A Scalable, Parallel Implementation of Weighted, Non-Linear Compact Schemes

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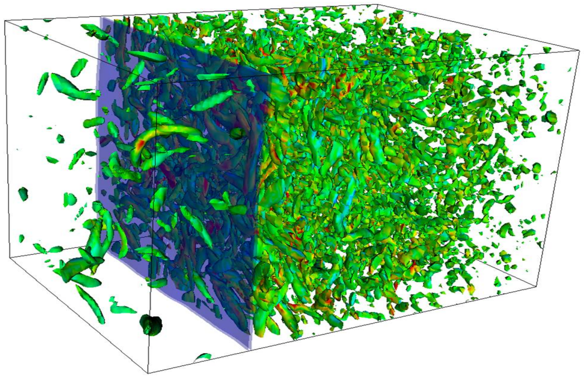
Motivation

Numerical Solution of Compressible Turbulent Flows

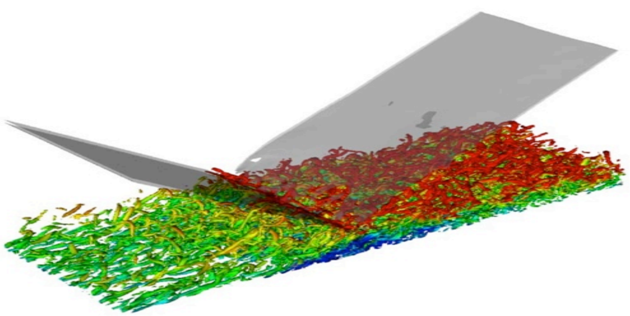
- Atmospheric flows, Aircraft and Rotorcraft wake flows
- Characterized by **large range of length scales**
- Convection and interaction of eddies
- Compressibility → **Shock waves** & **Shocklets**
- Thin shear layers → **High gradients** in flow



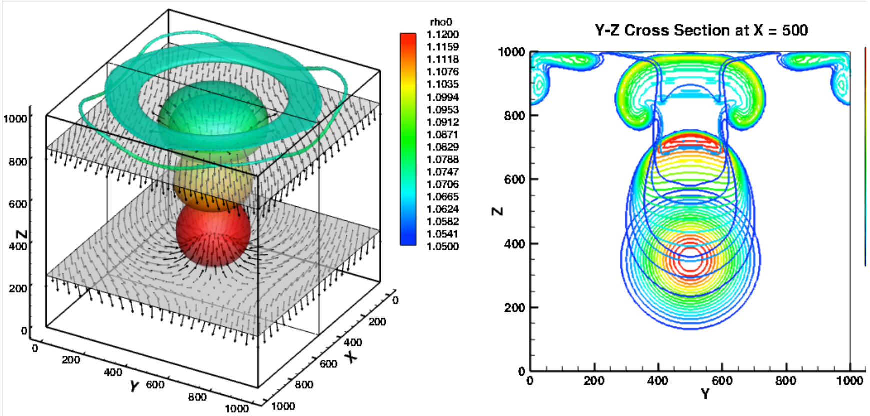
Shock-Turbulence Interaction (Stanford University)

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**

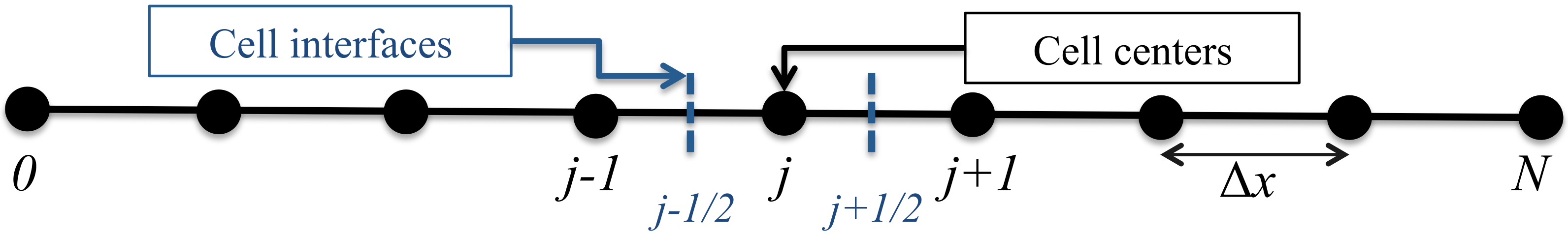


Shock-Turbulent Boundary Layer Interaction (Brandon Morgan, Stanford University and Nagi Mansour, NASA)



