Scalable Non-Linear Compact Schemes

Debojyoti Ghosh **Emil M. Constantinescu** **Jed Brown**

Mathematics & Computer Science
Argonne National Laboratory

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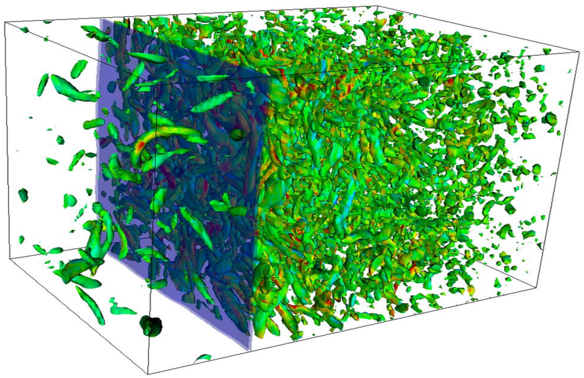
Motivation

Numerical Solution of Compressible Turbulent Flows

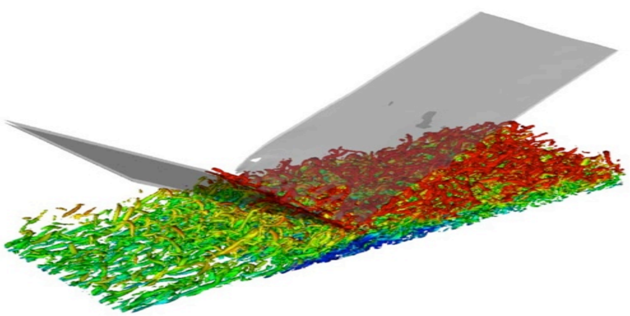
- Atmospheric flows, Aircraft and Rotorcraft wake flows
- Characterized by **large range of length scales**
- Convection and interaction of eddies
- Compressibility → **Shock waves** & **Shocklets**
- Thin shear layers → **High gradients** in flow



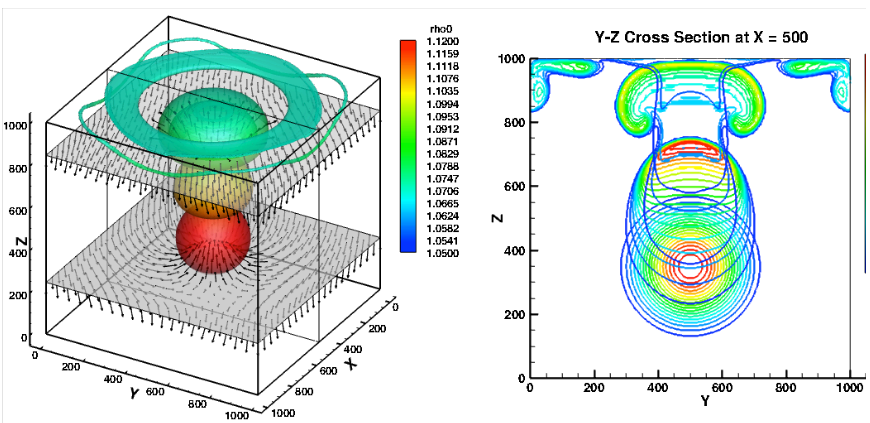
Shock-Turbulence Interaction (Stanford University)

High order accurate finite-difference solver

- High spectral resolution for **accurate capturing of smaller length scales**
- Non-oscillatory solution across shock waves and shear layers
- Low dissipation errors for **preservation of flow structures over large distances**

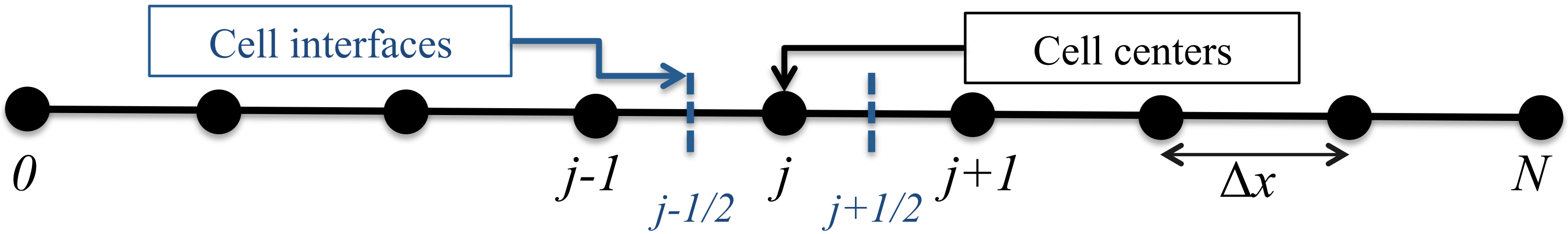


Shock-Turbulent Boundary Layer Interaction (Brandon Morgan, Stanford University and Nagi Mansour, NASA)



Rising Thermal Bubble in Hydrostatically Balanced Atmosphere

Background



Conservative finite-difference discretization of a Hyperbolic Conservation Law

$$u_t + f(u)_x = 0; \;\; f'(u) \in \Re \quad \Rightarrow \quad \frac{du_j}{dt} + \frac{1}{\Delta x}\left[f(x_{j+1/2},t) - f(x_{j-1/2},t) \right] = 0$$

Compressible Turbulent Flows

Weighted Essentially Non-Oscillatory (WENO) Schemes

Compact Finite-Difference Schemes

Hybrid Compact-WENO Schemes

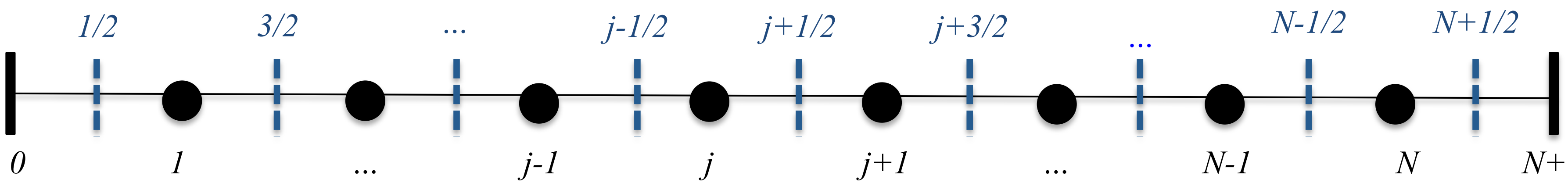
Disadvantages: loss of spectral resolution near discontinuities

Weighted Compact Non-Linear Schemes

Disadvantage: Relatively Poor spectral resolution

Compact-Reconstruction WENO (CRWENO) Schemes

Compact-Reconstruction WENO (CRWENO) Schemes



General form of a **conservative compact scheme**:

$$\mathrm{A}\left(\hat{f}_{j+1/2-m},\ldots,\hat{f}_{j+1/2},\ldots,\hat{f}_{j+1/2+m}\right)=\mathrm{B}\left(f_{j-n},\ldots,f_{j},\ldots,f_{j+n}\right) \quad \Longrightarrow \quad [A]\hat{\mathbf{f}}=[B]\mathbf{f}$$

At each interface, r possible *(r)*-th order compact interpolations, combined using optimal weights c_k to yield *(2r-1)*-th order compact interpolation scheme:

