Compact-Reconstruction WENO Schemes – Theory, Implementation and Applications

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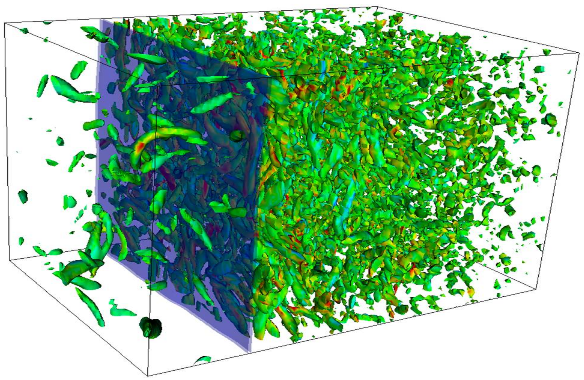
Motivation

Numerical Solution of Compressible Turbulent Flows

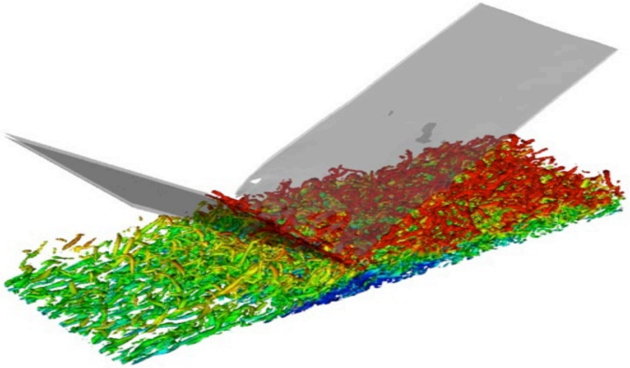
- Aircraft and Rotorcraft wake flows
- Characterized by **large range of length scales**
- Convection and interaction of eddies
- Compressibility → **Shock waves** & **Shocklets**
- Thin shear layers → **High gradients** in flow



Shock-Turbulence Interaction
(Stanford University CTR)

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**



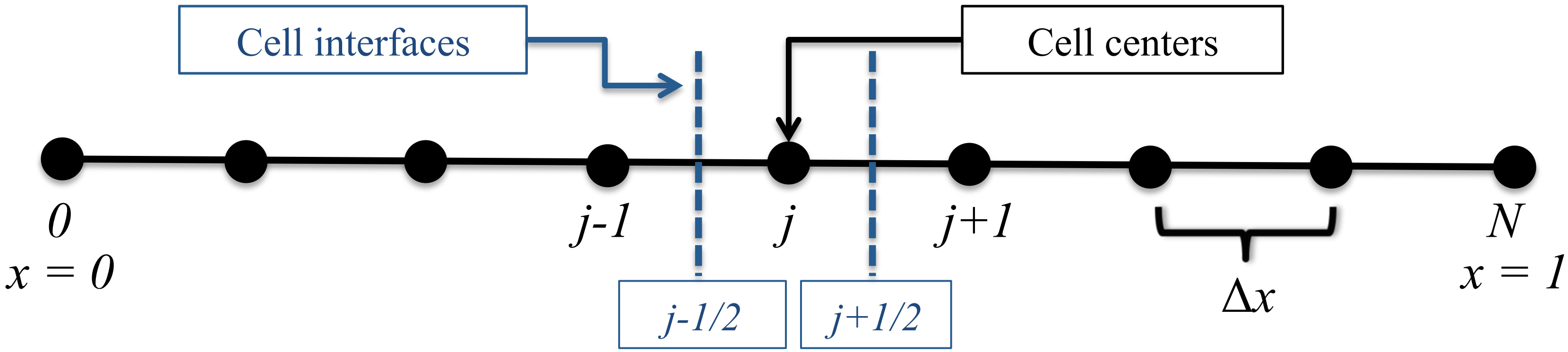
Shock-Turbulent Boundary Layer Interaction
(Brandon Morgan, Stanford University and Nagi Mansour, NASA)

Outline

- **Compact-Reconstruction WENO Schemes**
  - Background and other high-resolution, non-oscillatory schemes in the literature
  - Description of the CRWENO scheme, especially the 5^{th} order CRWENO schemes
  - Numerical analysis
- **Applications demonstrating the numerical properties**
  - Scalar conservation laws
  - Inviscid Euler equations
  - Aerodynamic flow problems
  - DNS of benchmark turbulent flows
- **Implementation and Computational Cost**
  - Computational efficiency on a single processor
  - Review of existing parallelizing strategies
  - Parallel implementation of the CRWENO5 scheme
  - Performance and scalability
- **Concluding Remarks**

Background

- **Hyperbolic Conservation Law** $$u_t + f(u)_x = 0;\ \ f'(u) \in \Re$$



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

- **Reconstruction** $$f_{j+1/2} = \mathrm{f}\left(f_i : i = j-m, \ldots, j+n \right)$$

High-Order Finite Difference Schemes

- **Weighted Essentially Non-Oscillatory Schemes**
  - Liu, Osher & Chan (*JCP, 1994*) and Jiang & Shu (*JCP, 1996*)
  - Solution-dependent combination of r interpolation stencils of r^{th}-order accuracy – **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 → **non-oscillatory behavior**
  - Poor spectral resolution, even for very high orders of accuracy
- **Compact Finite-Difference Schemes**
  - Lele (*JCP, 1992*) (Non-conservative discretization of the flux derivative)
  - Coupling between neighboring flux derivative approximations
  - Requires the solution of a **banded (tridiagonal/penta-diagonal) system of equations** (linear compact schemes → constant coefficients → LU decomposition can be pre-computed)
  - **High spectral resolution** for the same order of convergence
  - Linear compact schemes need some form of limiting for solutions with discontinuities

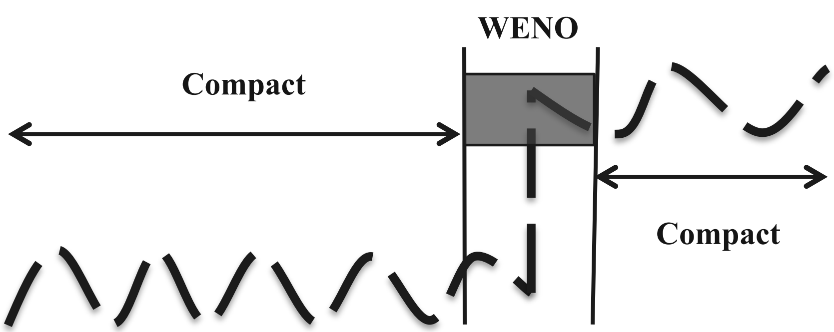
High-Resolution Non-Oscillatory Schemes

Compressible Turbulent Flows

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

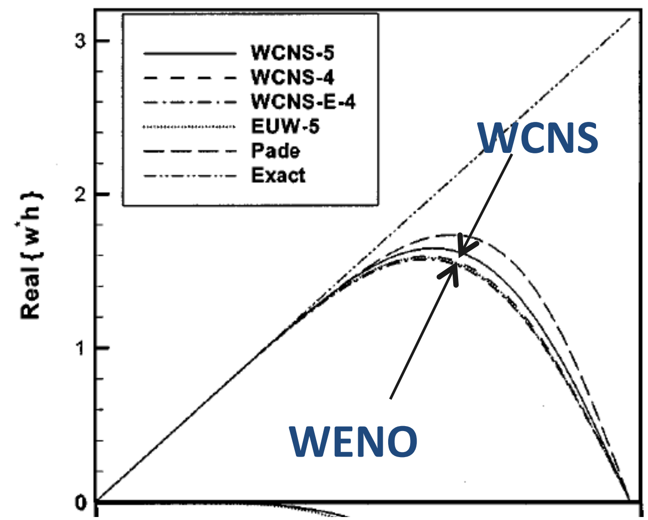
Hybrid Compact-WENO Schemes

- Smoothness indicator **marks out regions near discontinuities**
- *Adams & Sherriff (1996), Pirozzoli (2002), Ren et. al. (2003)*
- **Disadvantages**: arbitrary parameter for switching, loss of spectral resolution near discontinuities



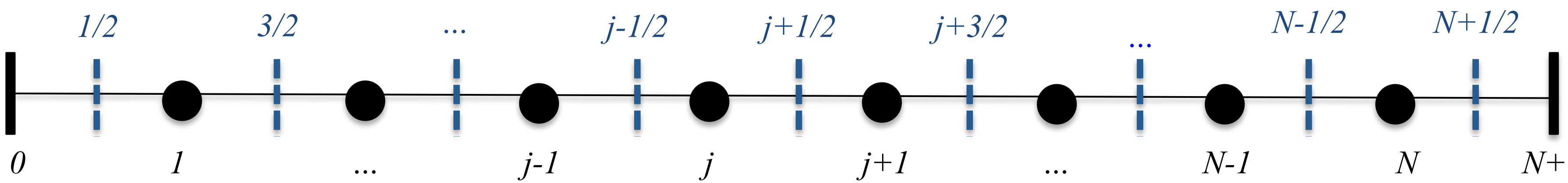
Weighted Compact Non-Linear Schemes

- Non-conservative finite-difference formulation over a staggered mesh
- *Deng & Zhang (2000), Wang & Huang (2002), Zhang, Jiang & Shu (2008)*



Deng & Zhang, 2000, *JCP.*

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:

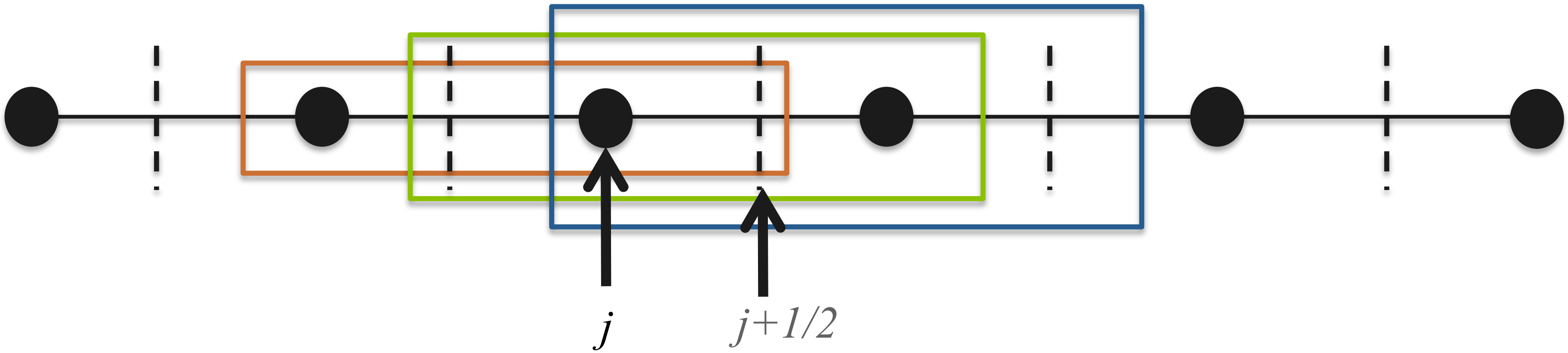
$$\sum_{k=1}^{r} c_k\,\mathrm{A}_k^r\left(\hat{f}_{j+1/2-m},\ldots,\hat{f}_{j+1/2+m}\right)=\sum_{k=1}^{r} c_k\,\mathrm{B}_k^r\left(f_{j-n},\ldots,f_{j+n}\right)$$

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

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

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

5th Order CRWENO Scheme (CRWENO5)



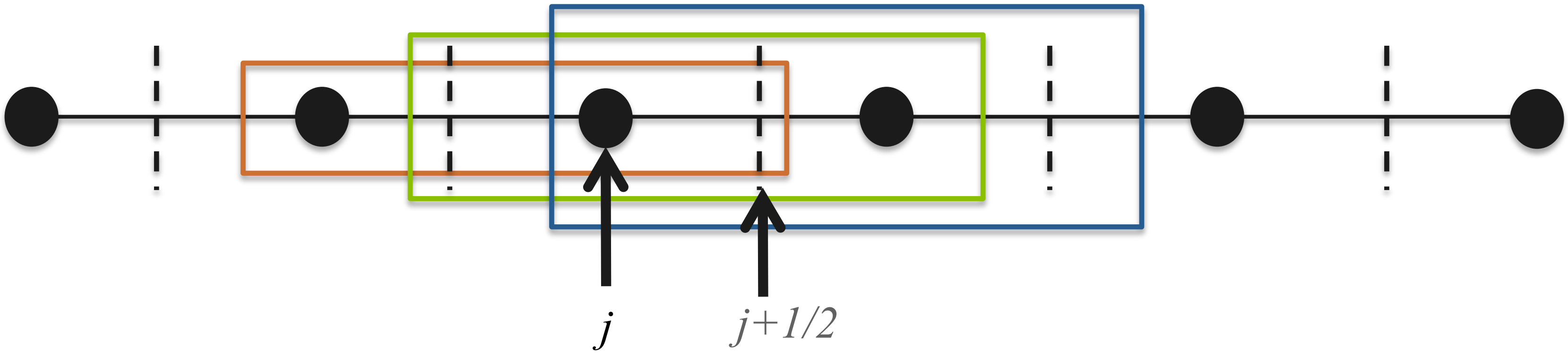
$$\frac{2}{3}f_{j-1/2}+\frac{1}{3}f_{j+1/2}=\frac{1}{6}f_{j-1}+\frac{5}{6}f_j \quad\longrightarrow\quad c_1=\frac{2}{10}$$

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

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

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

5^{th} Order CRWENO Scheme (CRWENO5)



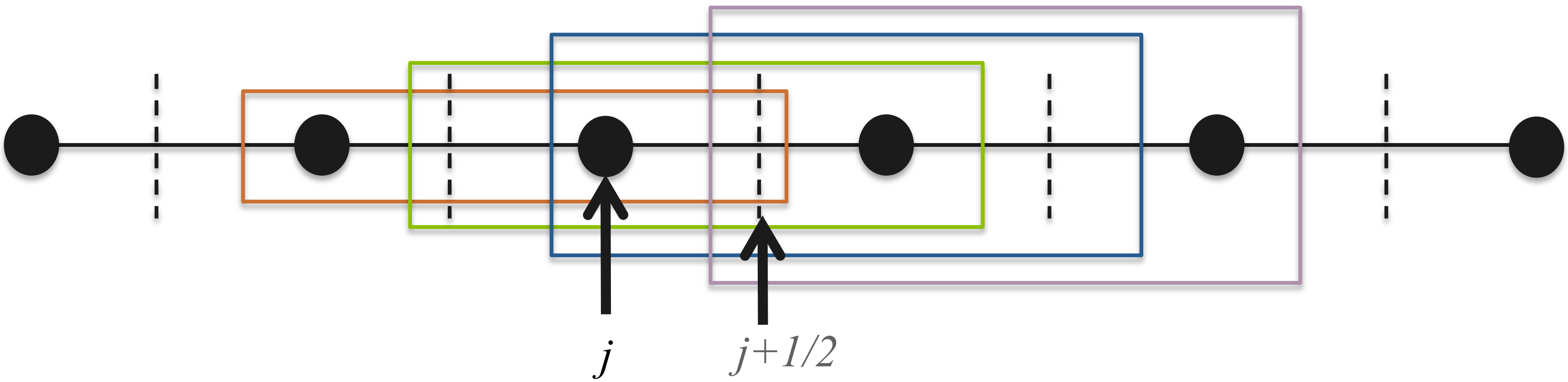
$$\frac{2}{3}f_{j-1/2}+\frac{1}{3}f_{j+1/2}=\frac{1}{6}f_{j-1}+\frac{5}{6}f_j \quad \longrightarrow \quad \cancel{c_1=\frac{2}{10}} \quad \omega_1$$