Rising Thermal Bubble in Hydrostatically Balanced Atmosphere

Background



Conservative finite-difference discretization of a Hyperbolic Conservation Law

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

Compressible Turbulent Flows

Weighted Essentially Non-Oscillatory (WENO) Schemes

Compact Finite-Difference Schemes

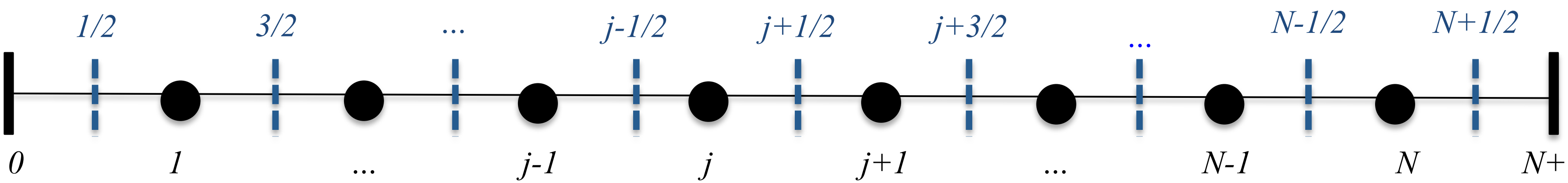
Hybrid Compact-WENO Schemes
Disadvantages: loss of spectral resolution near discontinuities

Weighted Compact Non-Linear Schemes
Disadvantage: Relatively Poor spectral resolution

Compact-Reconstruction WENO (CRWENO) Schemes

Ghosh & Baeder, SIAM J. Sci. Comput., 2012

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 $(2r\text{-}1)$-th order compact interpolation scheme:

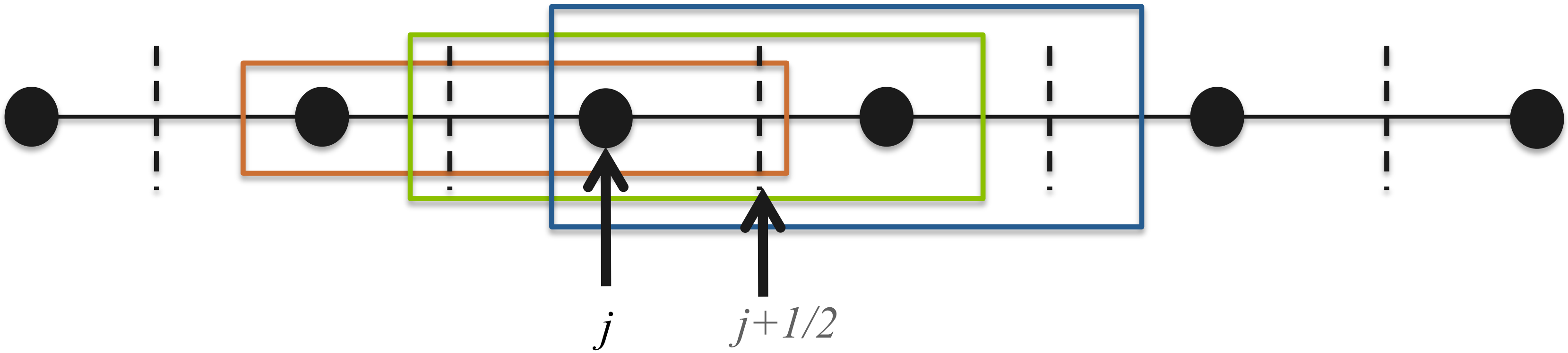
$$\sum_{k=1}^{r} c_k\,\mathrm{A}_k^r\left(\hat{f}_{j+1/2-m},\ldots,\hat{f}_{j+1/2+m}\right)=\sum_{k=1}^{r} c_k\,\mathrm{B}_k^r\left(f_{j-n},\ldots,f_{j+n}\right)$$

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

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)



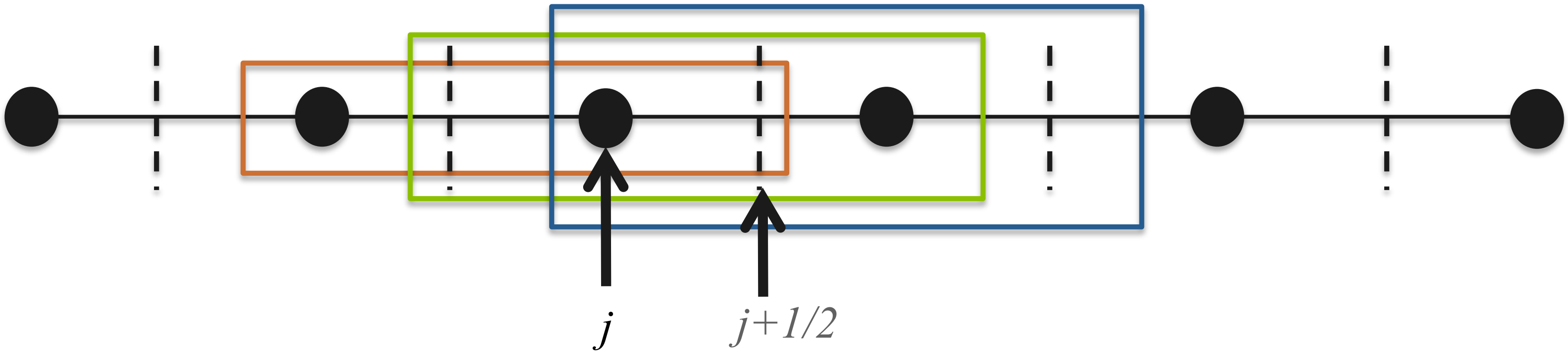
$$\frac{2}{3} f_{j-1/2} + \frac{1}{3} f_{j+1/2} = \frac{1}{6} f_{j-1} + \frac{5}{6} f_j \longrightarrow c_1 = \frac{2}{10}$$