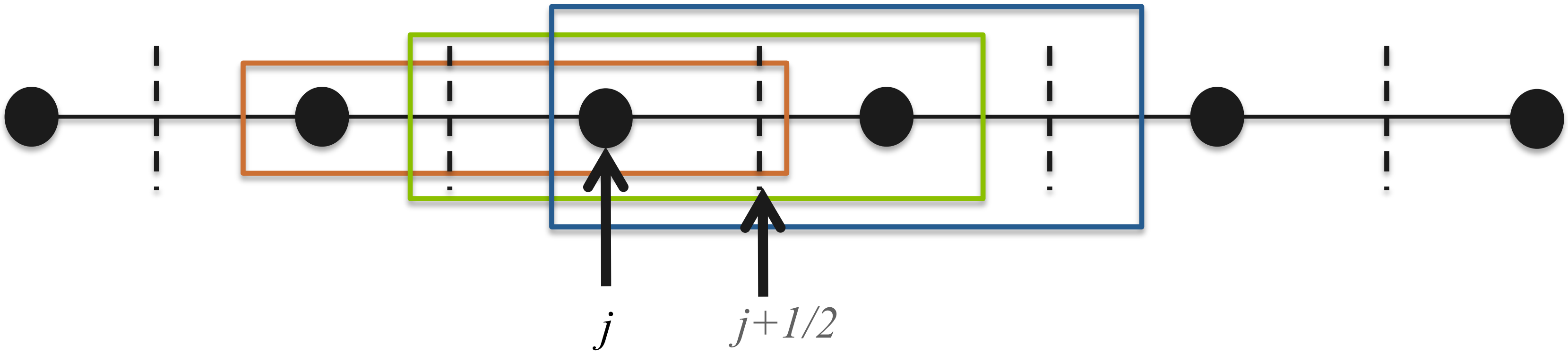
$$\sum_{k=1}^{r} c_k\,\mathrm{A}_k^r\left(\hat{f}_{j+1/2-m},\ldots,\hat{f}_{j+1/2+m}\right)=\sum_{k=1}^{r} c_k\,\mathrm{B}_k^r\left(f_{j-n},\ldots,f_{j+n}\right)$$

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

Apply WENO algorithm on the optimal weights c_k – scale them according to local smoothness

$$\sum_{k=1}^{r} \omega_k\,\mathrm{A}_k^r\left(\hat{f}_{j+1/2-m},\ldots,\hat{f}_{j+1/2+m}\right)=\sum_{k=1}^{r} \omega_k\,\mathrm{B}_k^r\left(f_{j-n},\ldots,f_{j+n}\right) \qquad \alpha_k=\frac{c_k}{\left(\beta_k+\varepsilon\right)^p};\ \omega_k=\alpha_k \Big/ \sum_k \alpha_k$$

5^{th} Order CRWENO Scheme (CRWENO5)



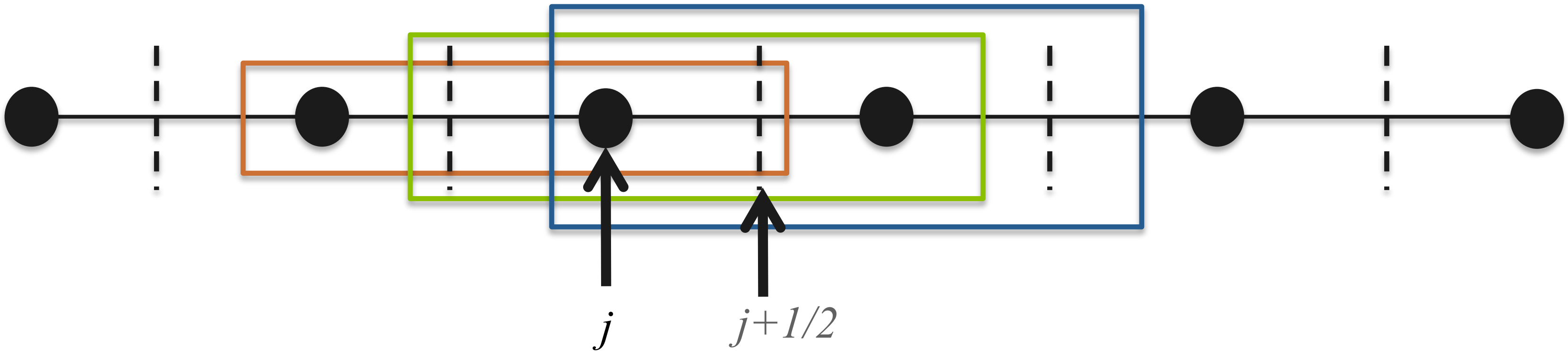
$$\frac{2}{3} f_{j-1/2} + \frac{1}{3} f_{j+1/2} = \frac{1}{6} f_{j-1} + \frac{5}{6} f_j \quad \longrightarrow \quad c_1 = \frac{2}{10}$$

$$\frac{1}{3} f_{j-1/2} + \frac{2}{3} f_{j+1/2} = \frac{5}{6} f_j + \frac{1}{6} f_{j+1} \quad \longrightarrow \quad c_2 = \frac{5}{10}$$

$$\frac{2}{3} f_{j+1/2} + \frac{1}{3} f_{j+3/2} = \frac{1}{6} f_j + \frac{5}{6} f_{j+1} \quad \longrightarrow \quad c_3 = \frac{3}{10}$$

$$\frac{3}{10} f_{j-1/2} + \frac{6}{10} f_{j+1/2} + \frac{1}{10} f_{j+3/2} = \frac{1}{30} f_{j-1} + \frac{19}{30} f_j + \frac{10}{30} f_{j+1}$$

5^{th} Order CRWENO Scheme (CRWENO5)



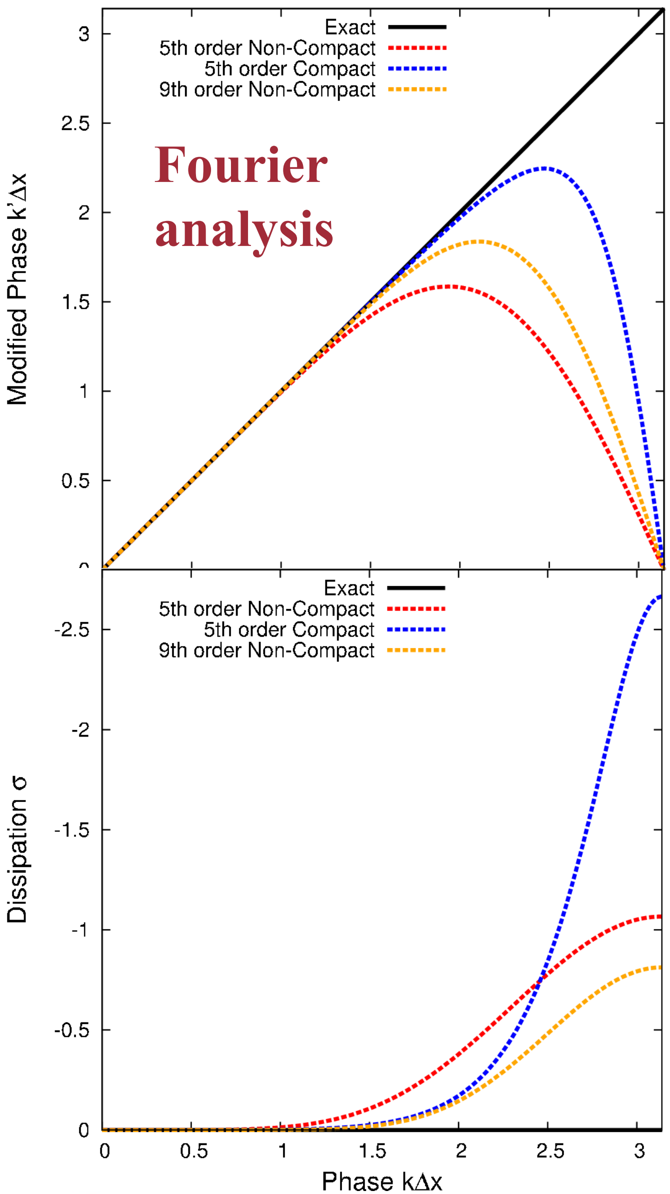
$$\frac{2}{3} f_{j-1/2} + \frac{1}{3} f_{j+1/2} = \frac{1}{6} f_{j-1} + \frac{5}{6} f_j \qquad \omega_1$$

$$\frac{1}{3} f_{j-1/2} + \frac{2}{3} f_{j+1/2} = \frac{5}{6} f_j + \frac{1}{6} f_{j+1} \qquad \omega_2$$

$$\frac{2}{3} f_{j+1/2} + \frac{1}{3} f_{j+3/2} = \frac{1}{6} f_j + \frac{5}{6} f_{j+1} \qquad \omega_3$$

$$\left(\frac{2}{3}\omega_1 + \frac{1}{3}\omega_2\right) f_{j-1/2} + \left(\frac{1}{3}\omega_1 + \frac{2}{3}(\omega_2 + \omega_3)\right) f_{j+1/2} + \frac{1}{3}\omega_3 f_{j+3/2} = \frac{\omega_1}{6} f_{j-1} + \frac{5(\omega_1 + \omega_2)}{6} f_j + \frac{\omega_2 + 5\omega_3}{6} f_{j+1}$$