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

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

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

Low Dissipation CRWENO5 scheme (CRWENO5-LD)



$$\frac{2}{3}f_{j-1/2}+\frac{1}{3}f_{j+1/2}=\frac{1}{6}f_{j-1}+\frac{5}{6}f_j \quad\rightarrow\quad c_1=\frac{3}{20}$$

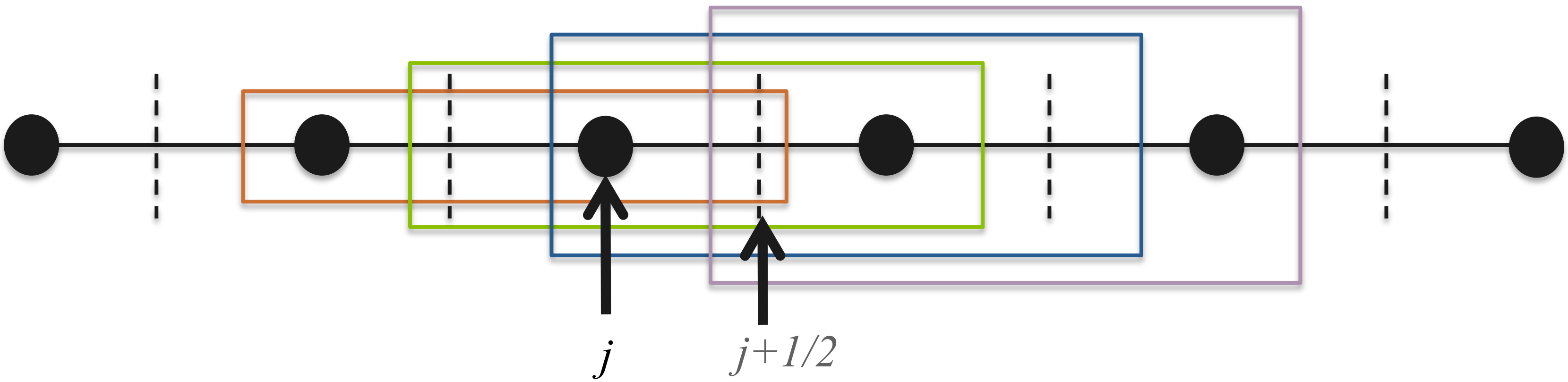
$$\frac{1}{3}f_{j-1/2}+\frac{2}{3}f_{j+1/2}=\frac{5}{6}f_j+\frac{1}{6}f_{j+1} \quad\rightarrow\quad c_2=\frac{9}{20}$$

$$\frac{2}{3}f_{j+1/2}+\frac{1}{3}f_{j+3/2}=\frac{1}{6}f_j+\frac{5}{6}f_{j+1} \quad\rightarrow\quad c_3=\frac{7}{20}$$

$$\frac{1}{3}f_{j+1/2}+\frac{2}{3}f_{j+3/2}=\frac{5}{6}f_{j+1}+\frac{1}{6}f_{j+2} \quad\rightarrow\quad c_4=\frac{1}{20}$$

$$\frac{5}{20}f_{j-1/2}+\frac{12}{20}f_{j+1/2}+\frac{3}{20}f_{j+3/2}=\frac{3}{120}f_{j-1}+\frac{67}{120}f_j+\frac{49}{120}f_{j+1}+\frac{1}{120}f_{j+2}$$

Low Dissipation CRWENO5 scheme (CRWENO5-LD)



$$\frac{2}{3}f_{j-1/2} + \frac{1}{3}f_{j+1/2} = \frac{1}{6}f_{j-1} + \frac{5}{6}f_j \longrightarrow \cancel{c_1 = \frac{3}{20}} \quad \omega_1$$

$$\frac{1}{3}f_{j-1/2} + \frac{2}{3}f_{j+1/2} = \frac{5}{6}f_j + \frac{1}{6}f_{j+1} \longrightarrow \cancel{c_2 = \frac{9}{20}} \quad \omega_2$$

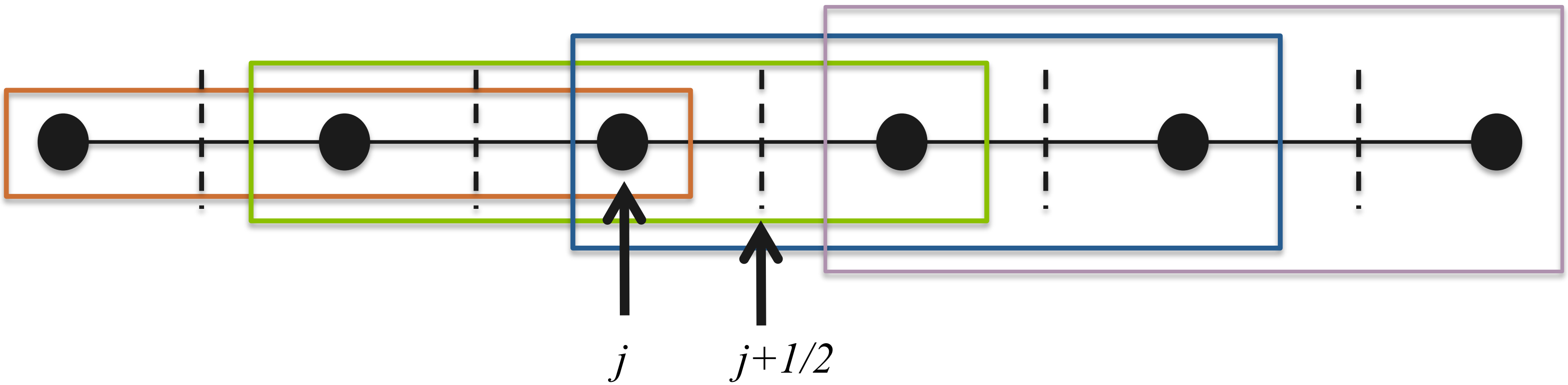
$$\frac{2}{3}f_{j+1/2} + \frac{1}{3}f_{j+3/2} = \frac{1}{6}f_j + \frac{5}{6}f_{j+1} \longrightarrow \cancel{c_3 = \frac{7}{20}} \quad \omega_3$$

$$\frac{1}{3}f_{j+1/2} + \frac{2}{3}f_{j+3/2} = \frac{5}{6}f_{j+1} + \frac{1}{6}f_{j+2} \longrightarrow \cancel{c_4 = \frac{1}{20}} \quad \omega_4$$

$$\left(\frac{2}{3}\omega_1 + \frac{1}{3}\omega_2\right)f_{j-1/2} + \left(\frac{1}{3}\omega_1 + \frac{2}{3}(\omega_2+\omega_3) + \frac{1}{3}\omega_4\right)f_{j+1/2} + \left(\frac{1}{3}\omega_3 + \frac{2}{3}\omega_4\right)f_{j+3/2} = \frac{\omega_1}{6}f_{j-1} + \frac{5(\omega_1+\omega_2)+\omega_3}{6}f_j + \frac{\omega_2+5(\omega_3+\omega_4)}{6}f_{j+1} + \frac{\omega_4}{6}f_{j+2}$$

Smoothness Indicators

Weights are calculated based on **smoothness indicators** of corresponding explicit stencils **(same as WENO5 scheme)**



$$\left.\begin{aligned} \beta_1 &= IS(f_{j-2}, f_{j-1}, f_j) \\ \beta_2 &= IS(f_{j-1}, f_j, f_{j+1}) \\ \beta_3 &= IS(f_j, f_{j+1}, f_{j+2}) \\ \beta_4 &= IS(f_{j+1}, f_{j+2}, f_{j+3}) \end{aligned}\right\} \quad \alpha_k = \frac{c_k}{(\beta_k + \varepsilon)^p}; \; \omega_k = \frac{\alpha_k}{\sum_k \alpha_k}; \; k = 1,2,3$$

$$\beta_4 = \max(\beta_3, \beta_4)$$

(Avoid downwind interpolation)

CRWENO5-LD

Numerical Analysis – Accuracy and Convergence

Underlying optimal (linear) schemes:

$$f_{j+1/2} = \frac{1}{30} f_{j-2} - \frac{13}{60} f_{j-1} + \frac{47}{60} f_j + \frac{27}{60} f_{j+1} - \frac{1}{20} f_{j+2}$$ WENO5

$$\frac{3}{10} f_{j-1/2} + \frac{6}{10} f_{j+1/2} + \frac{1}{10} f_{j+3/2} = \frac{1}{30} f_{j-1} + \frac{19}{30} f_j + \frac{10}{30} f_{j+1}$$ CRWENO5

$$\frac{5}{20} f_{j-1/2} + \frac{12}{20} f_{j+1/2} + \frac{3}{20} f_{j+3/2} = \frac{3}{120} f_{j-1} + \frac{67}{120} f_j + \frac{49}{120} f_{j+1} + \frac{1}{120} f_{j+2}$$ CRWENO5-LD

Dissipation and dispersion errors

Dissipation

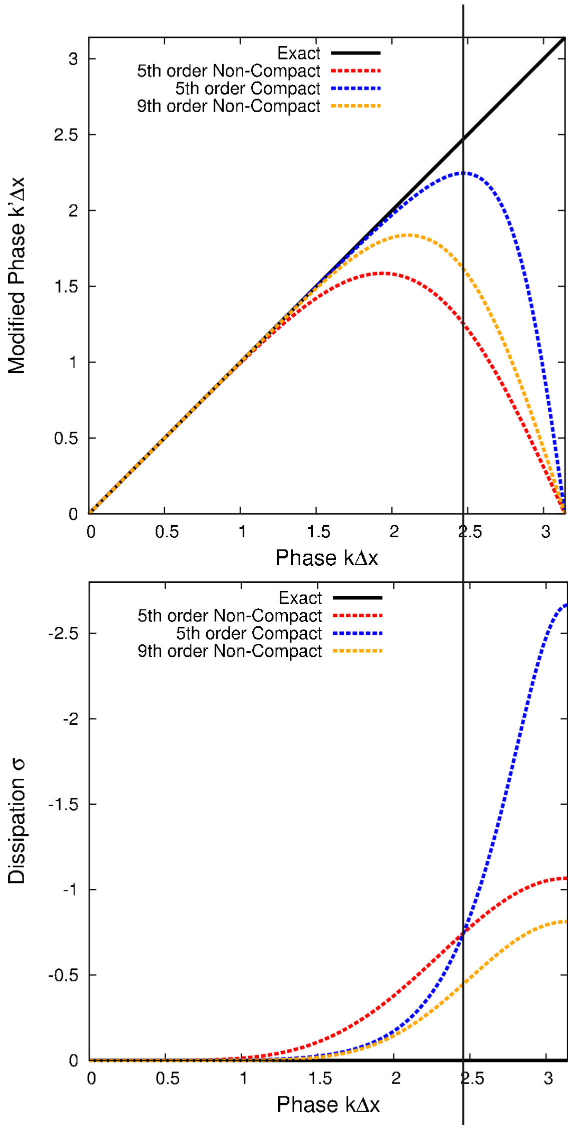
WENO5	CRWENO5	CRWENO5-LD
$\frac{1}{60} \left.\frac{\partial^6 f}{\partial x^6}\right\|_j \Delta x^5$	$\frac{1}{600} \left.\frac{\partial^6 f}{\partial x^6}\right\|_j \Delta x^5$	$\frac{1}{1200} \left.\frac{\partial^6 f}{\partial x^6}\right\|_j \Delta x^5$

Dispersion

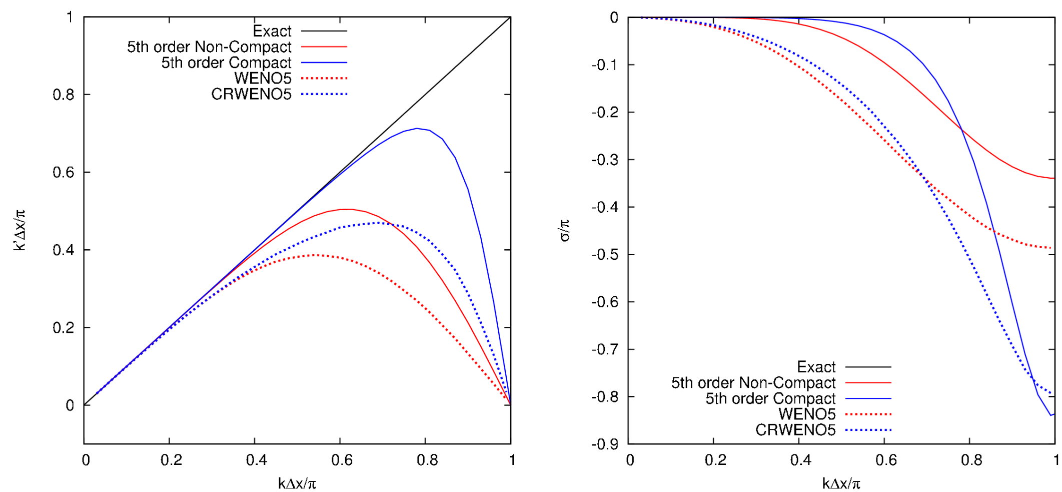
WENO5	CRWENO5, CRWENO5-LD
$\frac{1}{140} \left.\frac{\partial^7 f}{\partial x^7}\right\|_j \Delta x^6$	$\frac{1}{2100} \left.\frac{\partial^7 f}{\partial x^7}\right\|_j \Delta x^6$