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

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

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

5th Order CRWENO Scheme (CRWENO5)



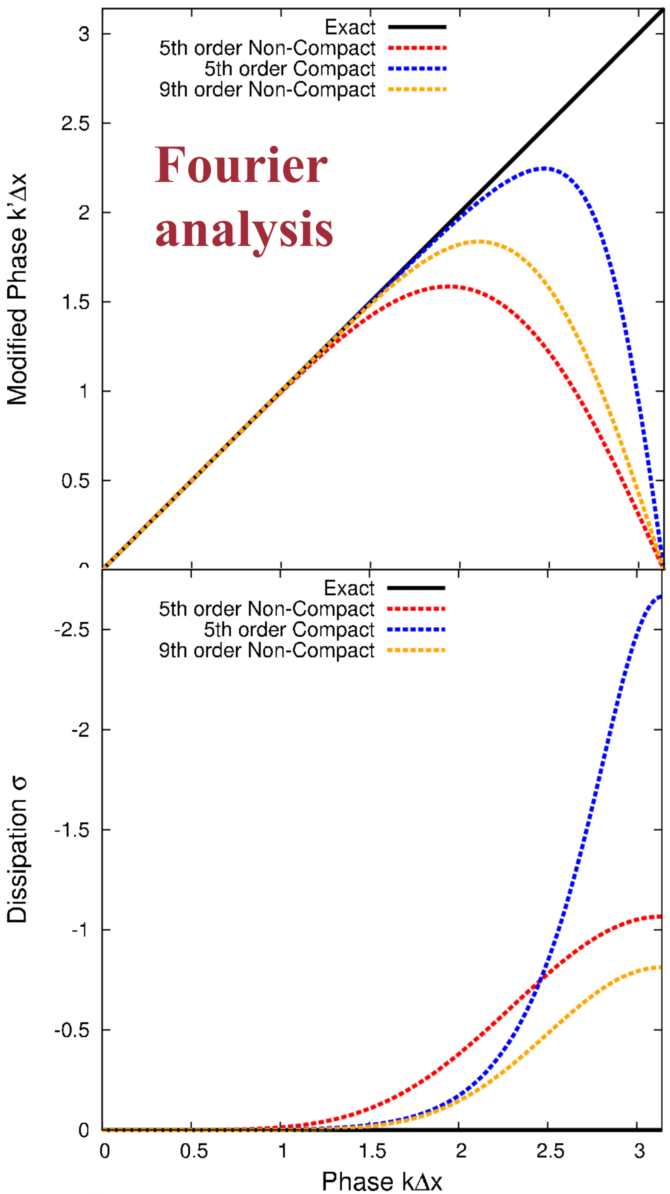
$$\frac{2}{3} f_{j-1/2} + \frac{1}{3} f_{j+1/2} = \frac{1}{6} f_{j-1} + \frac{5}{6} f_j \longrightarrow \cancel{c_1 = \frac{2}{10}} \quad \omega_1$$

$$\frac{1}{3} f_{j-1/2} + \frac{2}{3} f_{j+1/2} = \frac{5}{6} f_j + \frac{1}{6} f_{j+1} \longrightarrow \cancel{c_2 = \frac{5}{10}} \quad \omega_2$$

$$\frac{2}{3} f_{j+1/2} + \frac{1}{3} f_{j+3/2} = \frac{1}{6} f_j + \frac{5}{6} f_{j+1} \longrightarrow \cancel{c_3 = \frac{3}{10}} \quad \omega_3$$