Numerical Analysis



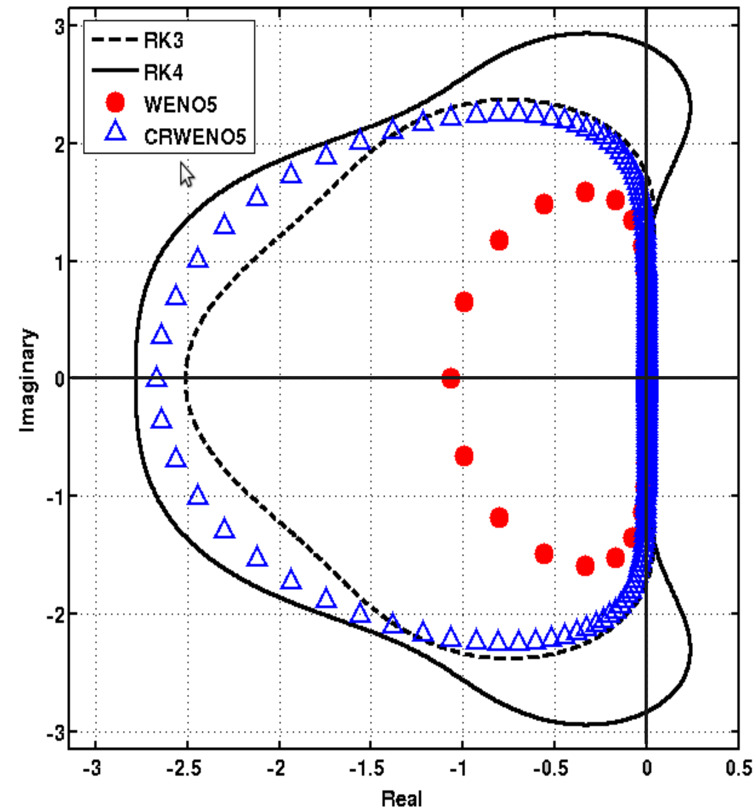
Taylor Series

WENO5

$$\frac{1}{60}\frac{\partial^6 f}{\partial x^6}\bigg|_j \Delta x^5$$

CRWENO5

$$\frac{1}{600}\frac{\partial^6 f}{\partial x^6}\bigg|_j \Delta x^5$$



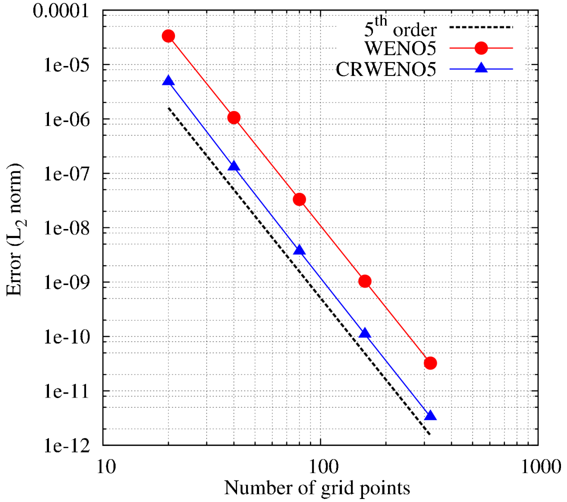
➔ WENO5 requires **~ 1.5 times more grid points per dimension** to yield a solution of comparable accuracy as the CRWENO5 scheme.

➔ Time step size limit is **~ 1.6 times smaller** for CRWENO than WENO5

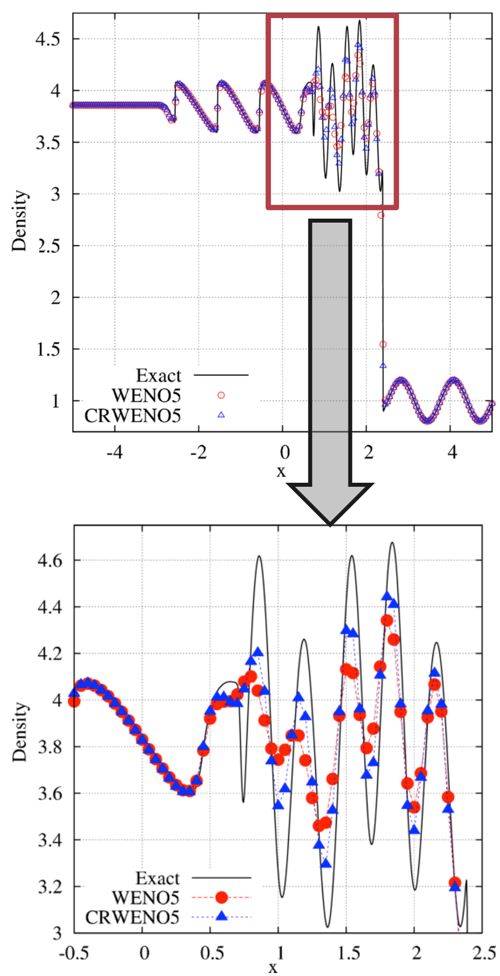
Preliminary Results

doi:10.1137/110857659
doi:10.1007/s10915-014-9818-0
doi:10.2514/6.2012-2832

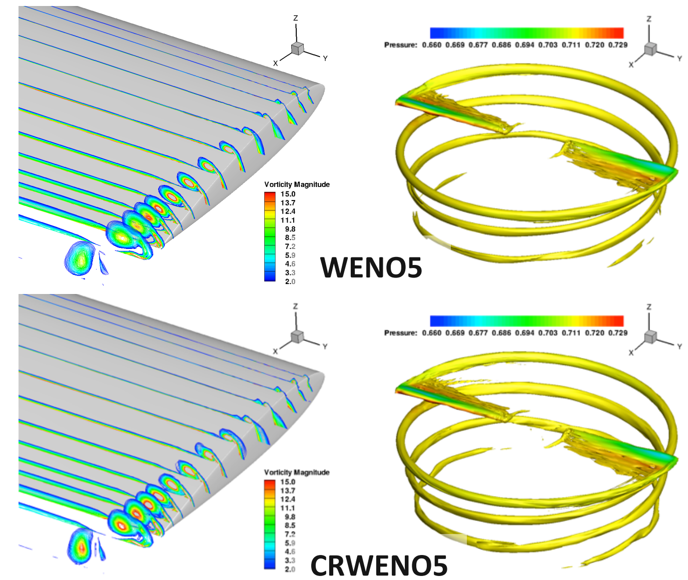
Periodic density wave advection



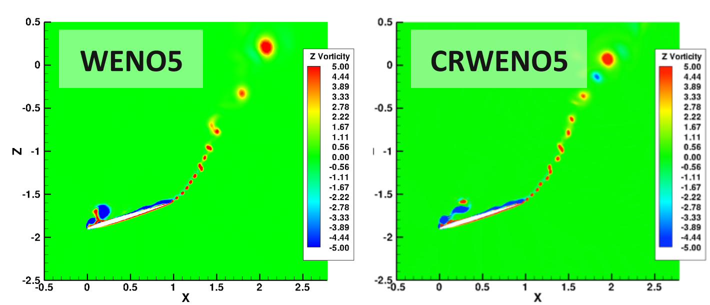
Shu-Osher Problem



Flow around Harrington Rotor



Vortex shedding from a flapping wing



- **Lower absolute errors** for smooth problems for the same order of convergence
- **Resolution of small length scales** improved
- **Better preservation** of flow features (shed vortices)

Scalable Parallel Implementation

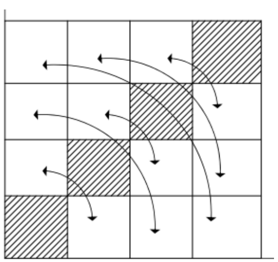
CRWENO5 needs a tridiagonal solution at each time-integration stage/step

Treat sub-domain boundary as physical boundary

- Decouple system of equations across processors (biased compact or non-compact schemes at MPI boundaries)
- **Drawback:** Numerical properties of the scheme function of number of processors
- **Good for small number of processors, numerical errors grow or spectral resolution falls as number of processors increase for same problem size**

Data Transposition

- Transpose pencils of data such that entire system of equations is collected on one processor.
- **Huge communication cost**