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

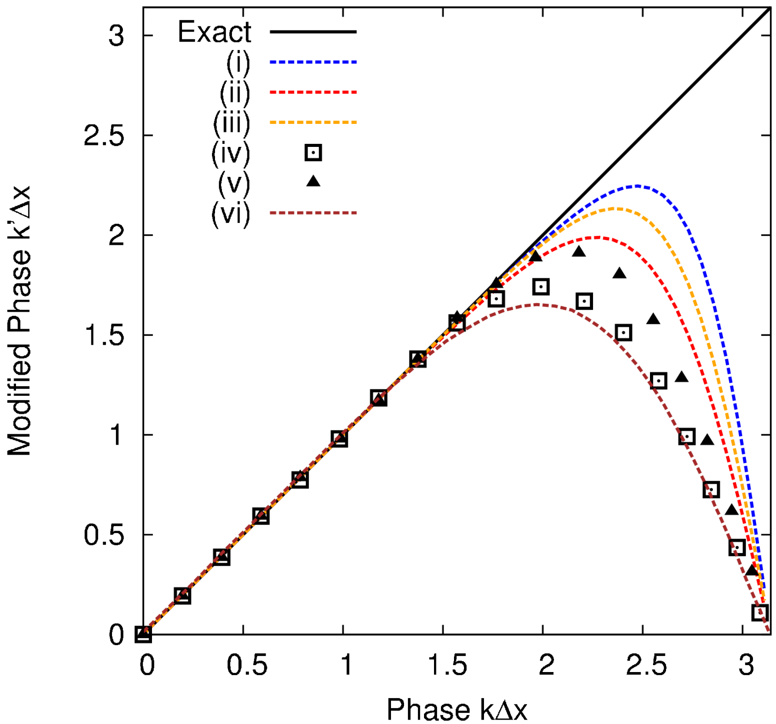
Numerical Analysis – Spectral Resolution



- **Linear Analysis**
  - 5th order compact scheme (CRWENO5) shows higher spectral resolution than the 5th (WENO5) and 9th order (WENO9) non-compact schemes.
  - Lower dissipation at small and moderate wavenumbers for the compact scheme
  - Higher dissipation for the compact scheme at incorrectly aliased wavenumbers
- **Non-Linear Analysis**
  - *Fauconnier & Dick (J. Comput. Appl. Math., 2013)*
  - Same qualitative trends, but resolution and dissipation compromised due to non-linear weights



Numerical Analysis – Comparison



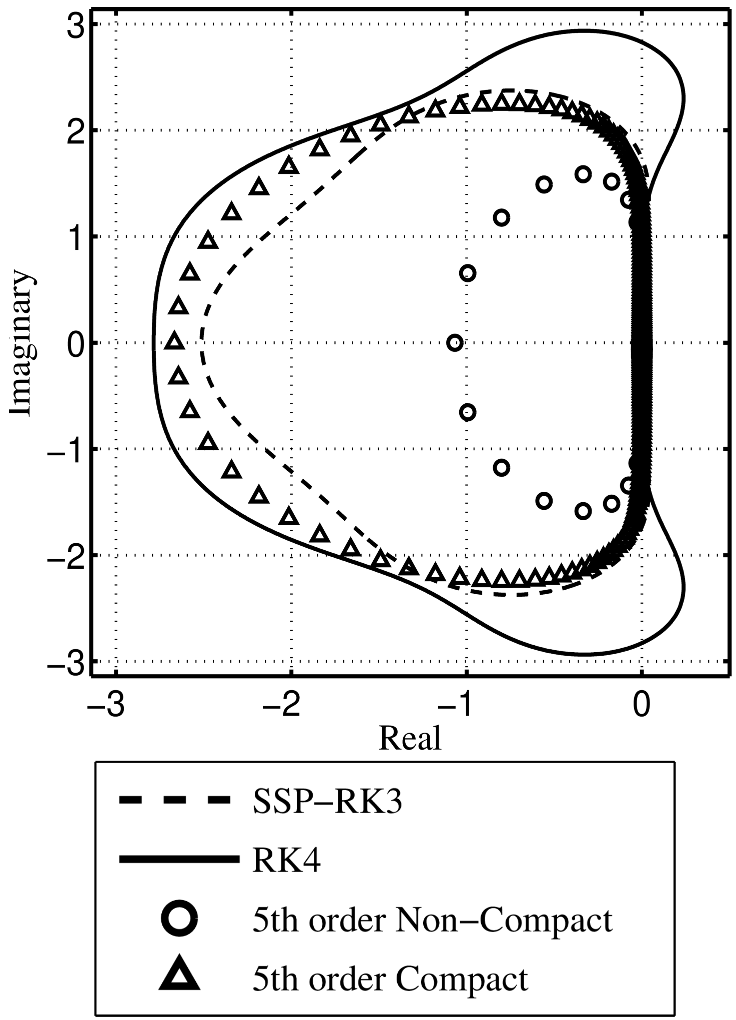
i. CRWENO5
ii. 6^{th} order central compact (Lele, 1992)
iii. 8^{th} order central compact (Lele, 1992)
iv. WENO-SYMBO (*r=3*) (Martin, et. al., 2006)
v. WENO-SYMBO (*r=4*) (Martin, et. al., 2006)
vi. WCNS5 (Deng & Zhang, 2000)

Comparison of **spectral resolution** and **bandwidth resolving efficiency** – CRWENO5 scheme with high-resolution schemes in literature

Bandwidth Resolving Efficiency

WENO5 (Jiang & Shu, 1996)	**0.35**
WENO7 (Balsara & Shu, 2000)	**0.42**
WENO9 (Balsara & Shu, 2000)	**0.48**
CRWENO5	**0.61**
6th-order central compact (Lele, 1992)	**0.50**
8th-order central compact (Lele, 1992)	**0.58**
WENO-SYMBO (r = 3) (Martin, et. al., 2006)	**0.49**
WENO-SYMBO (r = 4) (Martin, et. al., 2006)	**0.56**

Time-Integration and Stability

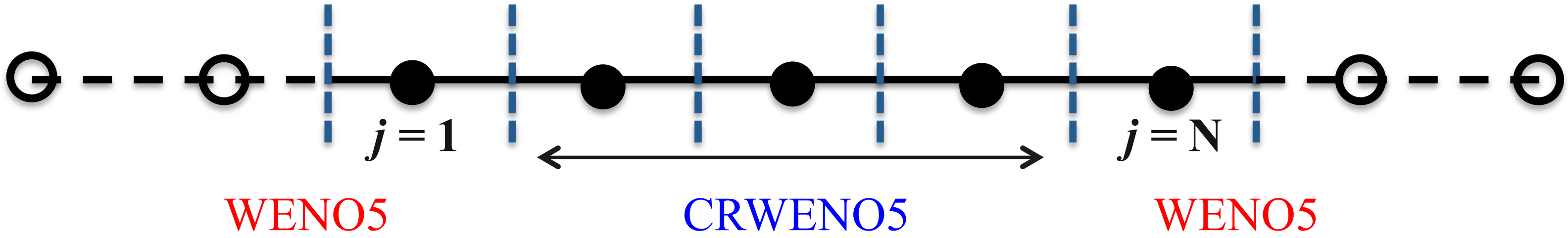


Linear Stability Analysis

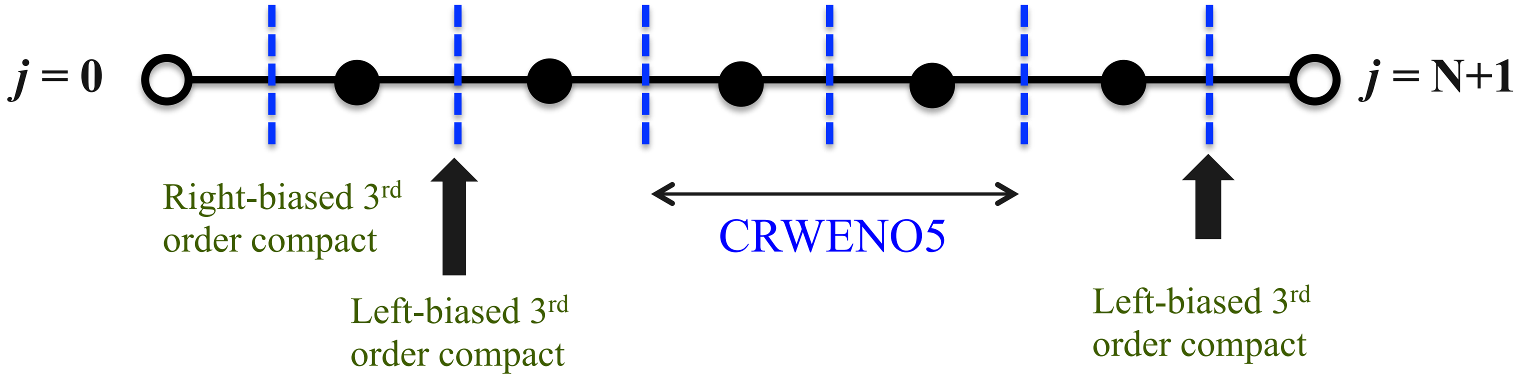
- CRWENO5 scheme has a lower linear stability limit than the WENO5 scheme → Smaller timestep restriction for explicit time integration
- CFL restriction for **3rd order SSP Runge-Kutta** scheme
  - WENO5: ~ 1.5
  - CRWENO5: ~ 0.9
- CFL restriction for **4th order Runge Kutta** scheme
  - WENO5: ~ 1.8
  - CRWENO5: ~ 1.1
- Time step size limit is **~ 1.6 times smaller** for CRWENO than WENO5

Boundary Treatment

Cell interface aligned with physical boundary – Boundary conditions implemented on “**ghost cells**”



Cell center coincident on physical boundary – **Reduced-order / interior-biased interpolation scheme** at interfaces near the boundary



Applications

Scalar Conservation Laws

Inviscid Euler Equations

Aerodynamic Applications

DNS of Benchmark Turbulent Flows

Scalar Conservation Laws

Schemes validated for the **linear advection equation** and the **inviscid Burgers equation**

Smooth problems

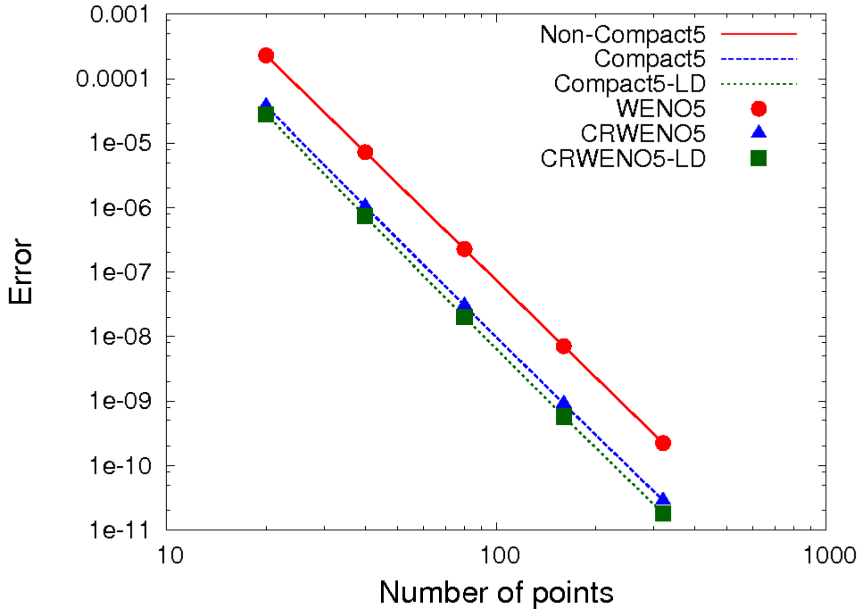
- 5^{th} order convergence verified for the new schemes
- Errors for CRWENO5 order of magnitude lower than WENO5, errors for CRWENO5-LD half those of CRWENO5 (consistent with Taylor series analysis)

Linear advection equation

$u_0(x) = \sin(2\pi x); 0 \leq x \leq 1$

(Periodic domain)

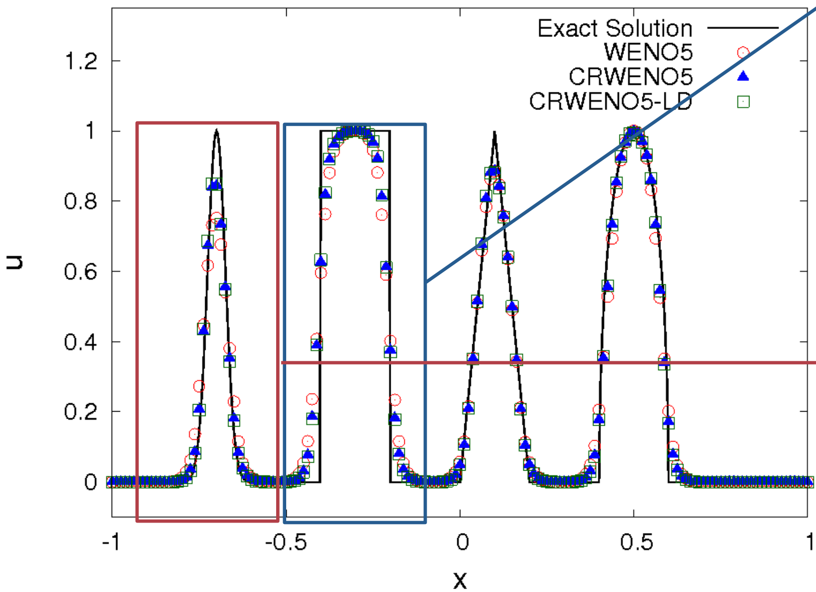
Solution obtained after 1 cycle with SSP-RK3 time-stepping



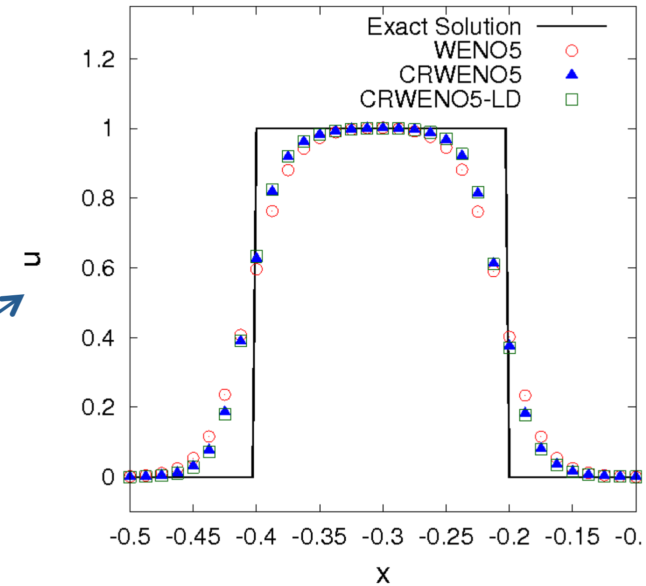
Scalar Conservation Laws

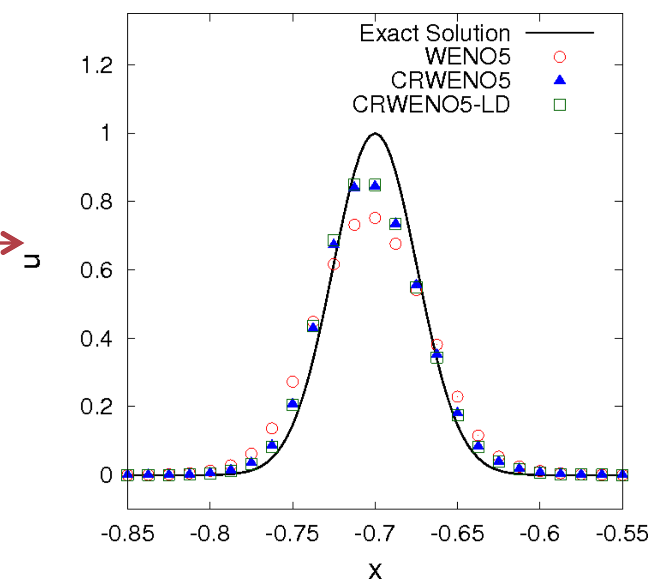
Discontinuous problems

- Non-oscillatory behavior validated across discontinuities
- CRWENO schemes show better resolution of discontinuous data