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

Numerical Analysis



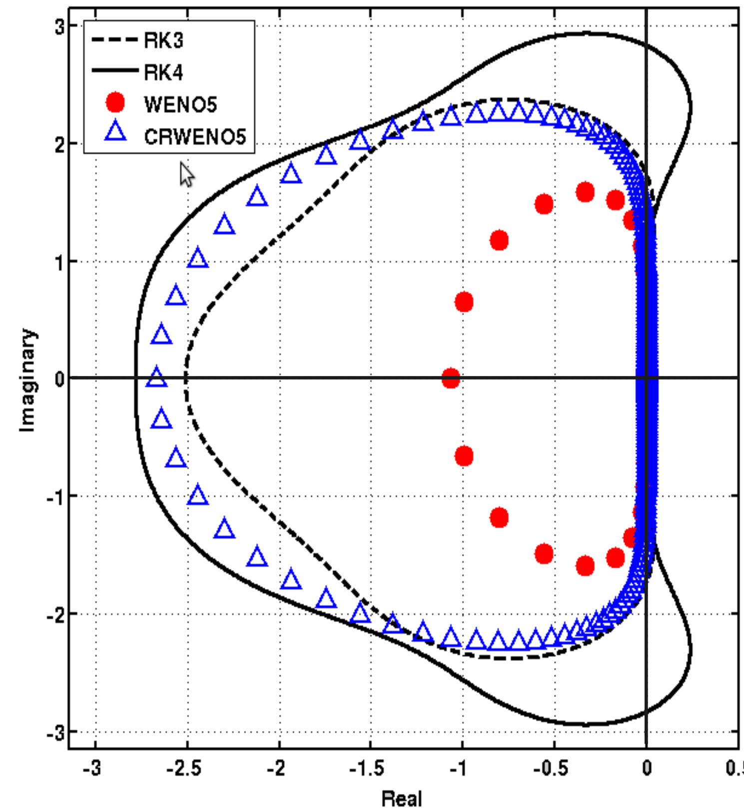
Taylor Series

WENO5

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

CRWENO5

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



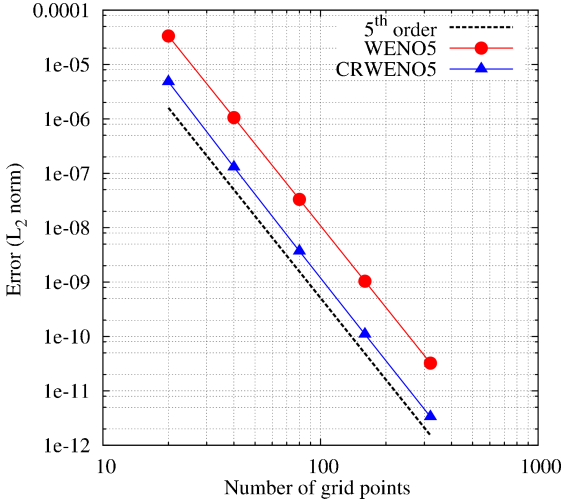
➔ WENO5 requires **~ 1.5 times more grid points per dimension** to yield a solution of comparable accuracy as the CRWENO5 scheme.