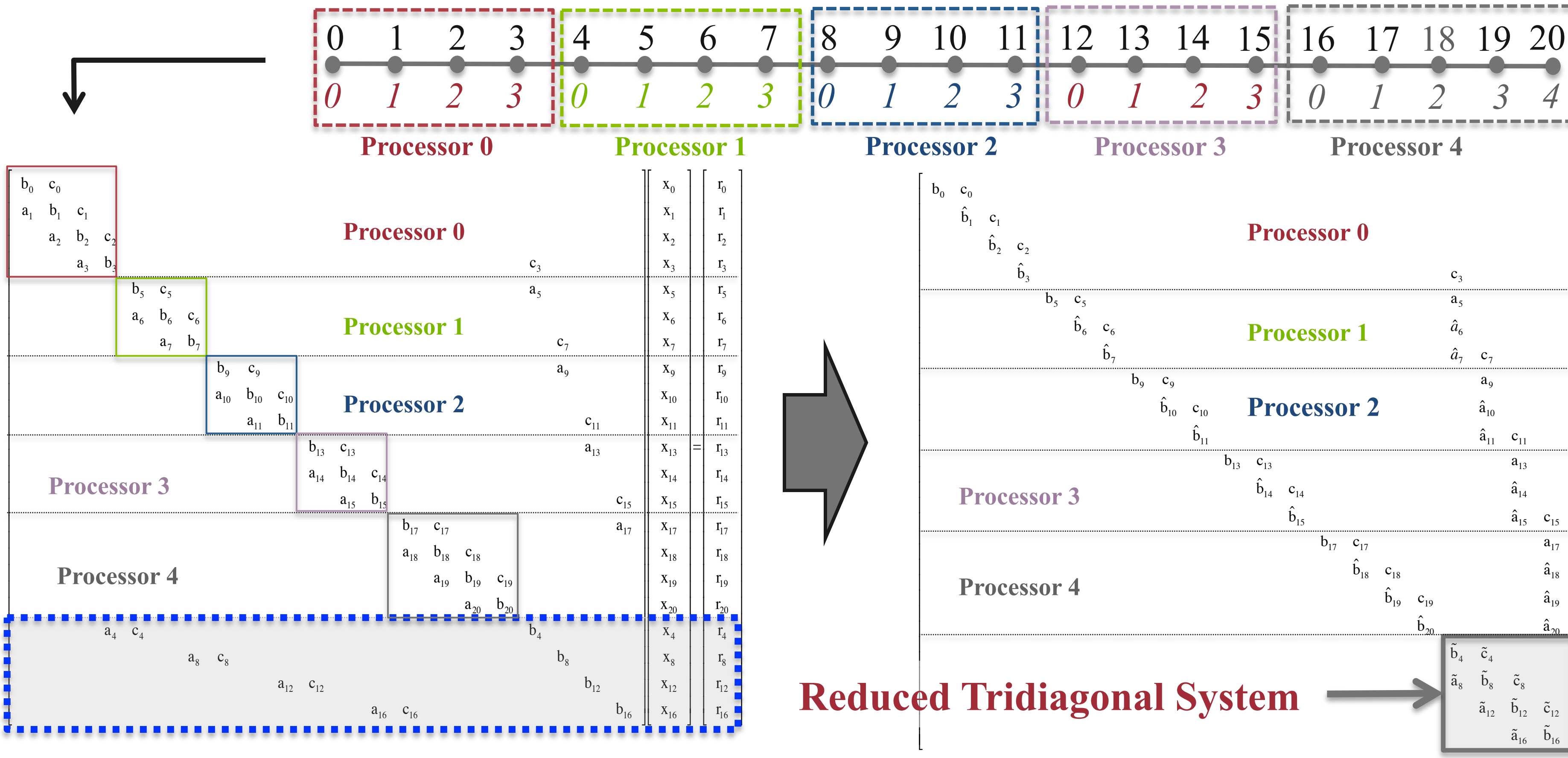


Parallel Implementation of the Thomas Algorithm

- **Pipelined Thomas Algorithm** (PTA) (*Povitsky & Morris, JCP, 2000*): Used a complicated static schedule to use idle times of processors to carry out computations – **Trade-off between computation & communication efficiencies**
- **Parallel Diagonally Dominant** (PDD) (*Sun & Moitra, NASA Tech. Rep., 1996*): Solve a perturbed linear system that introduces an error due to assumption of diagonal dominance
- Other implementations of tridiagonal solvers not applied to compact schemes
- **Increased mathematical complexity compared to the serial Thomas algorithm**

Existing approaches do not scale well!

Parallel Tridiagonal Solver



Solution of reduced system is critical to scalability

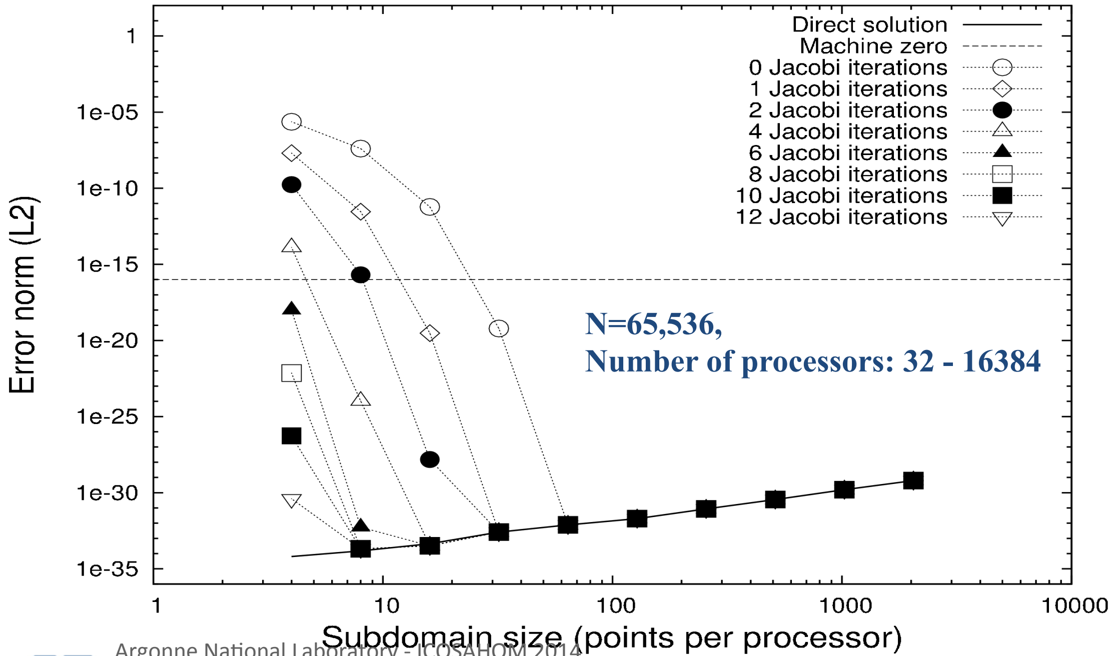
- One row on each processor → **Communication intensive**
- **Direct/Exact** solutions to the reduced system (**Cyclic Reduction / Recursive-Doubling Algorithm, Gather-and-Solve) - <u>Do not scale well!</u>**

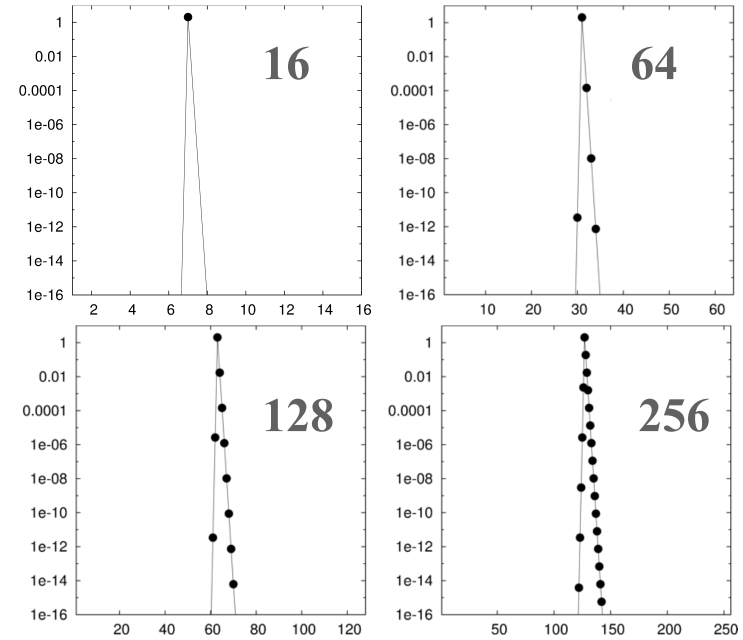
Iterative Sub-structuring Method

Iterative Solution of the Reduced System

Reduced system represents the **coupling between the first interface of every subdomain** through an approximation to a **hyperbolic flux.**