Linear Advection equation

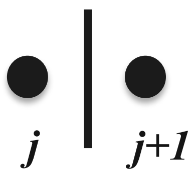




CRWENO for Euler Equations

Extension of scalar reconstruction schemes to vectors

- Component-wise reconstruction
- Characteristic-based reconstruction



U^{avg} (Roe averaged)

$\hookrightarrow \lambda^k_{j+1/2}, \mathbf{l}^k_{j+1/2}, \mathbf{r}^k_{j+1/2}$

Eigenvalues, left and right eigenvectors

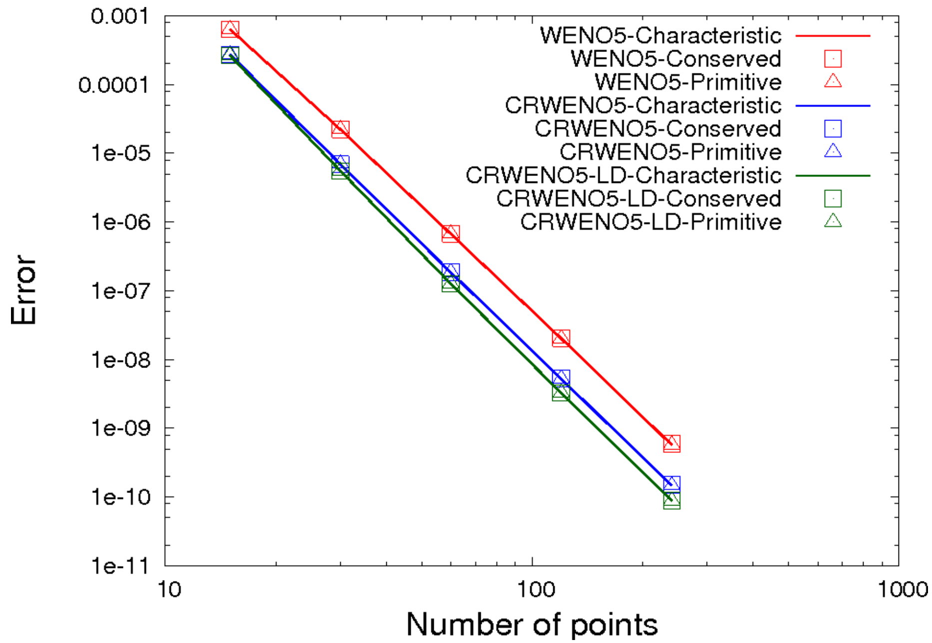
$$a\alpha^k_{j-1/2} + b\alpha^k_{j+1/2} + c\alpha^k_{j+3/2} = \tilde{a}\alpha^k_{j-1} + \tilde{b}\alpha^k_{j} + \tilde{c}\alpha^k_{j+1} \qquad \left(\alpha^k_i = \mathbf{l}^k_{j+1/2} \bullet \mathbf{f}_i\right)$$

$$\begin{aligned} & a(l^{k1}_{j+1/2} f^1_{j-1/2} + l^{k2}_{j+1/2} f^2_{j-1/2} + l^{k3}_{j+1/2} f^3_{j-1/2}) \\ + & b(l^{k1}_{j+1/2} f^1_{j+1/2} + l^{k2}_{j+1/2} f^2_{j+1/2} + l^{k3}_{j+1/2} f^3_{j+1/2}) \quad = \tilde{a}\alpha^k_{j-1} + \tilde{b}\alpha^k_{j} + \tilde{c}\alpha^k_{j+1} \\ + & c(l^{k1}_{j+1/2} f^1_{j+3/2} + l^{k2}_{j+1/2} f^2_{j+3/2} + l^{k3}_{j+1/2} f^3_{j+3/2}) \end{aligned}$$

Results in a **block tri-diagonal linear system** along each dimension (as compared to tri-diagonal system for conserved/primitive reconstruction)

Inviscid Euler Equations (1D)

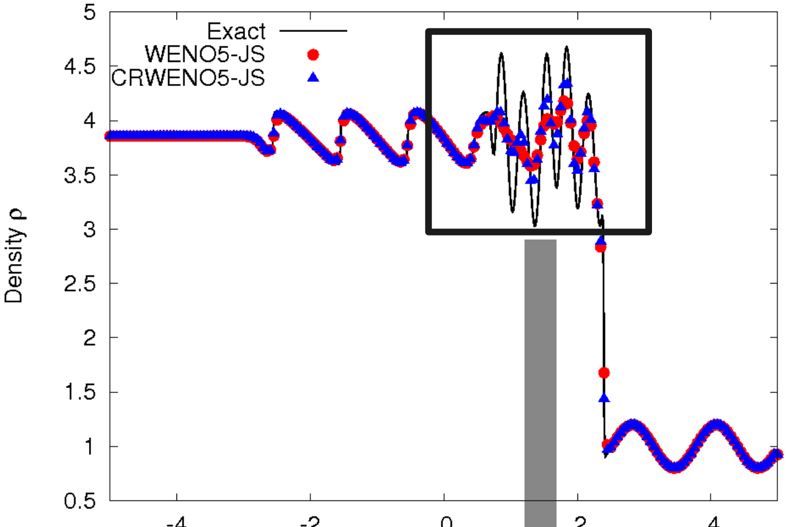
Entropy Wave Advection

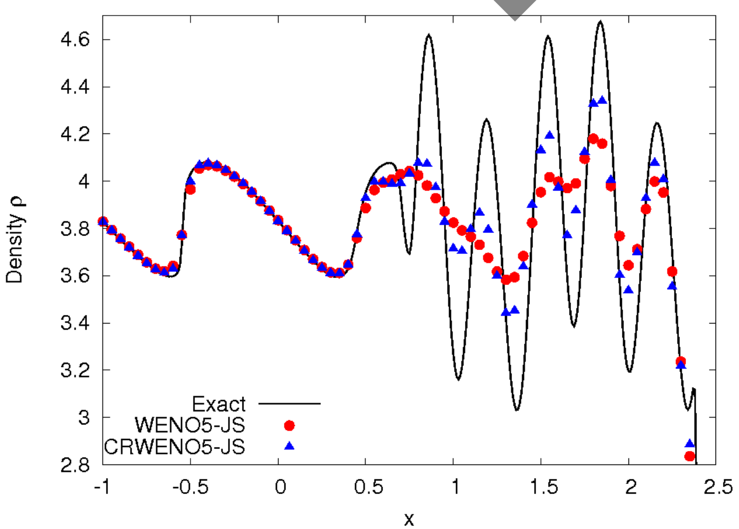


- CRWENO5 errors **1/10th** that of WENO5 for smooth solution
- **Improved resolution of small length-scale** waves and discontinuities

Shu-Osher Problem

(Characteristic-based reconstruction)

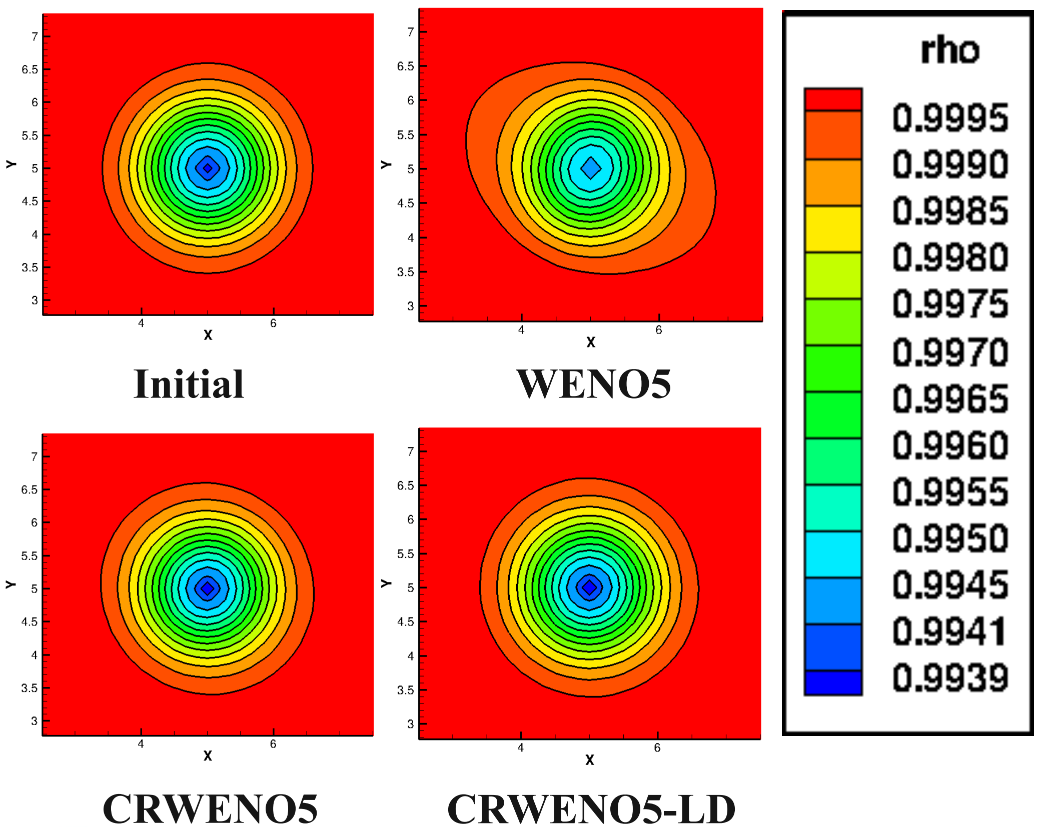


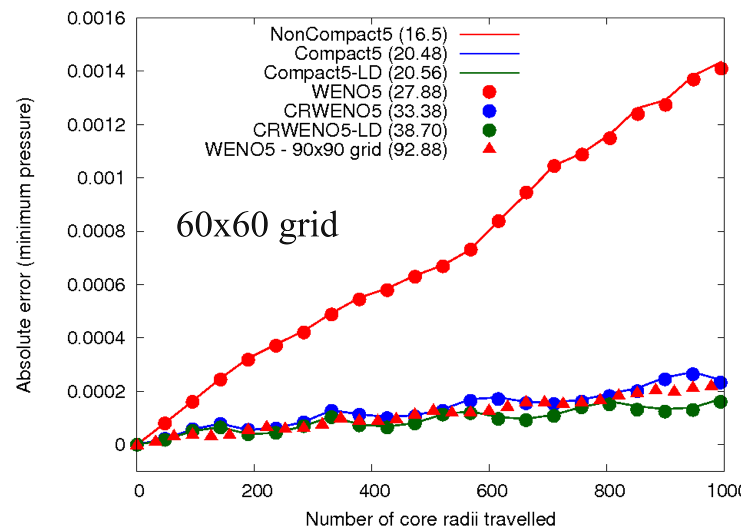


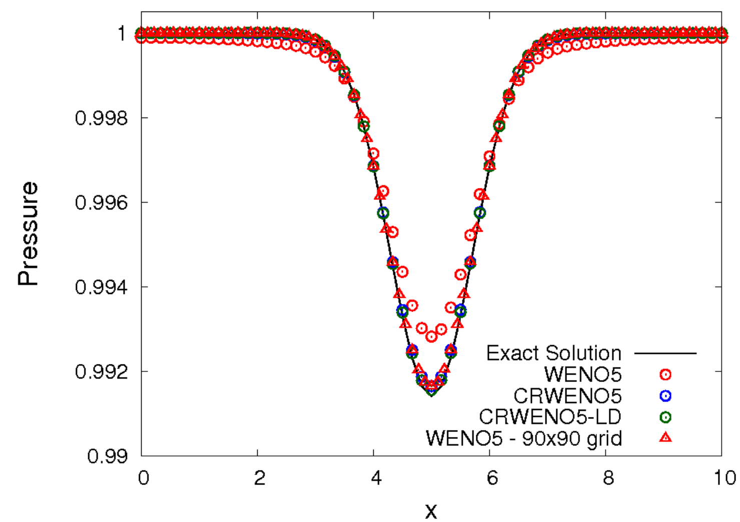
Inviscid Euler Equations (2D)

Isentropic Vortex Convection: Solution after travelling 1000 core radii

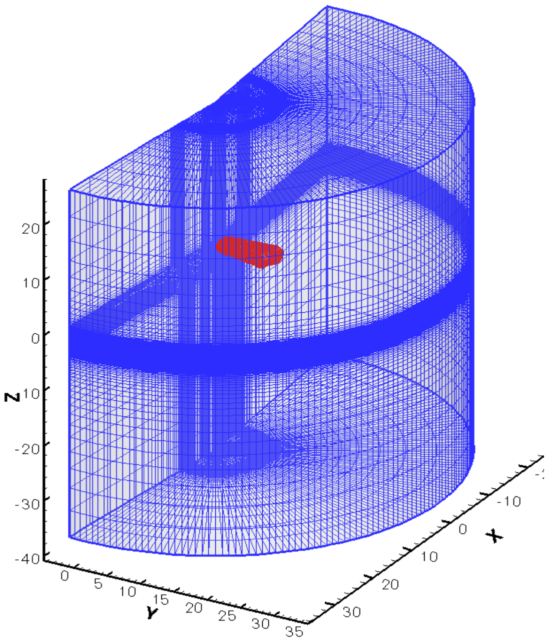
Compact schemes show better shape and strength preservation for long term convection





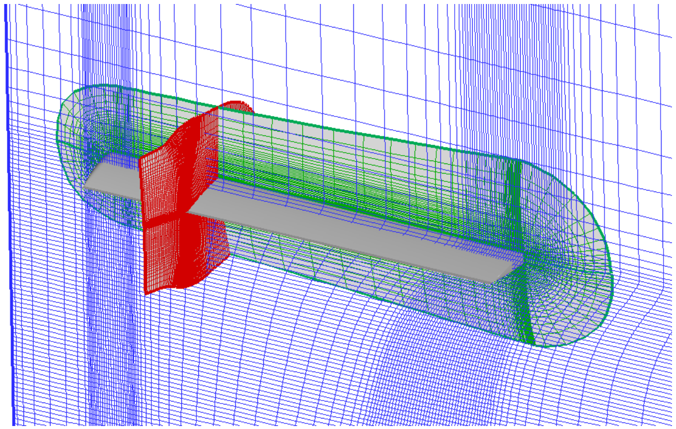


Flow around Harrington 2-Bladed Rotor



Cylindrical Background Mesh

127 x 116 x 118 points



Blade Mesh –

C-O type, 267x78x56 points

Flow Conditions:

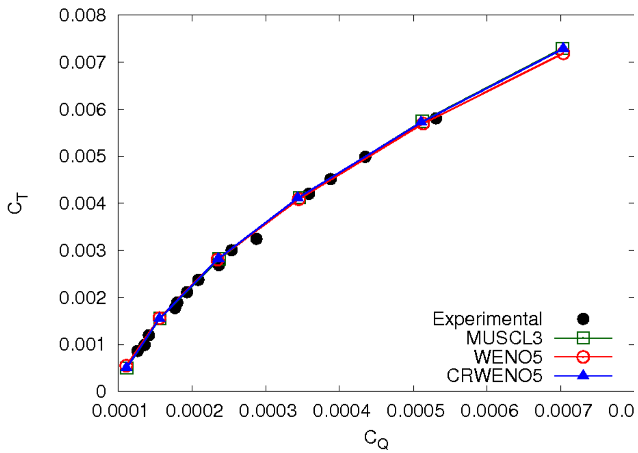
- M_{tip}: 0.352
- Re_{tip}: 3.5 million

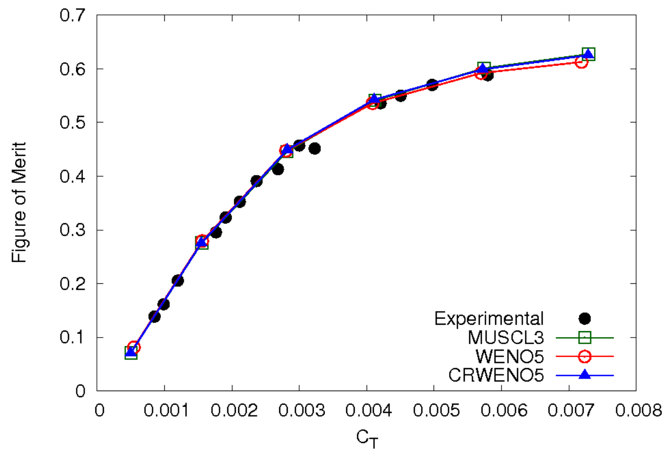
Validation of thrust & power coefficients and figure of merit

Rotor Geometry:

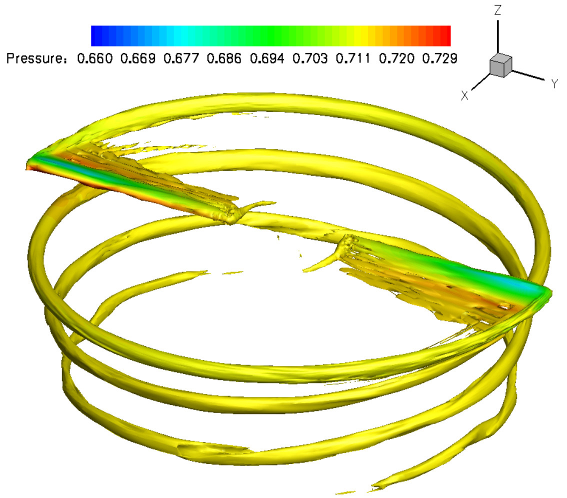
- Aspect Ratio – 8.33
- Airfoil section – NACA

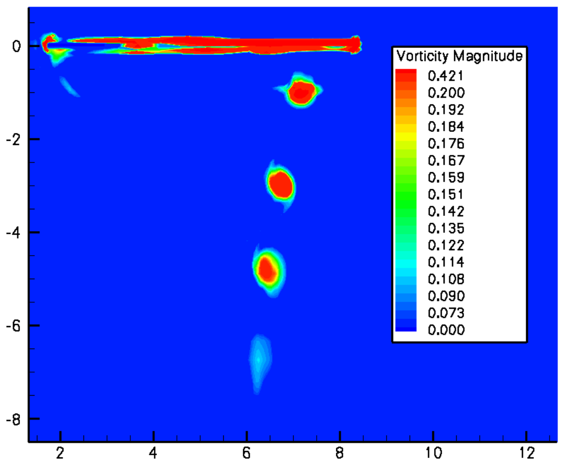
(t/c: 27.5% @ 0.2R, 15% @ R)



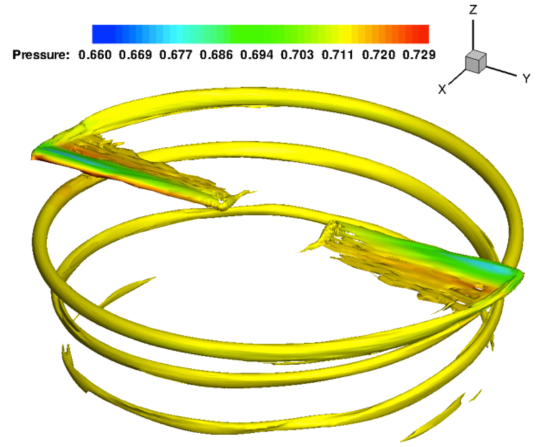


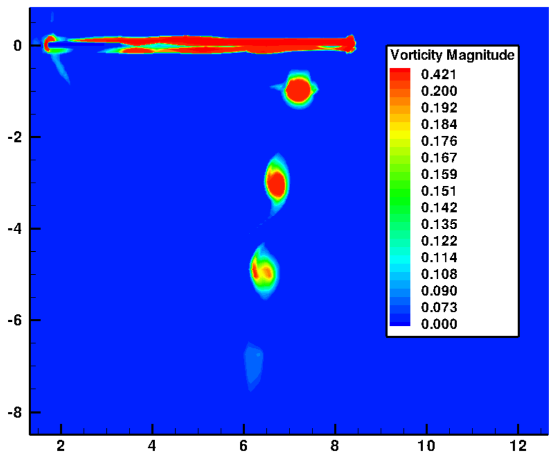
Harrington 2-Bladed Rotor (Near-Blade and Wake Flowfield)



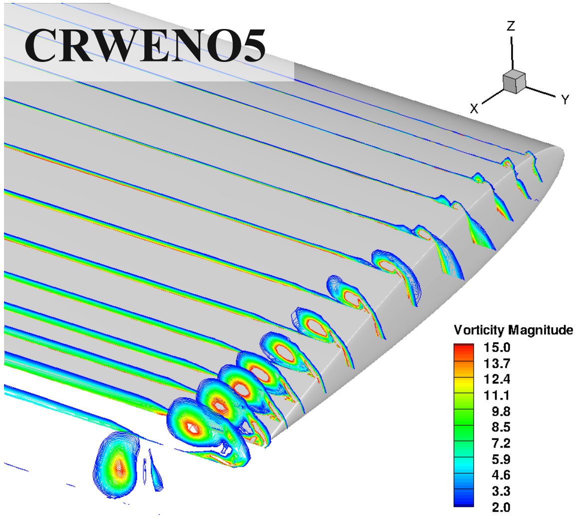


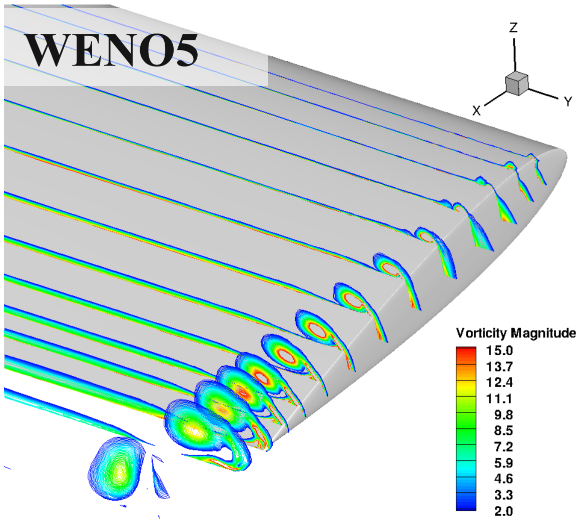
CRWENO5



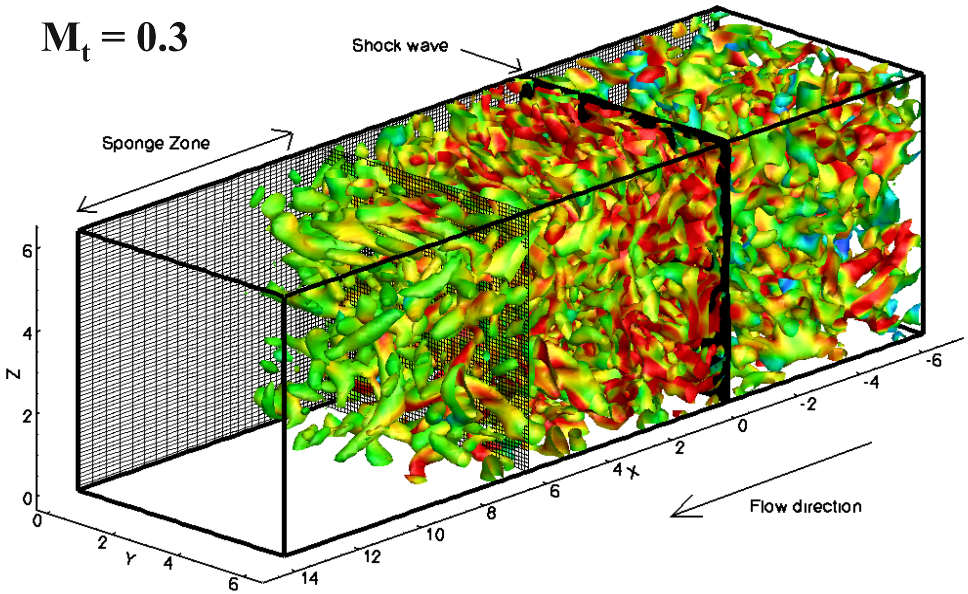


WENO5

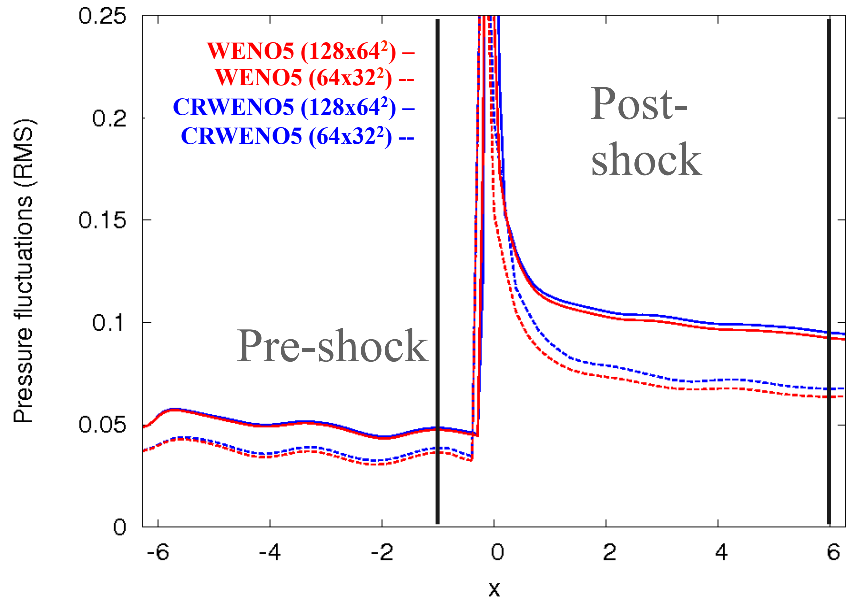




Shock – Turbulence Interaction



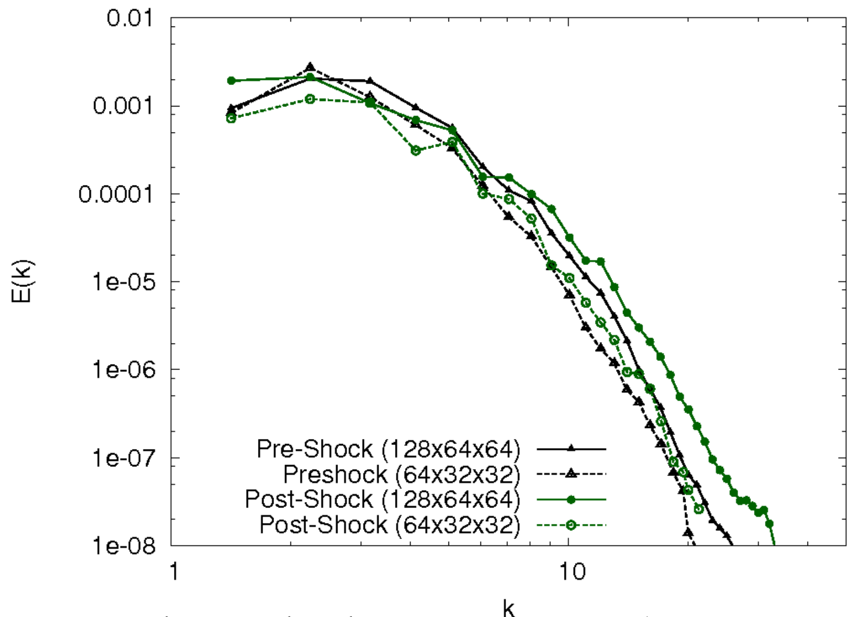
Iso-surfaces of 2nd invariant of velocity tensor, colored by vorticity magnitude



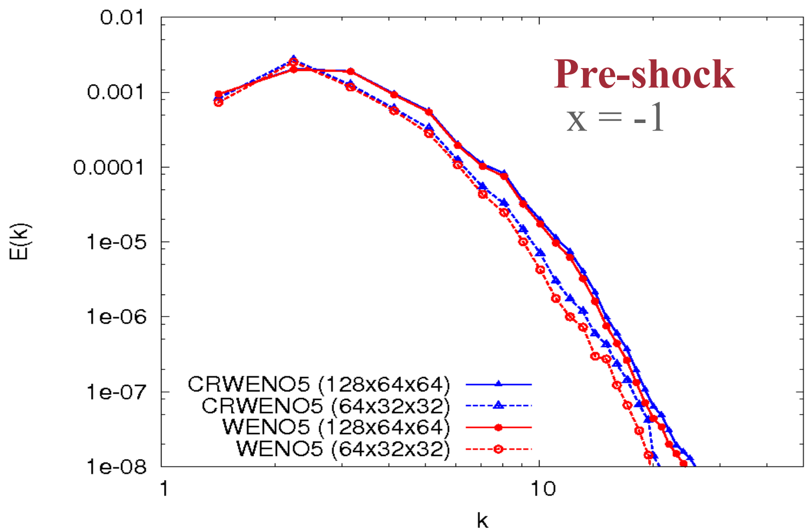
Stream-wise pressure fluctuations (RMS)