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

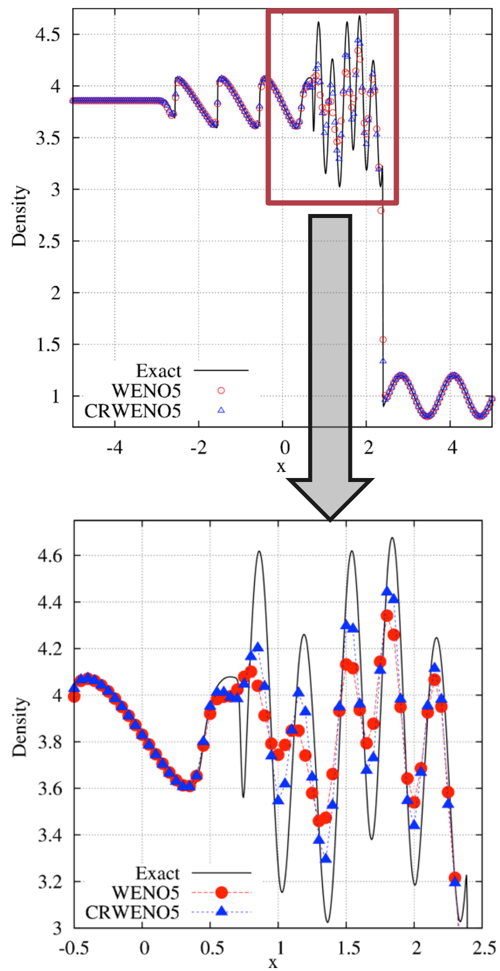
Preliminary Results

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

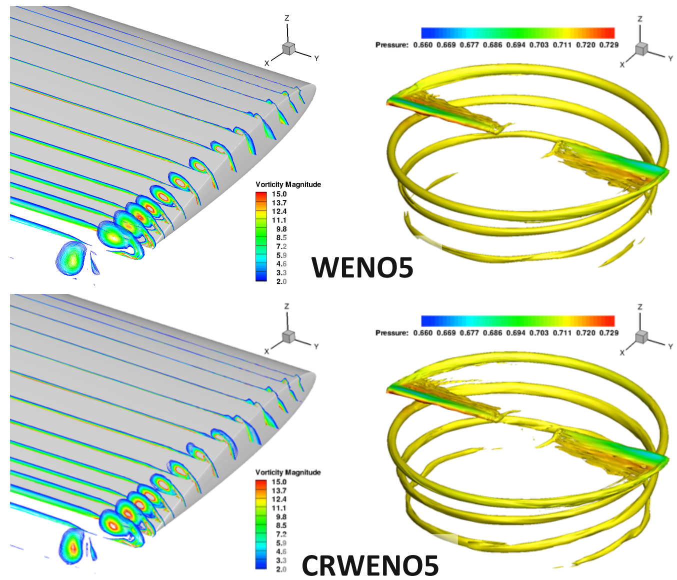
Periodic density wave advection



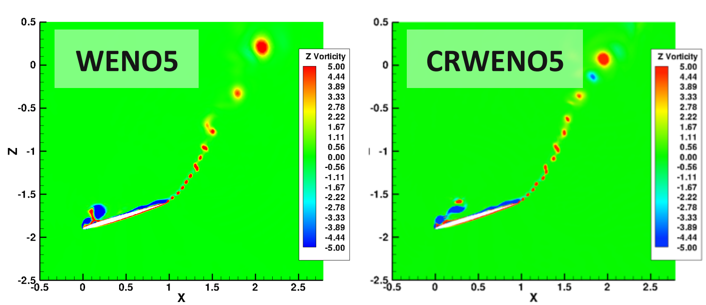
Shu-Osher Problem



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

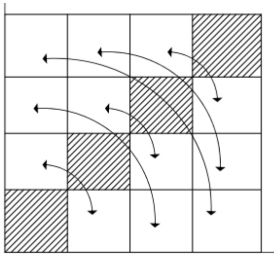
CRWENO5 needs a tridiagonal solution at each time-integration stage/step