- For large subdomain sizes, **very diagonally dominant**
- **Diagonal dominance decreases** as **sub-domain size grows smaller** (Number of processors increase for same problem size)





Non-machine-zero elements of an arbitrarily chosen column of the inverse of the reduced system (N=1024)

Number of Jacobi iterations required for an "exact" solution **increases as sub-domain size grows smaller.**

→ Cost of the tridiagonal solver increases

Performance Analysis

Governing Equations: Inviscid Euler Equations

Platform: ALCF *Vesta* (IBM BG/Q)

CRWENO5 scheme on N points per dimension

- On a single processor, CRWENO5 is more efficient (***error vs. wall time***).
- Cost of the tridiagonal solver increases as number of processors increases
- At a **critical sub-domain size**, the CRWENO5 becomes less efficient than the WENO5 scheme.

WENO5 scheme on *f*N points per dimension

- $f > 1$ ($f \sim 1.5$ for smooth solutions) – WENO5 yields solutions of comparable accuracy/resolution with f times more points
- Non-compact scheme, so almost ideal scalability expected.

Same number of processors for the CRWENO5 scheme (on N points) and the WENO5 scheme (on *f*N points)

Given p processors, is it faster to obtain a solution of given accuracy/resolution with the WENO5 or CRWENO5 scheme?

Performance Comparison for a Smooth Problem

Periodic Advection of a Sinusoidal Density Wave

1D

WENO5 yields solutions with comparable accuracy with **~ 1.5 times as many points**

2D

WENO5 yields solutions with comparable accuracy with **$\sim 1.5^2 = 2.25$ times as many points**

- **Time step size Δt is taken the same** for the CRWENO5 scheme on N points and the WENO5 scheme on fN points because of the **linear stability limit.**
- Solutions are obtained after one cycle over the periodic domain with the SSP-RK3 scheme
- It is verified that the **errors are exactly the same for the various number of processors** considered → There are no parallelization errors (Number of Jacobi iterations are specified *a priori* to ensure this)

Effect of Dimensionality

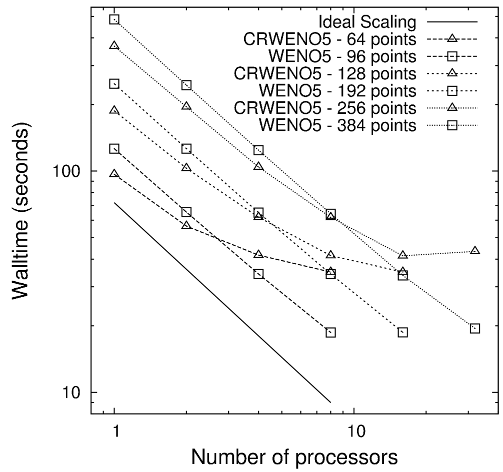
- The **factor by which the grid needs for WENO5 needs to be refined** to yield comparable solutions as CRWENO5 is f^D (f times per dimension)
- Several tridiagonal systems are solved for multi-dimensional problems →Higher arithmetic density → **Cost increases sub-linearly with number of systems**

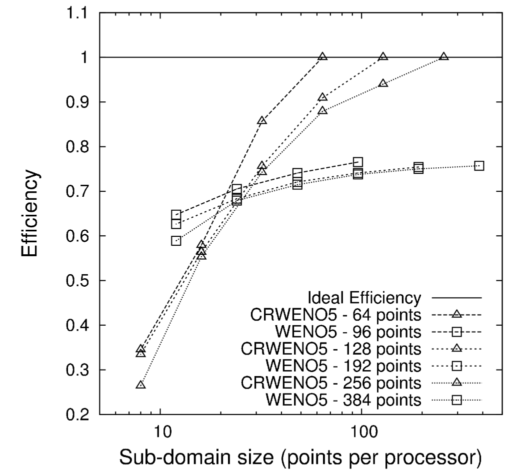
Performance Analysis for a Smooth Problem

1D

Cases: Number of grid points and number of processors considered

64 (96)	1	2	4	8		
128 (192)	1	2	4	8	16	
256 (384)	1	2	4	8	16	32

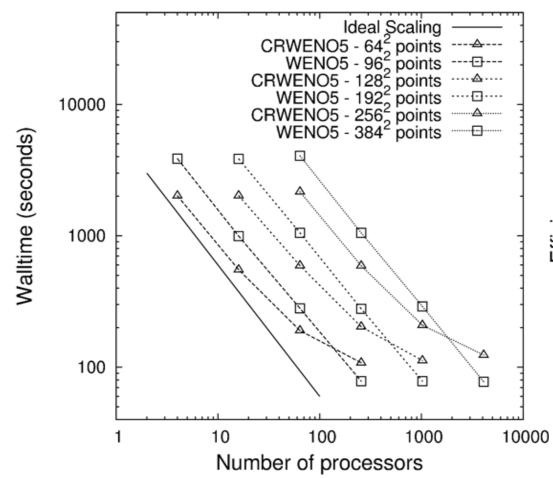


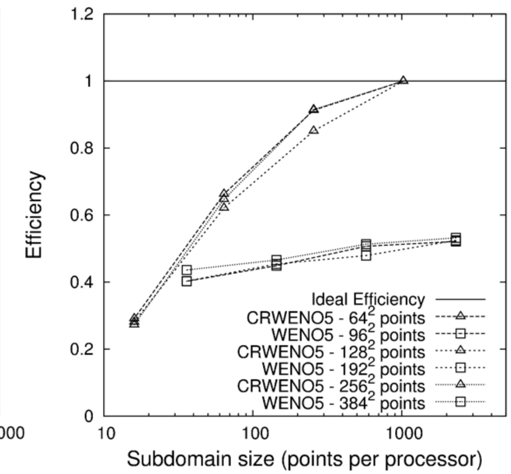


2D

Cases: Number of grid points and number of processors considered

64^2 (96^2)	4	16	64	256
128^2 (192^2)	16	64	256	1024
256^2 (384^2)	64	256	1024	4096