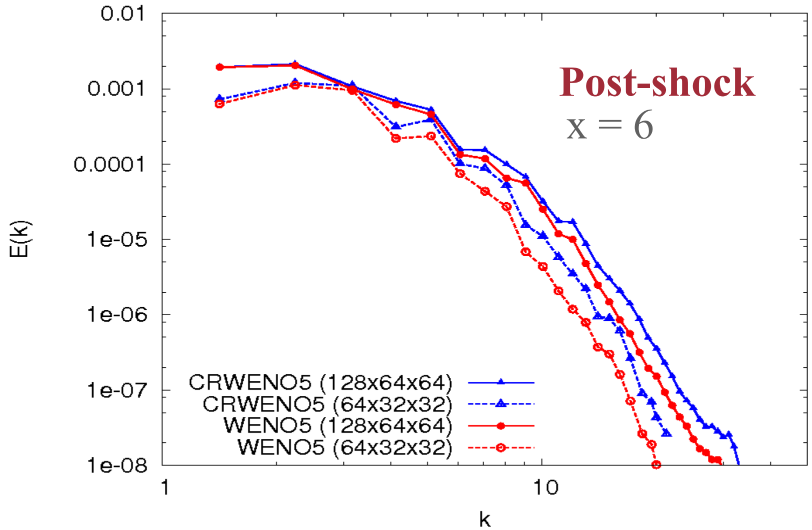
- **Inflow**: Fluctuations from isotropic turbulence decay added to mean flow at Mach 2
- Interaction with a shock wave **magnifies the turbulent fluctuations**
- Problem solved on two grids: 64x32x32 and 128x64x64 points (uniform)
- CRWENO5 → Lower dissipation → **Predicts higher levels of fluctuations on both grids**

Shock – Turbulence Interaction



Pre- and post-shock energy spectra (CRWENO5)





- Interaction with a shock wave amplifies intermediate and higher wavenumbers
- CRWENO5 shows improved resolution of the smaller length scales (both grids)

Implementation

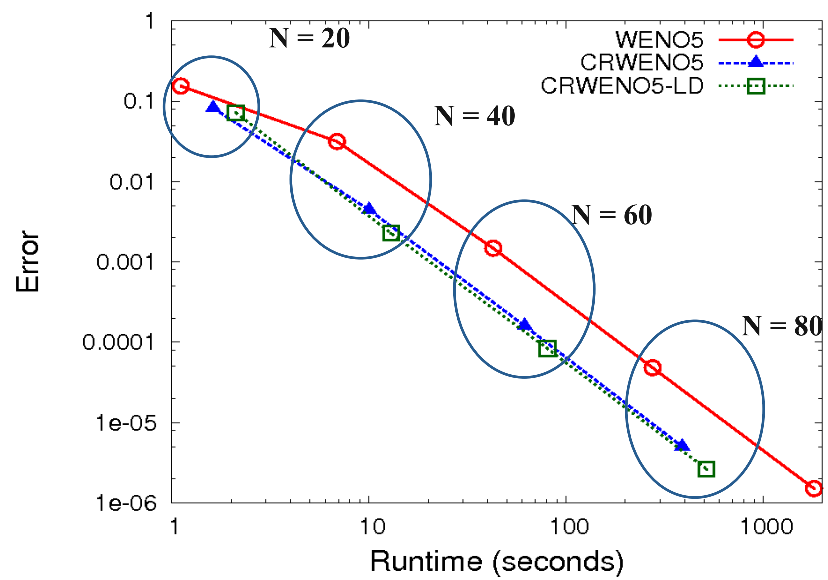
Computational Efficiency

Parallel Implementation

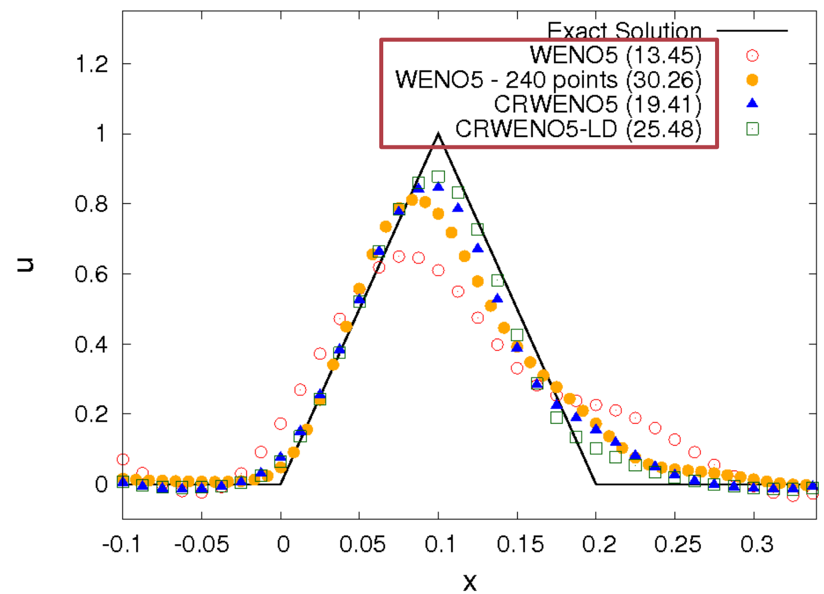
Scalability

Computational Efficiency on Single Processor
(Linear Advection Equation)

- CRWENO schemes **require solution to tridiagonal system** at each time-integration step/stage (solution-dependent weights) → Higher numerical cost for same number of points
- Higher accuracy (error is 1/10th that of WENO) → Comparable solution obtained on coarser mesh → Computationally more efficient



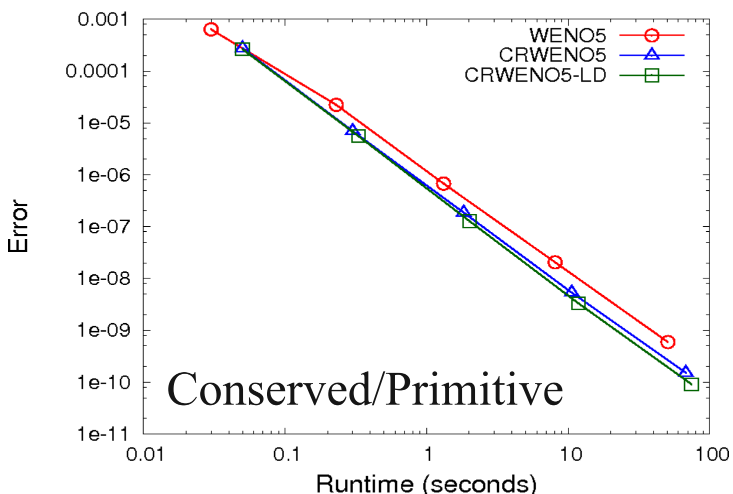
Error vs. runtime for periodic advection of a sine wave

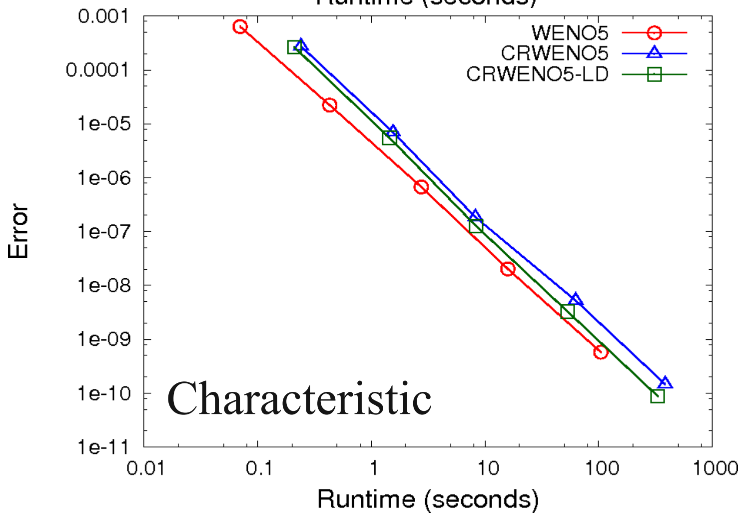


Periodic advection of a triangular wave after 100 cycles (160 point mesh)

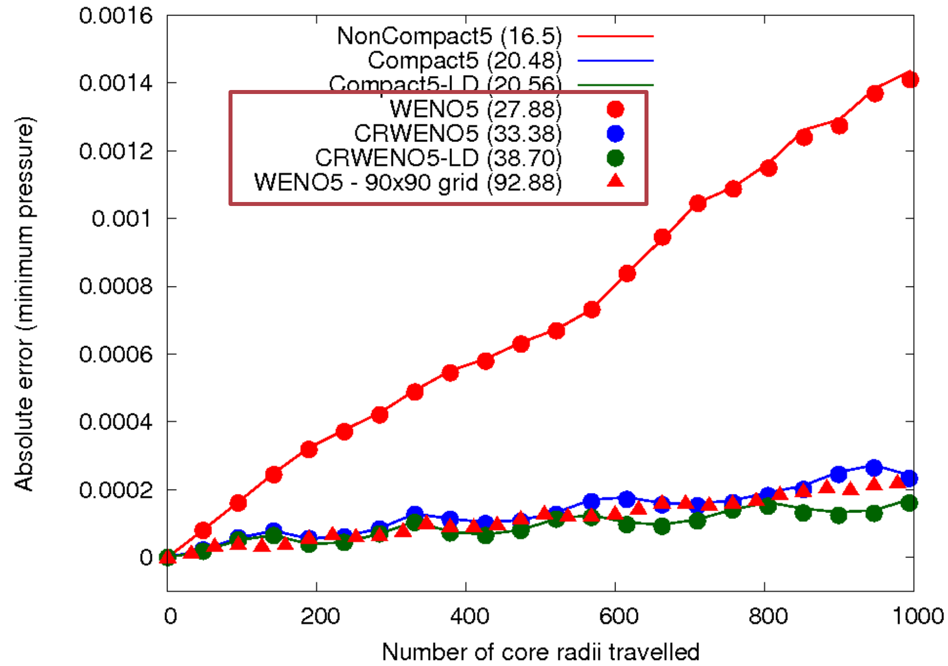
Computational Efficiency on Single Processor
(Inviscid Euler Equations)

Entropy Wave Advection





Isentropic Vortex Convection



CRWENO5 more efficient for component-wise reconstruction (scalar tridiagonal systems) but not for a characteristic-based reconstruction (block tridiagonal system)

Parallel Implementations of Non-Linear Compact Schemes (Distributed Memory)

Treat sub-domain boundary as physical boundary

- Decouple system of equations across processors
- *Chao, Haselbacher & Balachandar (JCP, 2009)*: Hybrid Compact-WENO scheme – Used the **5th order WENO scheme** at the MPI boundaries
- *Kim & Sandberg (Comp. & Fluids, 2012)*: Nonlinear compact scheme – Used **interior-biased compact schemes** at the 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**

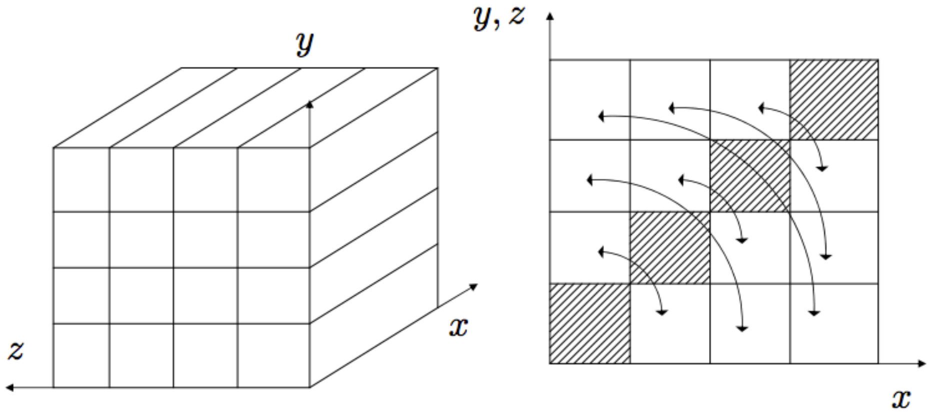
Parallel Implementation of the Thomas Algorithm

- **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**

Parallel Implementations of Non-Linear Compact Schemes (Distributed Memory)

Data Transposition

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



Shankar Ghosh, Ph.D. Thesis, University of Minnesota, 2008

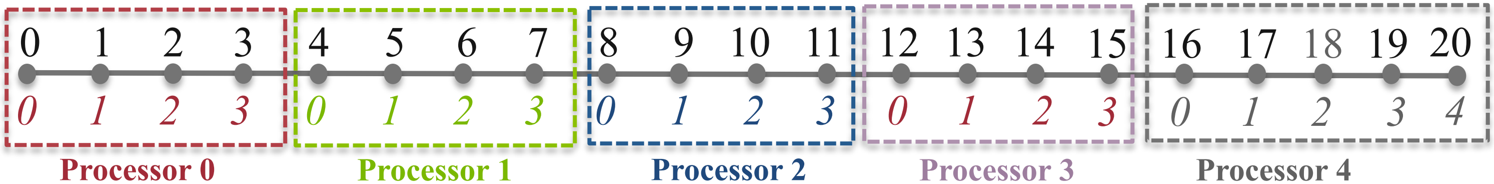
Existing approaches do not scale well!

Our approach:

– Avoid parallelization-induced approximations or errors
– No complicated schedule of computations
– Mathematical complexity comparable to serial Thomas algorithm
– Overall scheme retains higher computational efficiency observed on single processors for practical subdomain sizes.