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**

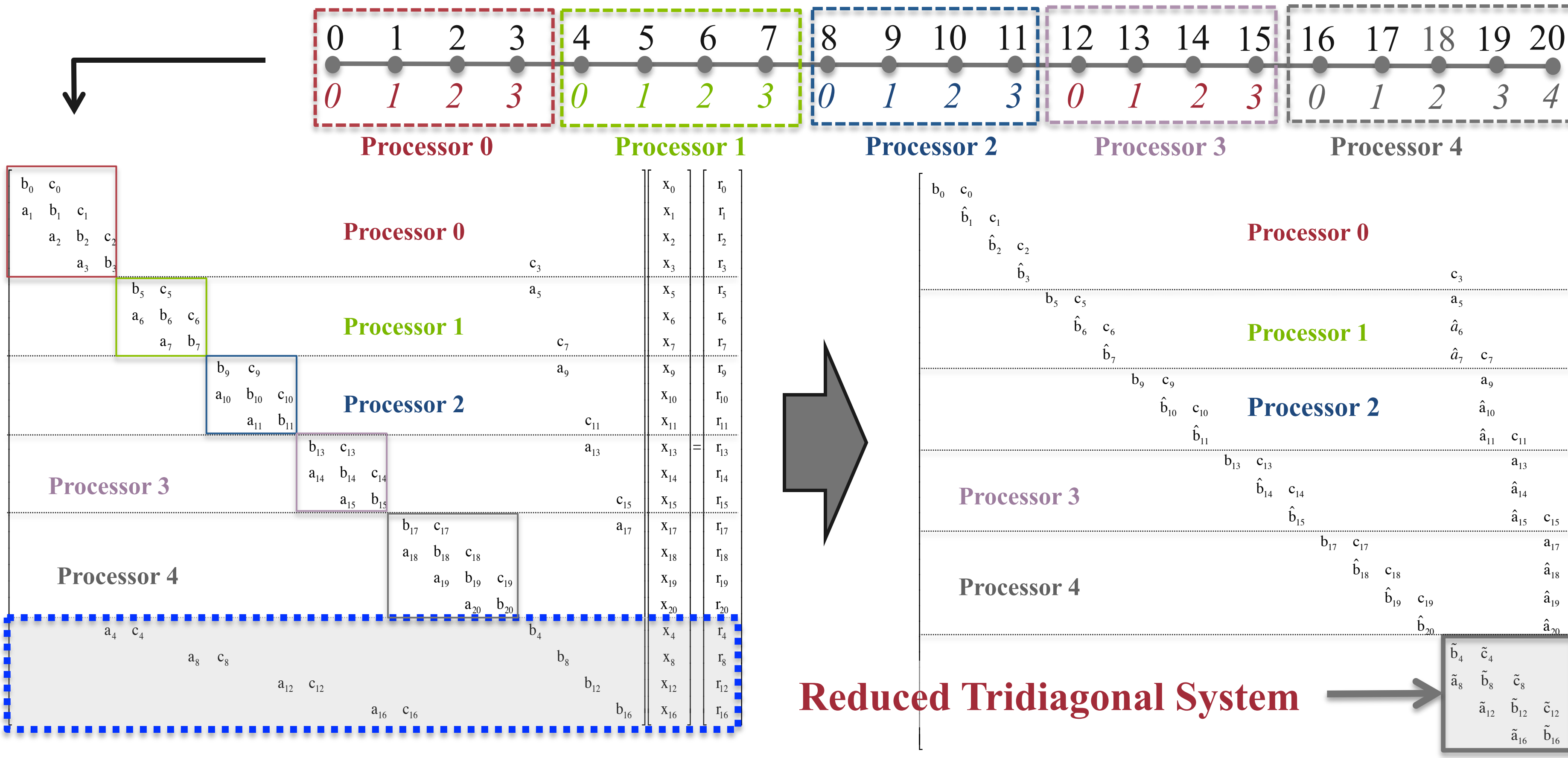


Parallel Implementation of the Thomas Algorithm

- **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

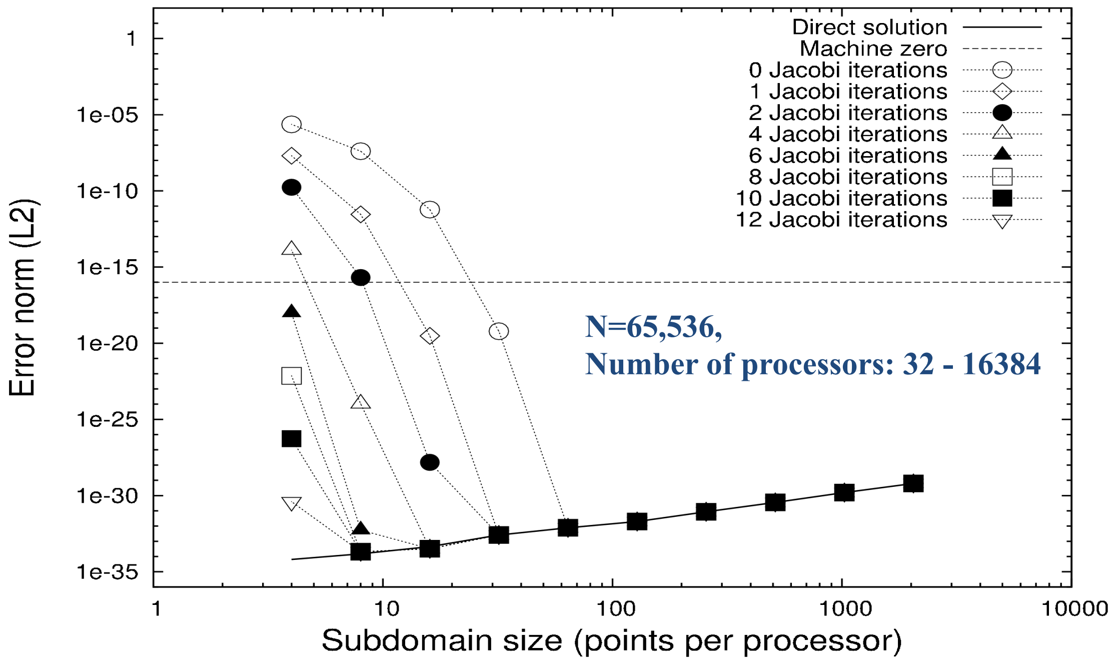
- One row on each processor → **Communication intensive**
- **Direct/Exact** solutions to the reduced system (**Cyclic Reduction / Recursive-Doubling Algorithm, Gather-and-Solve**) - **Do not scale well!**