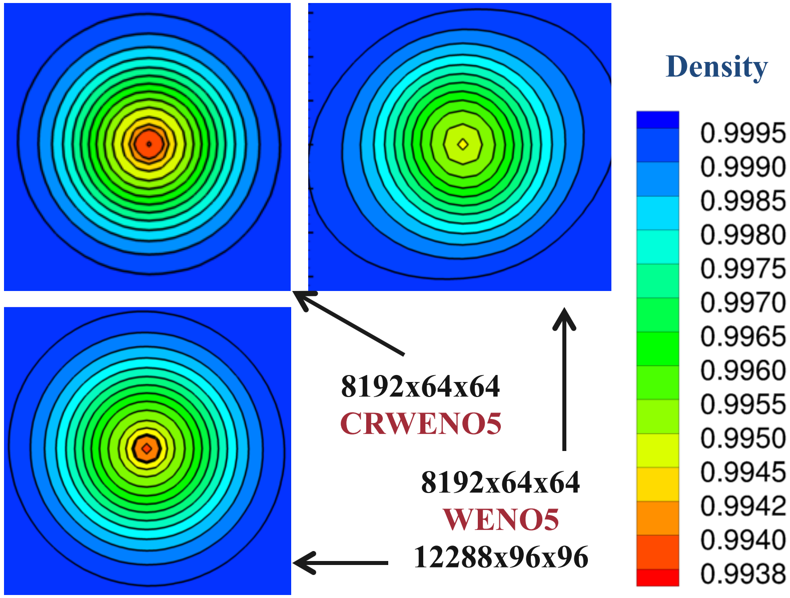




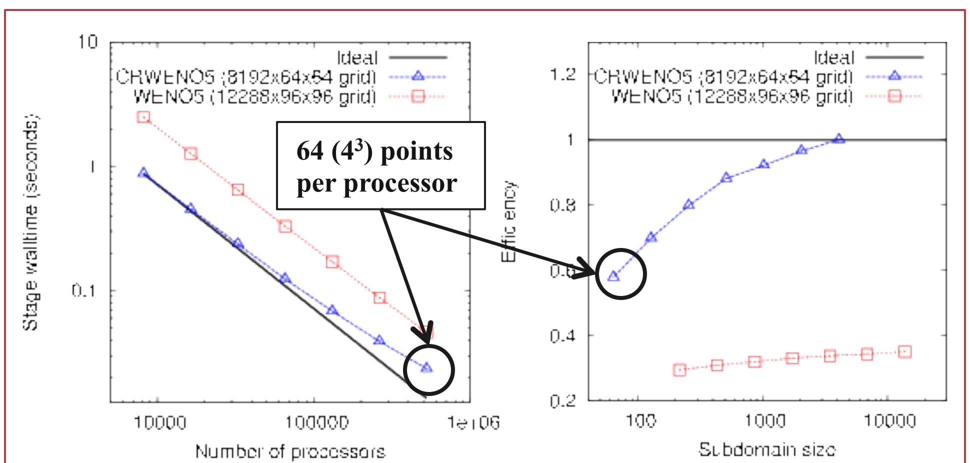
Note: Critical sub-domain size is insensitive to global problem size

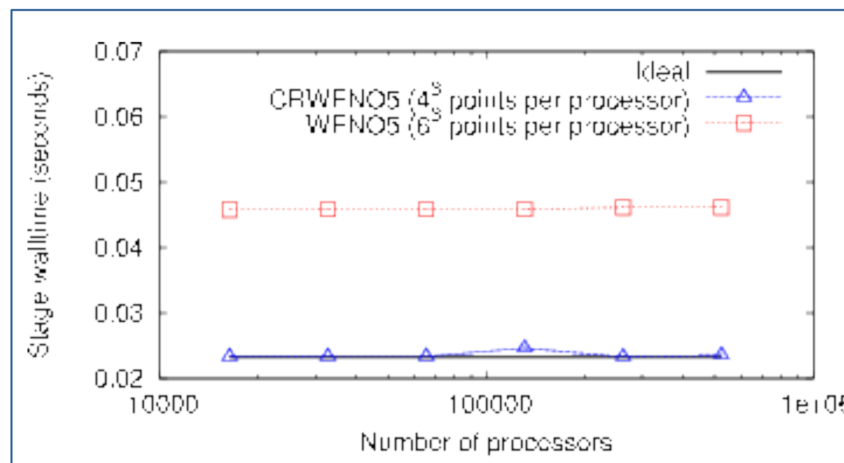
Scalability Results for Benchmark Flow Problems

Isentropic Vortex Convection – Vortex convects 1000x its core radius



- Verified that WENO5 yields a solution of comparable accuracy on a grid with ~ 1.5^3x (~ 3.4x) more grid points
- ALCF/*Mira* (IBM BG/Q) (**~ 8k to 500k cores**)
- **Strong Scaling:** At very small subdomain sizes, CRWENO5 does not scale as well, yet is more efficient / has lower absolute walltime
- **Weak Scaling:** CRWENO5 shows excellent weak scaling





Application: Atmospheric Modeling

Non-hydrostatic Unified Model of the Atmosphere (NUMA)

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

Giraldo, Restelli, Lauter, SIAM J. Sci. Comp. (2010)

$$\dot{\mathbf{q}} = \hat{\mathbf{S}}(\mathbf{q})$$

$$\dot{\mathbf{q}} = \left[\hat{\mathbf{S}}(\mathbf{q}) - \hat{\mathbf{L}}(\mathbf{q})\right] + \left[\hat{\mathbf{L}}(\mathbf{q})\right]$$

Non-Stiff

Stiff

Explicit time-integration schemes (SSPRK3, RK4)

Implicit-Explicit (IMEX) time-integration schemes (ARKIMEX)

$$\mathbf{L} = \begin{bmatrix} -\nabla(\rho\mathbf{u}) \\ \nabla P' + \rho g\hat{\mathbf{k}} \\ \nabla(-\frac{\Theta_0}{\rho_0}\rho\mathbf{u}) \end{bmatrix}$$

IMEX Formulation with WENO5/CRWENO5

Semi-discrete ODE $\dot{\mathbf{q}} - \hat{\mathbf{L}}(\mathbf{q}) = \hat{\mathbf{R}}(\mathbf{q})$ $\left(\hat{\mathbf{R}} = \hat{\mathbf{S}} - \hat{\mathbf{L}}\right)$

Even though L(q) is linear, the spatial discretization scheme is non-linear

Linearizing the WENO5/ CRWENO5 operator
Consistency of L and R

Example: 2-stage ARKIMEX method

$$Y^{(1)} = \mathbf{q}^n \quad \omega\left(\hat{\mathbf{S}}\left(\mathbf{q}^n\right)\right)$$

$$Y^{(2)} = \mathbf{q}^n + h\tilde{a}_{21}\hat{\mathbf{L}}\left(Y^{(1)}\right) + h\tilde{a}_{22}\hat{\mathbf{L}}\left(Y^{(2)}\right) + ha_{21}\hat{\mathbf{R}}\left(Y^{(1)}\right) \quad \omega\left(\hat{\mathbf{S}}\left(Y^{(1)}\right)\right)$$

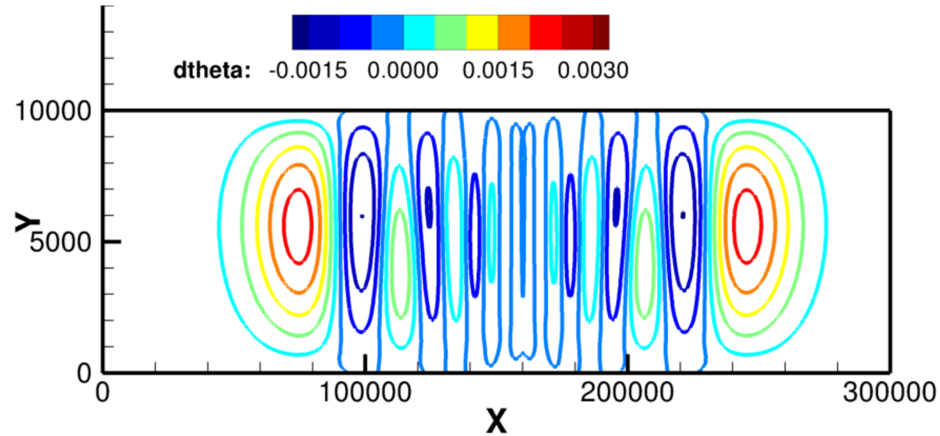
$$\mathbf{q}^{n+1} = \mathbf{q}^n + h\tilde{b}_1\hat{\mathbf{L}}\left(Y^{(1)}\right) + h\tilde{b}_2\hat{\mathbf{L}}\left(Y^{(2)}\right) + hb_1\hat{\mathbf{R}}\left(Y^{(1)}\right) + hb_2\hat{\mathbf{R}}\left(Y^{(2)}\right) \quad \omega\left(\hat{\mathbf{S}}\left(Y^{(2)}\right)\right)$$

PETSc TSARKIMEX

Non-Oscillatory? (for large time steps)

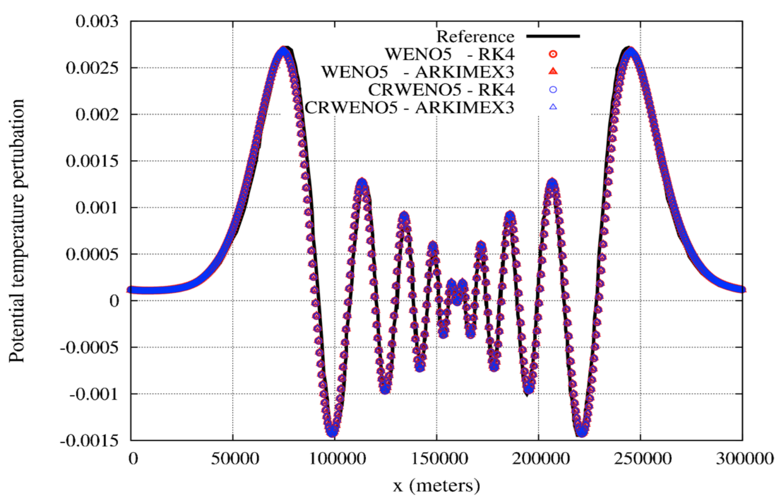
Inertia Gravity Waves

- **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
- Initial solution – **Potential temperature perturbation**
- Solutions obtained at 3000 s



