalues of the right-hand-side operators



Grid: 300x10 points, WENO5



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



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

Good agreement with results in literature.

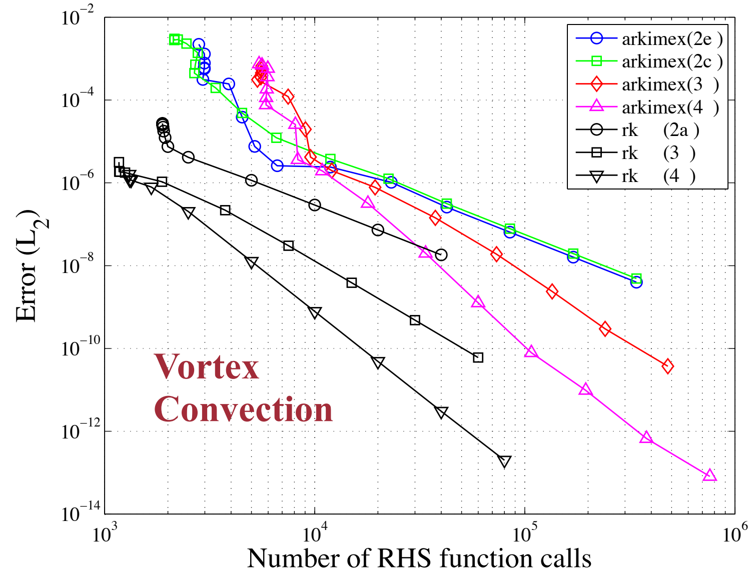
Purely imaginary eigenvalues for the explicit operator disagreeable!

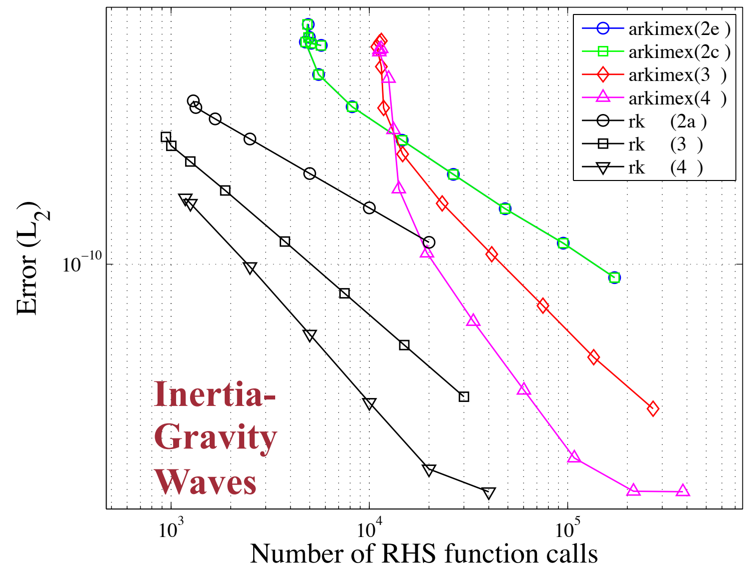
Conclusions

Characteristic-based flux splitting

(Work in progress)

- Partitioning of flux **separates the acoustic and entropy modes** → Allows **larger time step sizes** (determined by flow velocity, not speed of sound).
- **Comparison** to alternatives
  - **Vs. explicit time integration:** Larger time steps → 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).
- **(**) But** no preconditioning in current implementation → Semi-implicit not really more efficient (yet!)
  - **Implement and apply a pre-conditioner**
- **Apply to other low-Mach number flows?**





Error vs. total number of function calls for explicit and IMEX time-integrators with various time step sizes

Thank you!

Acknowledgements

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