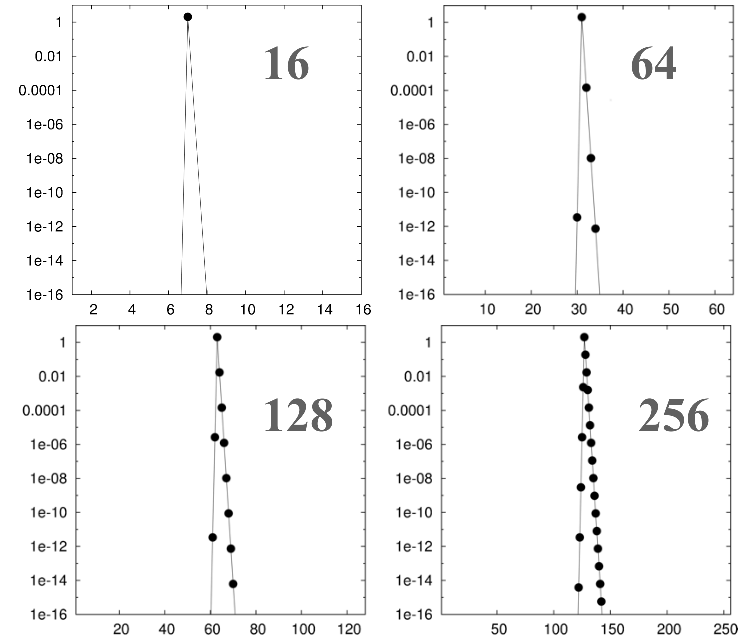
Iterative Sub-structuring Method

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

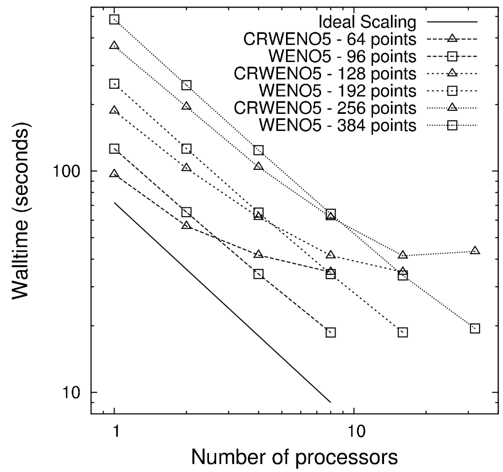
- The **factor by which the grid needs for WENO5 needs to be refined** to yield comparable solutions as CRWENO5 is f^D (f times per dimension)
- Several tridiagonal systems are solved for multi-dimensional problems →Higher arithmetic density → **Cost increases sub-linearly with number of systems**

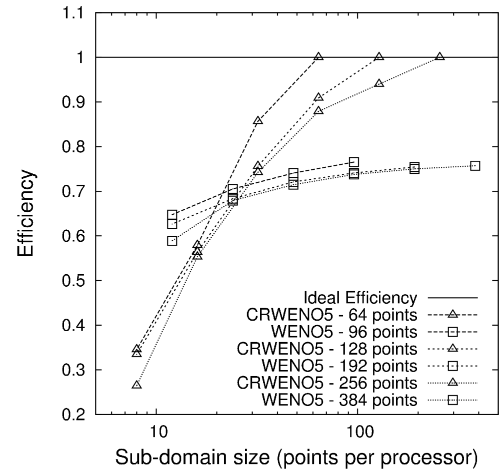
Performance Analysis for a Smooth Problem