Solution obtained with CRWENO5 and ARKIMEX 2C (CFL ~ 8.5)

Cross-sectional potential temperature perturbation (y = 5000)



- **Grid**: 1200 x 50 points
- **Explicit time-integration schemes:** SSPRK3 and RK4 (at CFL ~ 0.4)
- **IMEX time-integration schemes:** ARKIMEX 2C, 3, and 4 (at CFL ~ 8.5)
- **Spatial schemes:** WENO5 and CRWENO5
- Excellent agreement with reference solution
- CRWENO5 and WENO5 give similar resolution of perturbations

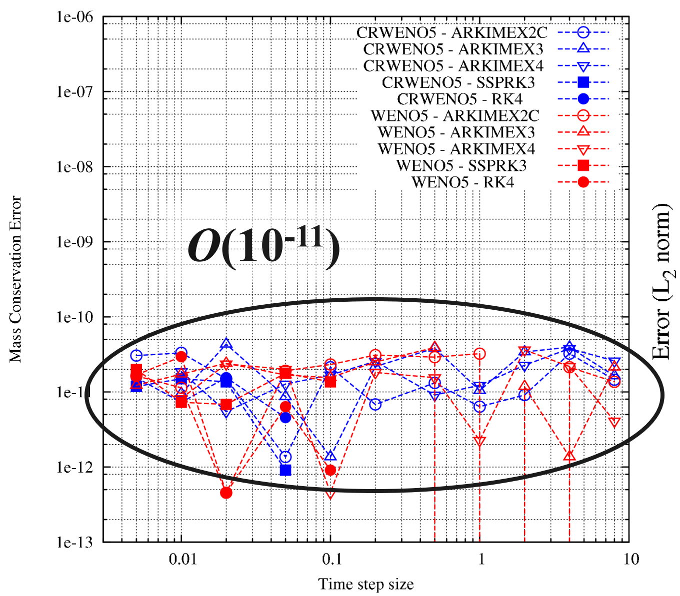
Reference solution: *Giraldo, Restelli, J. Comput. Phys. (2008)* – Spectral element method (10^{th} order polynomials and 250 m resolution)

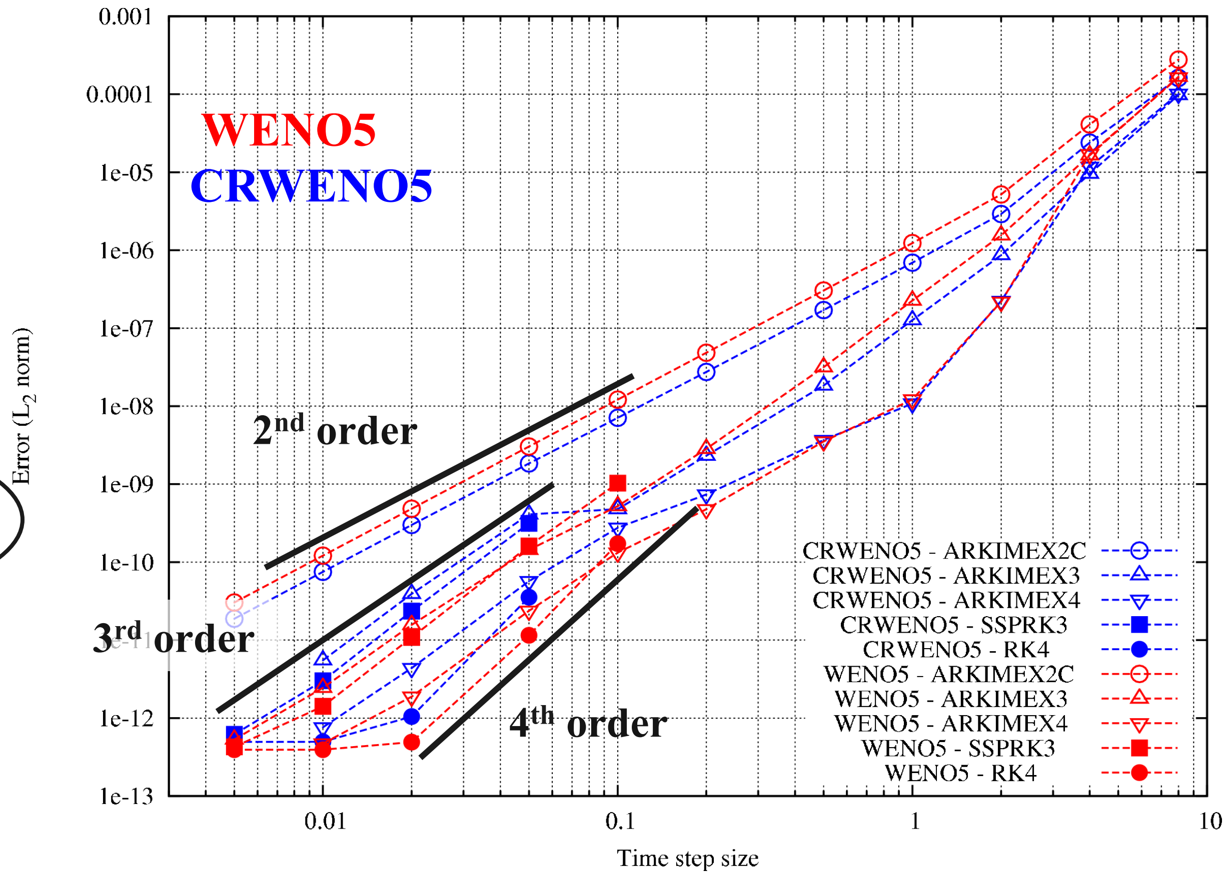
Inertia – Gravity Wave: Error Analysis

- **Grid:** 8192 x 256 (to minimize spatial discretization errors)
- **Optimal orders of convergence** observed for IMEX schemes
- IMEX methods stable over a large range of time step sizes