Parallel tridiagonal solver based on iterative sub-structuring

Parallel Tridiagonal Solver (1)

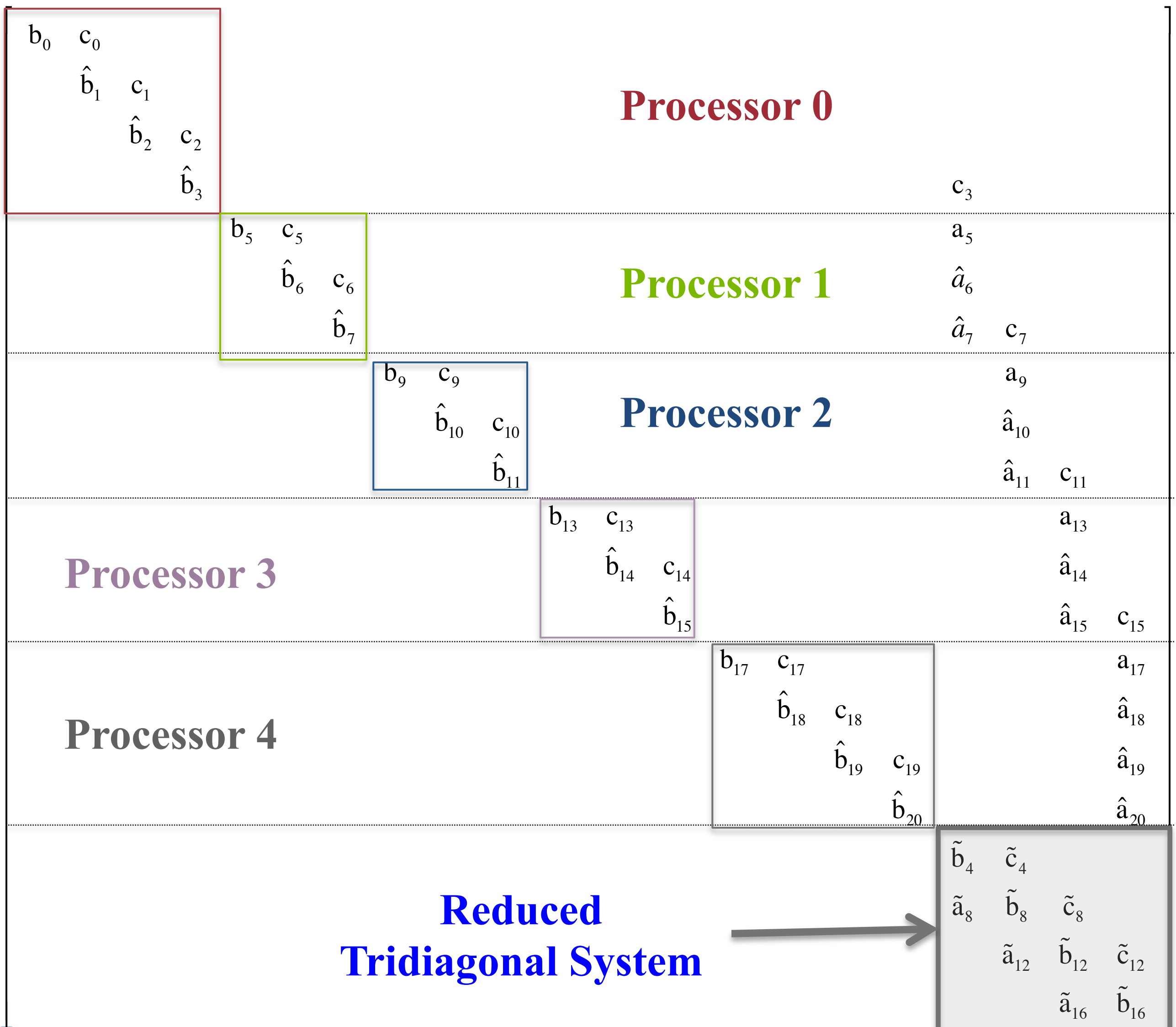


$$
\begin{array}{l|ccccccccccccccccccccc|}
 & b_0 & c_0 & & & & & & & & & & & & & & & & & & & \\
\text{Processor 0} & a_1 & b_1 & c_1 & & & & & & & & & & & & & & & & & & \\
 & & a_2 & b_2 & c_2 & & & & & & & & & & & & & & & & & \\
 & & & a_3 & b_3 & & & & & & & & & & & & & & c_3 & & & \\
\hline
 & & & & & b_5 & c_5 & & & & & & & & & & & & a_5 & & & \\
\text{Processor 1} & & & & & a_6 & b_6 & c_6 & & & & & & & & & & & & & & \\
 & & & & & & a_7 & b_7 & & & & & & & & & & & & c_7 & & \\
\hline
 & & & & & & & & b_9 & c_9 & & & & & & & & & & a_9 & & \\
\text{Processor 2} & & & & & & & & a_{10} & b_{10} & c_{10} & & & & & & & & & & & \\
 & & & & & & & & & a_{11} & b_{11} & & & & & & & & & & c_{11} & \\
\hline
 & & & & & & & & & & & b_{13} & c_{13} & & & & & & & & a_{13} & \\
\text{Processor 3} & & & & & & & & & & & a_{14} & b_{14} & c_{14} & & & & & & & & \\
 & & & & & & & & & & & & a_{15} & b_{15} & & & & & & & & c_{15} \\
\hline
 & & & & & & & & & & & & & & b_{17} & c_{17} & & & & & & a_{17} \\
 & & & & & & & & & & & & & & a_{18} & b_{18} & c_{18} & & & & & \\
\text{Processor 4} & & & & & & & & & & & & & & & a_{19} & b_{19} & c_{19} & & & & \\
 & & & & & & & & & & & & & & & & a_{20} & b_{20} & & & & \\
\hline
 & & & & a_4 & c_4 & & & & & & & & & & & & & b_4 & & & \\
 & & & & & & & a_8 & c_8 & & & & & & & & & & & b_8 & & \\
 & & & & & & & & & & a_{12} & c_{12} & & & & & & & & & b_{12} & \\
 & & & & & & & & & & & & & a_{16} & c_{16} & & & & & & & b_{16}
\end{array}
\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_5 \\ x_6 \\ x_7 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{13} \\ x_{14} \\ x_{15} \\ x_{17} \\ x_{18} \\ x_{19} \\ x_{20} \\ x_4 \\ x_8 \\ x_{12} \\ x_{16} \end{bmatrix}
=
\begin{bmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \\ r_5 \\ r_6 \\ r_7 \\ r_9 \\ r_{10} \\ r_{11} \\ r_{13} \\ r_{14} \\ r_{15} \\ r_{17} \\ r_{18} \\ r_{19} \\ r_{20} \\ r_4 \\ r_8 \\ r_{12} \\ r_{16} \end{bmatrix}
$$

Rearrangement of rows:

Eliminate interior rows on each processor

Parallel Tridiagonal Solver (2)



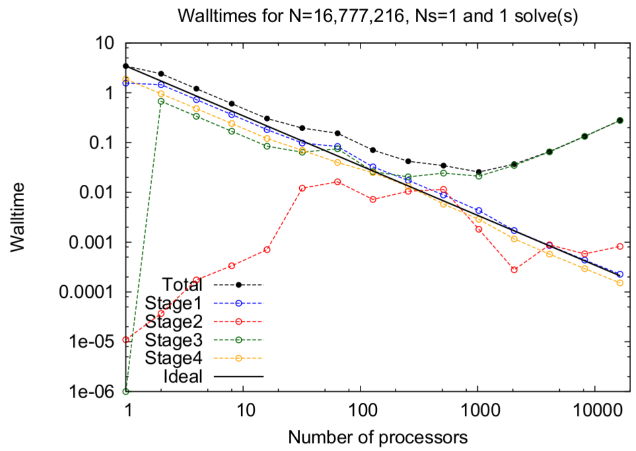
Elimination of interior rows on each process results in a reduced system of equations of size *p-1* (*p* being the number of processors)

Each processor (except rank 0) has 1 row of the reduced system.

Parallel Tridiagonal Solver (3)

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** – Gather the reduced system on one processor, solve, scatter the solution back (For multiple systems, each processor handles a set of systems)
- **Do not scale well!** (High communication cost)



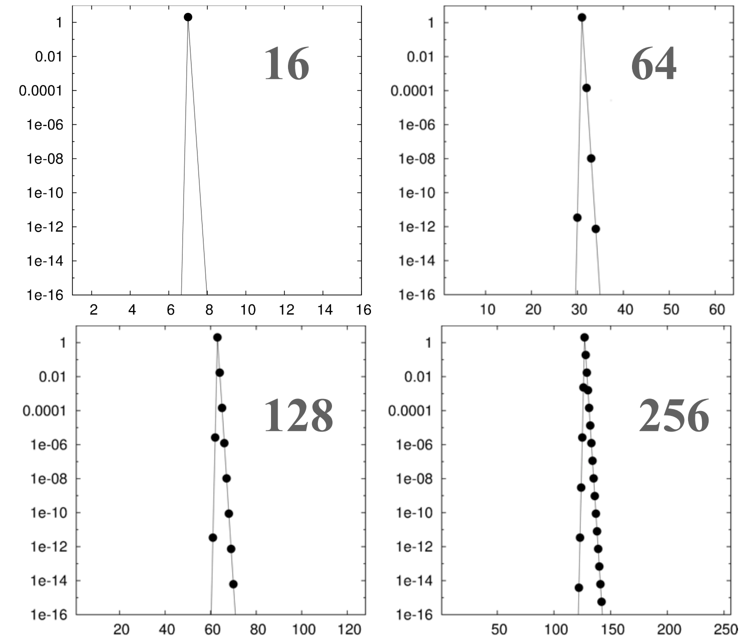
Iterative Sub-structuring Method

- Solve the reduced system using **Jacobi iterations**
- **But** solve till machine zero convergence → "Exact" solution (No parallelization-induced errors)
- Neighbor-to-neighbor communications required for each iteration
- Avoid collective communications by specifying *a priori* the number of iterations (instead of a norm-based exit criterion)

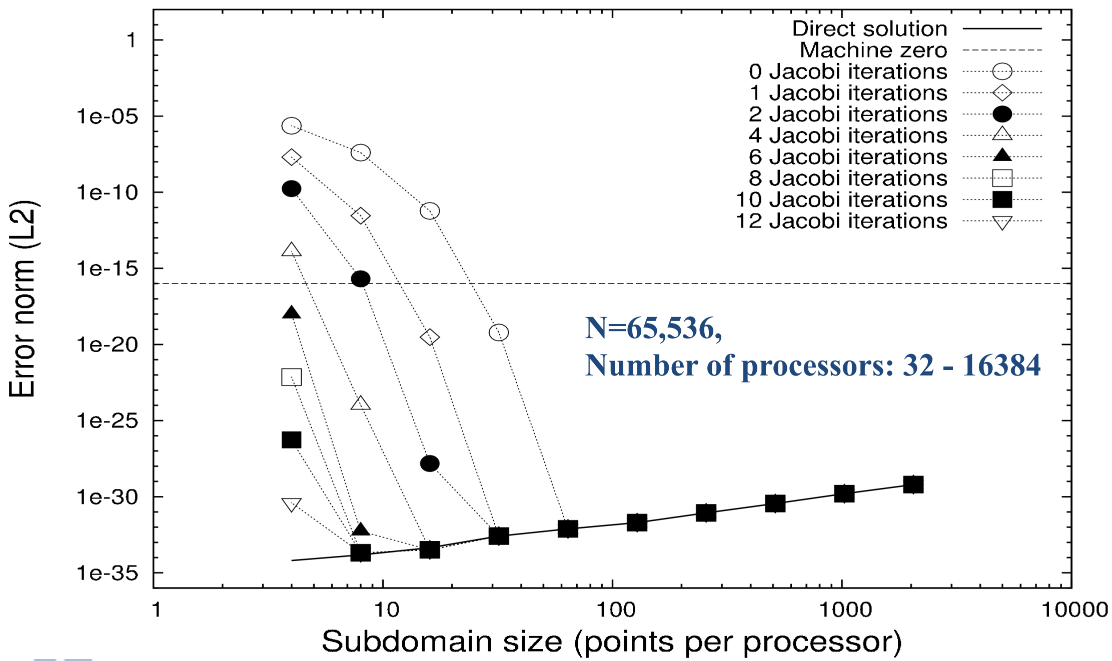
Iterative Solution of the Reduced System

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.
- 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

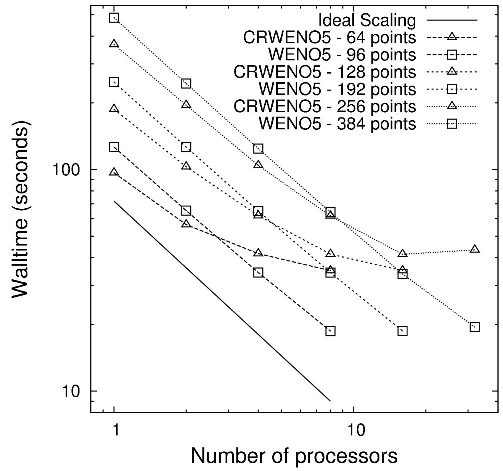
- The **factor by which the grid needs for WENO5 needs to be refined** to yield comparable solutions as CRWENO5 is f^D (f times per dimension)
- Several tridiagonal systems are solved for multi-dimensional problems →Higher arithmetic density → **Cost increases sub-linearly with number of systems**

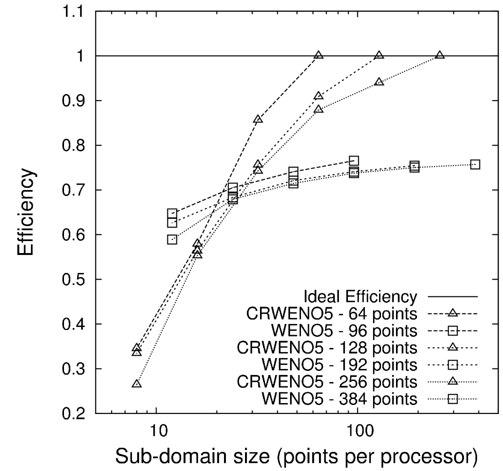
Performance Analysis for a Smooth Problem