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

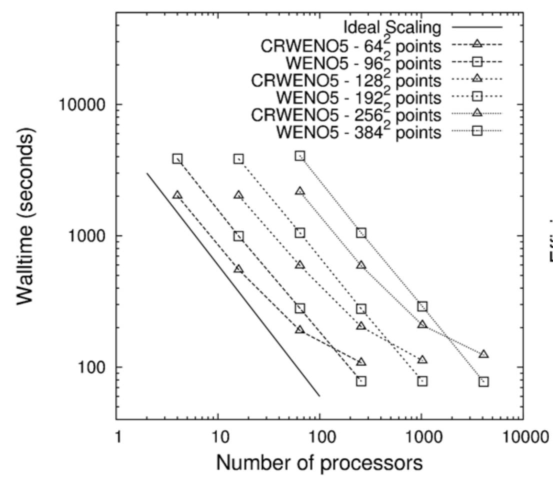


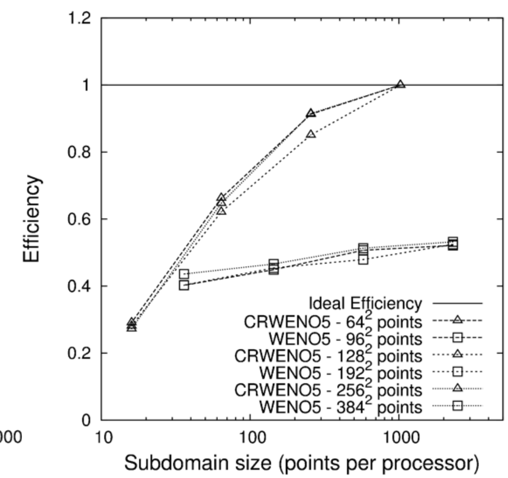


2D

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

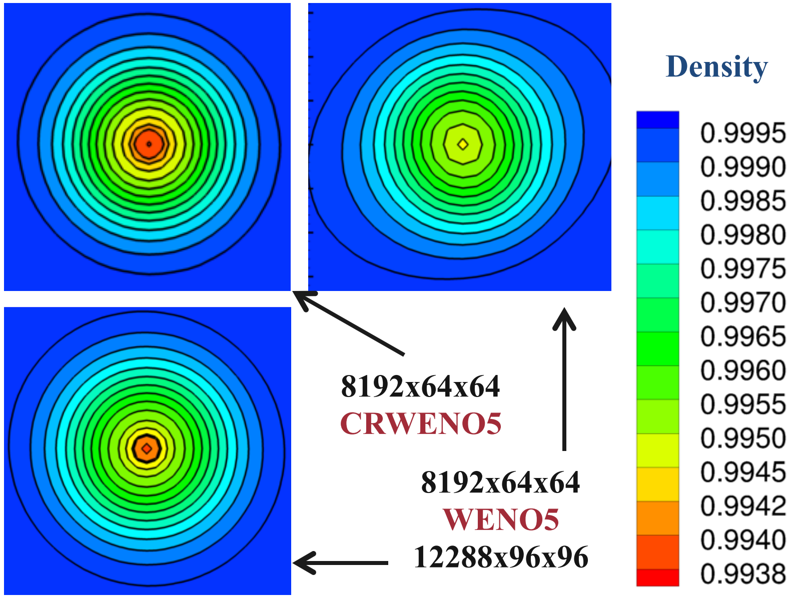




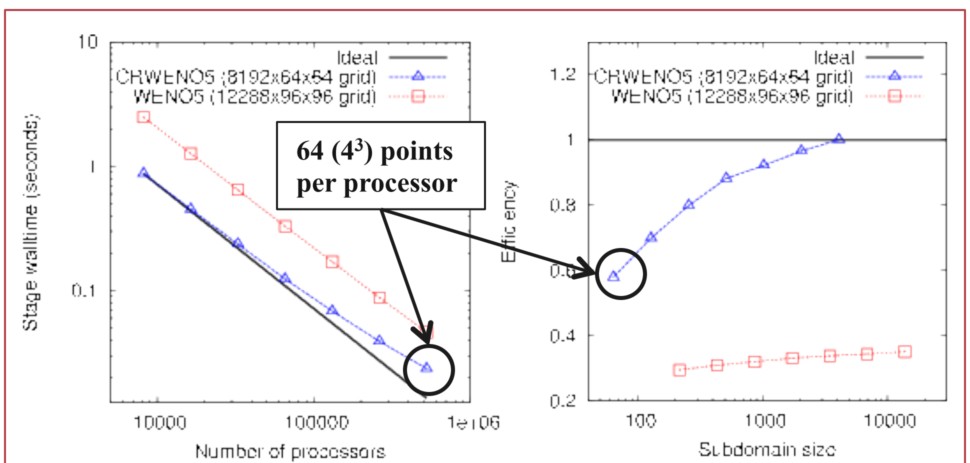
Note: Critical sub-domain size is insensitive to global problem size

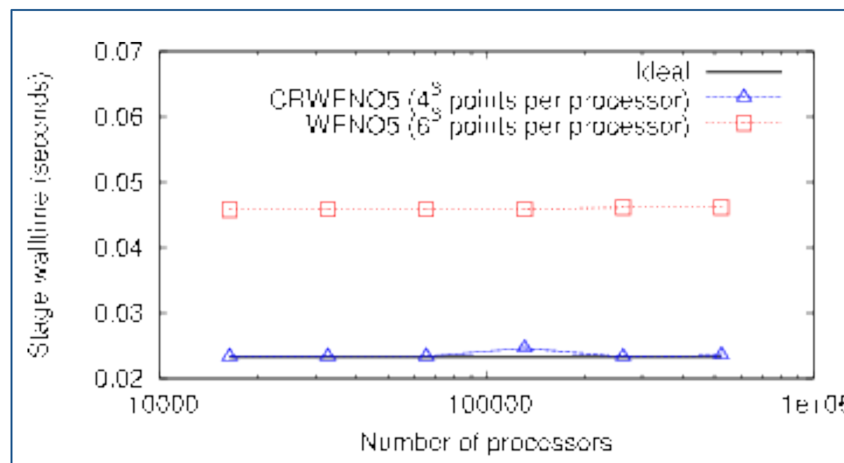
Scalability Results for Benchmark Flow Problems

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





Conclusions & Future Work

- **Parallel Implementation on Distributed Memory Platforms**
  - Based on an **iterative sub-structuring approach** to the tridiagonal system of equations
  - **No parallelization-induced errors** (however, need *a priori* estimate on the number of Jacobi iterations for the reduced system)
  - Avoids collective communication → **Excellent weak scaling**
  - Good strong scaling compared to a non-compact scheme; at very small subdomain sizes, **retains higher parallel efficiency** despite relatively poorer scaling
- **Future Work (Practical and Interesting Applications)**
  - DNS of shock-turbulence interaction and shock-turbulent boundary layer interaction
  - Apply the CRWENO5 scheme to benchmark atmospheric flow problems and compare solution and scalability with spectral element methods (popular in that community)
  - Implement this implementation of the CRWENO5 scheme in an existing, validated Navier-Stokes solver and apply to practical flow problems

Thank you!

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