Reference solution: SSPRK3 with time step size 0.0005

IMEX methods **conserve mass** for all time steps considered



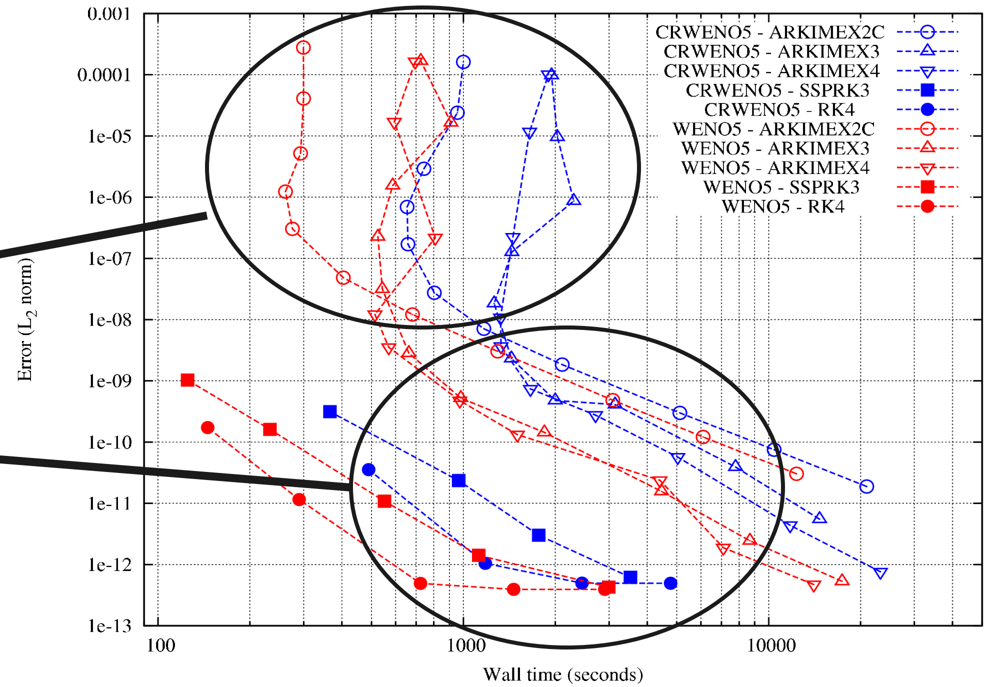


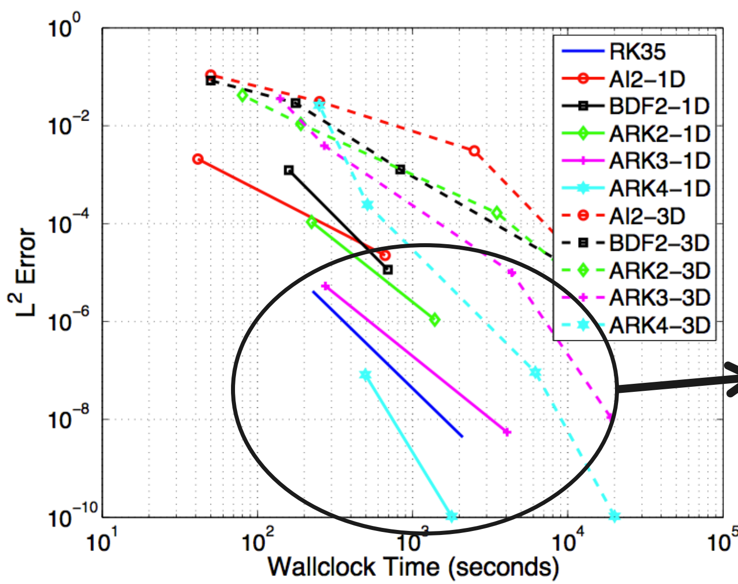
Inertia Gravity Waves: Computational Efficiency

Numerical cost vs. errors

IMEX and Explicit schemes

- Current implementation has no **preconditioning** – wall times stagnate for large time steps
- **Optimize** implementation: Evaluation of Jacobian, calculation of WENO weights

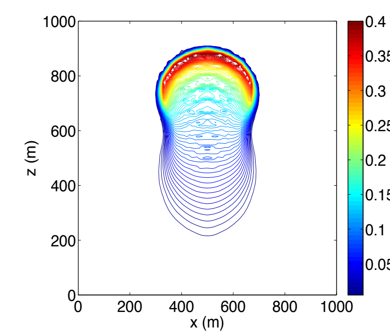




– *Giraldo, Kelly, Constantinescu, SIAM J. Sci. Comp. (2013)*

– Efficiency demonstrated for a **spectral element code** in 2D and 3D

– **ARKIMEX4** shown to be **more efficient** than RK35



Rising Thermal Bubble

Scalability and Adaptive Time-Stepping (Preliminary)

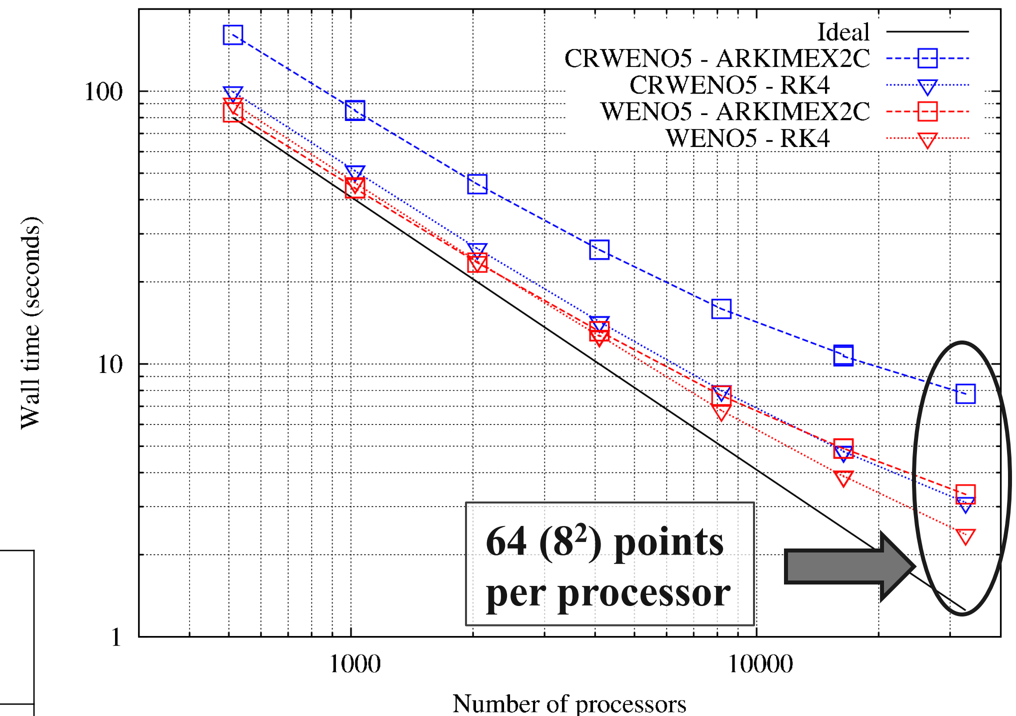
Strong Scaling: (ALCF/*Mira*)

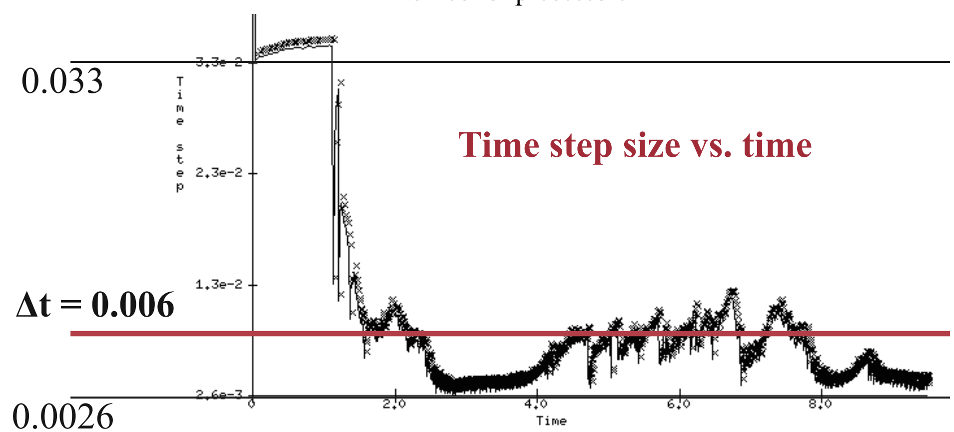
- **Grid:** 8192 x 256 points
- **RK4** at CFL ~ 0.4
- **ARKIMEX2c** at CFL ~ 8.5
- Number of cores: **512 to 32,768**

Adaptive Time Stepping:

- **Grid:** 1200 x 50 points
- **Tolerance:** 1e-10

	Constant Time Step ($\Delta t = 0.006$)	Adaptive Time Step	
Error	1.245E-07	6.727E-08	**~ 0.5x**
Time Steps	1653	1653	
Function Calls	36366	38896	**~1.1x**
GMRES Iterations	79674	87983	**~1.1x**





Conclusions

Compressible Turbulent Flows

Non-Oscillatory (WENO Schemes) ✚ **High Spectral Resolution** (Compact schemes)

- **Compact-Reconstruction WENO Schemes**
  - **High spectral resolution** – Improved resolution of small length scales
  - **Non-oscillatory interpolation** across discontinuities and steep gradients
  - **No parallelization-induced errors** (however, need *a priori* estimate on the number of Jacobi iterations for the reduced system)
  - Excellent strong and weak scaling compared to a non-compact scheme; at very small subdomain sizes, **retains higher parallel efficiency** despite relatively poorer scaling
- **WENO5/CRWENO5 + Implicit-Explicit Time Integration**
  - Achieves **theoretical orders of convergence**, stable for a large range of time step sizes
  - Need to **optimize implementation** (evaluation of Jacobian, application of pre-conditioner)
  - Preliminary scaling results encouraging – **Implicit in space and time scales well**
  - Error control through **adaptive time stepping** – preliminary results show promise

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