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

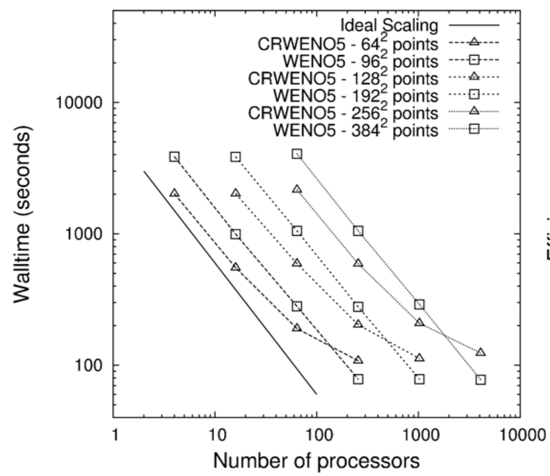


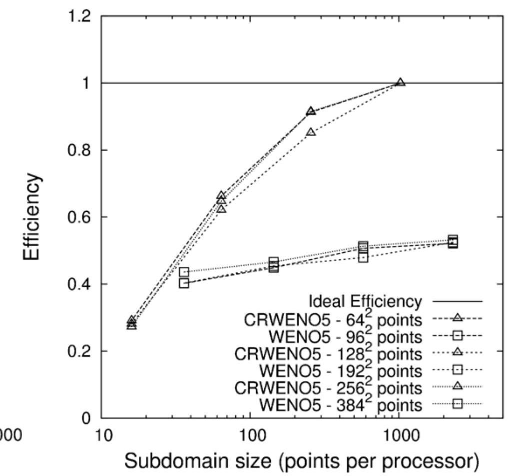


2D

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



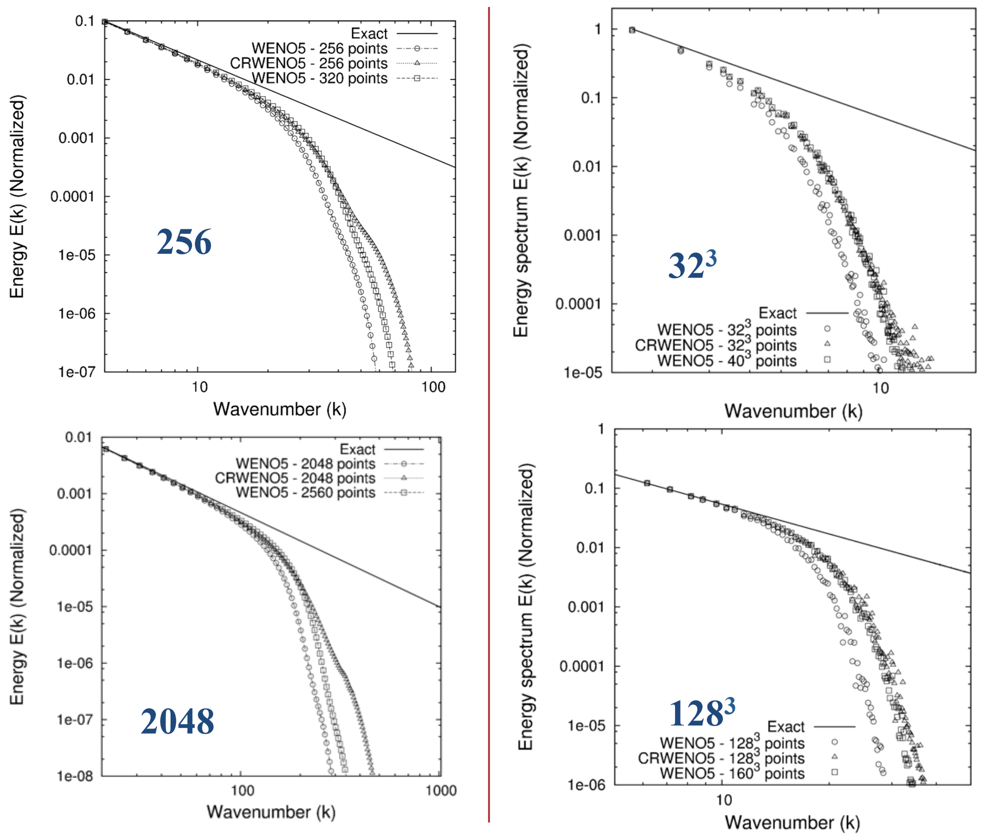


Note: Critical sub-domain size is insensitive to global problem size

Performance Comparison for a Non-Smooth Problem

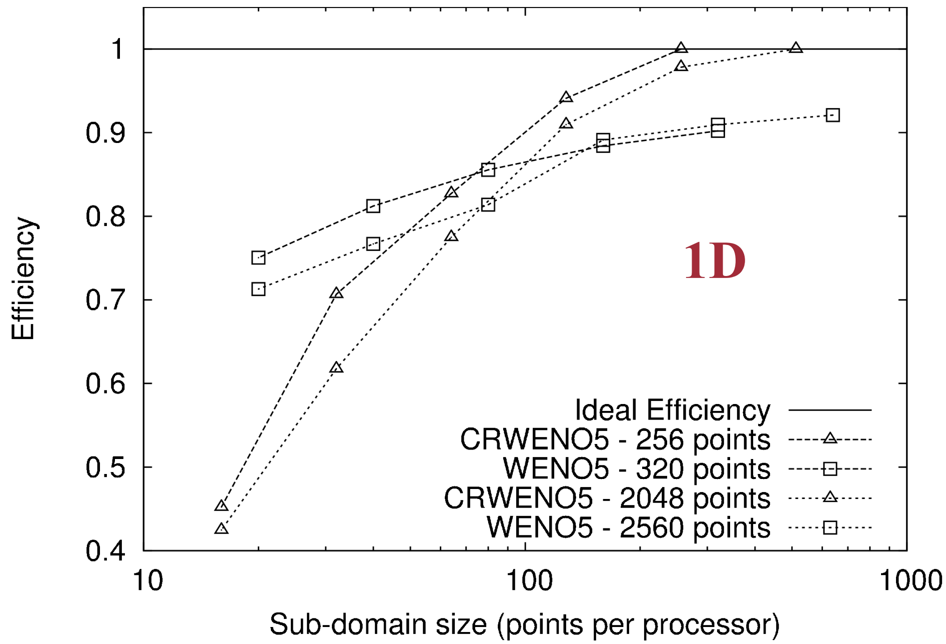
Periodic Advection of a Density Fluctuations (1D and 3D)

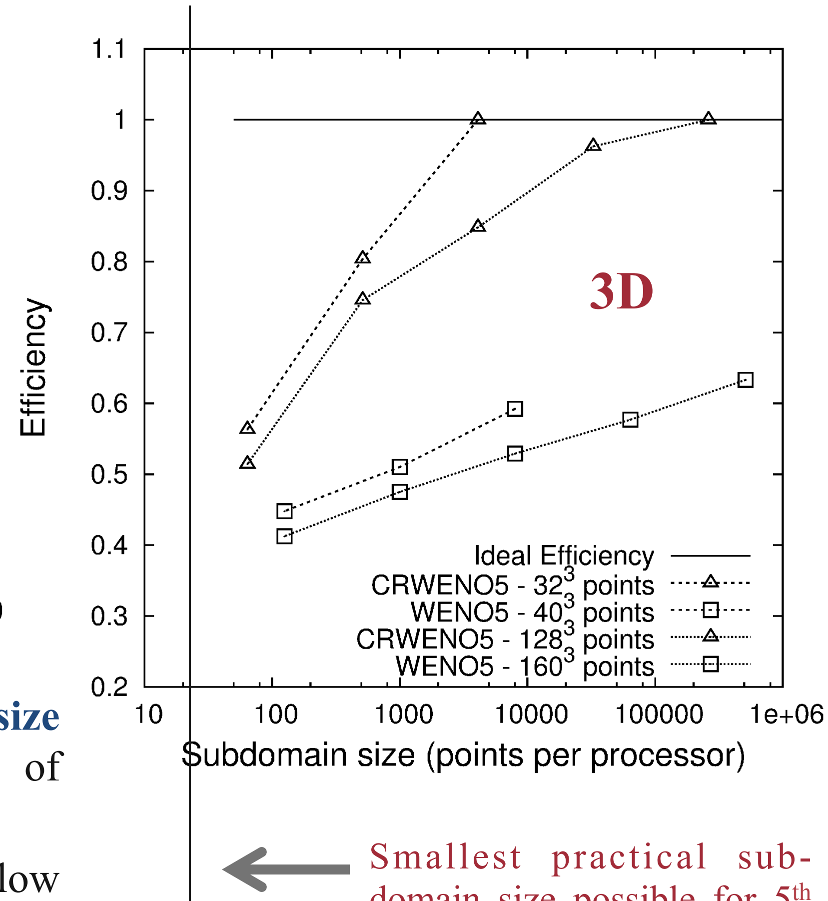
- Density is specified as the sum of sine waves with all grid-supported wavelengths
- Amplitude (as a function of wavelength) is representative of turbulent flows $A(k) \sim k^{-(5/3)}$
- Although solution is smooth, non-linear weights are not optimal



- Solutions obtained after 1 cycle over the periodic domain with the SSP-RK3 scheme
- Problems tried at **two different grid resolution** to demonstrate insensitivity of critical sub-domain size to global problem size.
- In 1D, WENO5 gives comparable resolution on grid with ~ **1.25x** more points
- In 2D, WENO5 gives comparable resolution on grid with ~ **1.25^3x (~ 2x)** more points

Performance Comparison for a Non-Smooth Problem





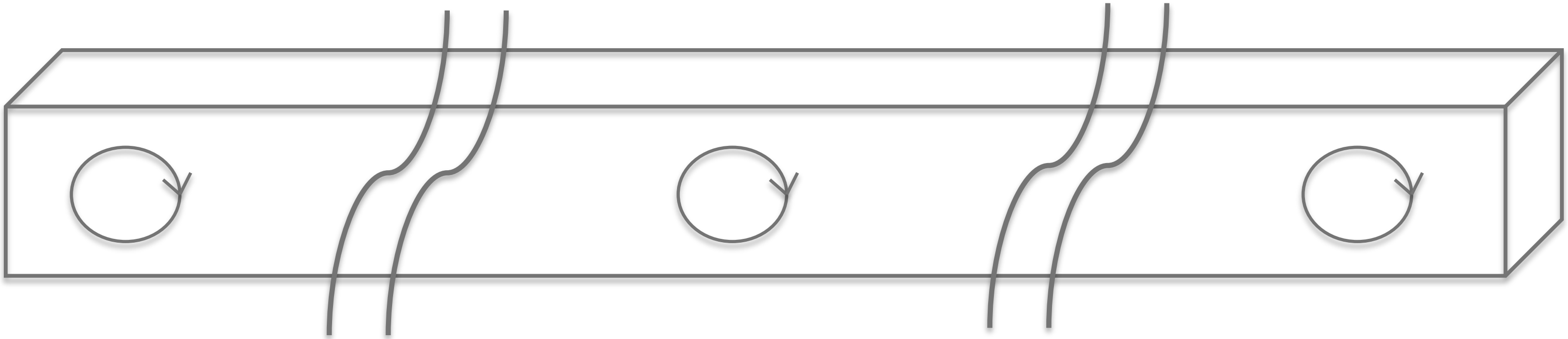
- For both 1D and 3D, **efficiency vs. sub-domain size insensitive to global problem size** and number of processors
- In 1D, there exists a **critical sub-domain size** below which WENO5 is more efficient
- In 3D, **CRWENO5 is more efficient than the WENO5** even with sub-domain sizes close to the smallest practically possible.

Smallest practical sub-domain size possible for 5th order schemes – 3 points per processor per dimension

Scalability Results for Benchmark Flow Problems

Isentropic Vortex Convection

- Long-term convection of a smooth flow feature over a large distance
- Convection over a long, 3D, cuboidal domain (instead of a smaller periodic domain)
- Periodic boundary conditions along z-direction to mimic 2D flow



Strong Scalability

Domain size: 1280 x 10 x 10 length units

CRWENO5 Grid: 8192 x 64 x 64 (~ 33 million points)

WENO5 Grid: 12288 x 96 x 96 (~ 113 million points)

Number of processors:

512 x 4 x 4 (8192) – Subdomain size 16^3 (24^3)

2048 x 16 x 16 (524288) – Subdomain size 4^3 (6^3)

Weak Scalability

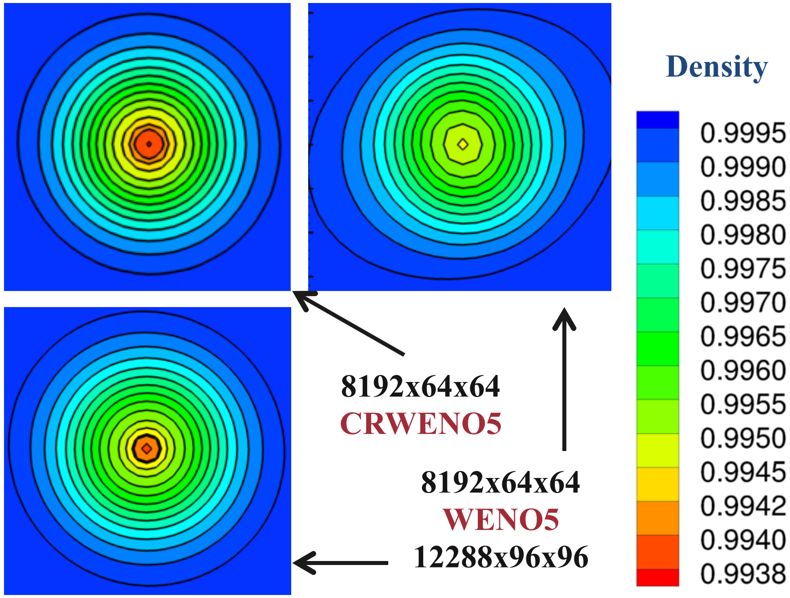
Subdomain size: 4^3 (CRWENO5), 6^3 (WENO5)

Domain:

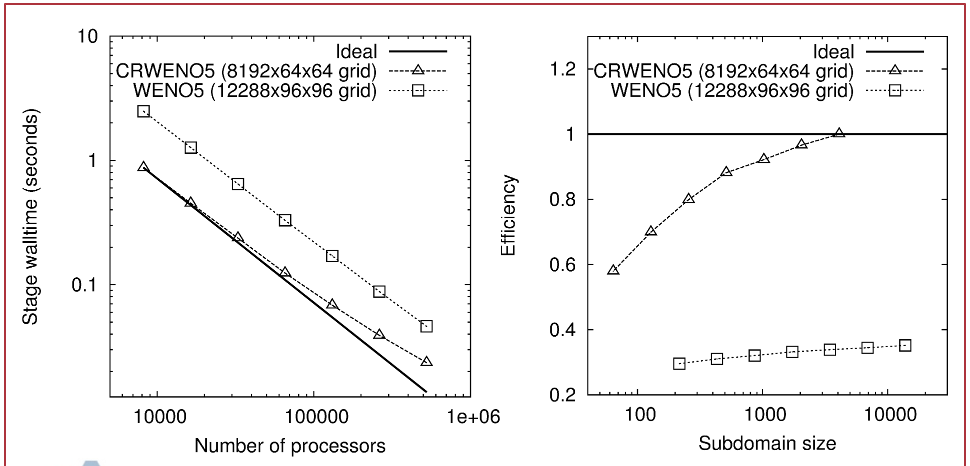
From 40 x 10 x 10 length units, 256 x 64 x 64 points for CRWENO5, 64 x 16 x 16 processors

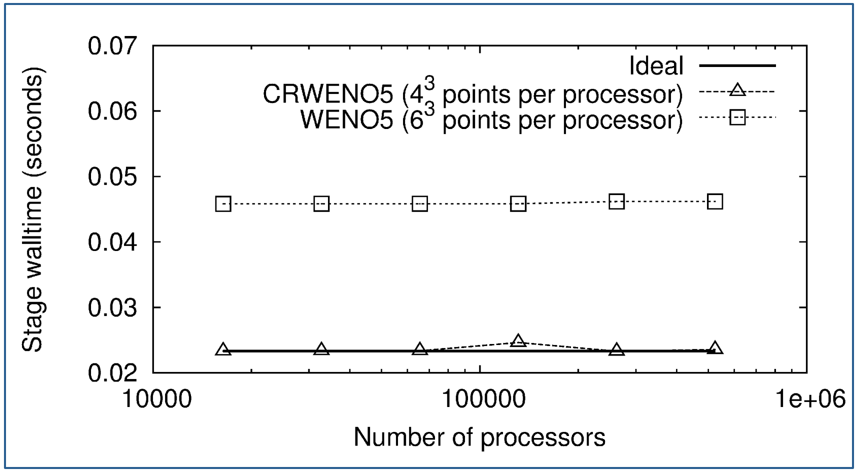
To 1280 x 10 x 10 length units, 8192 x 64 x 64 points for CRWENO5, 2048 x 16 x 16 processors

Scalability Results for Benchmark Flow Problems



- Verified that WENO5 yields a solution of comparable accuracy on a grid with ~ 1.53x (~ 3.4x) more grid points
- ALCF/*Mira* (IBM BG/Q)
- **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

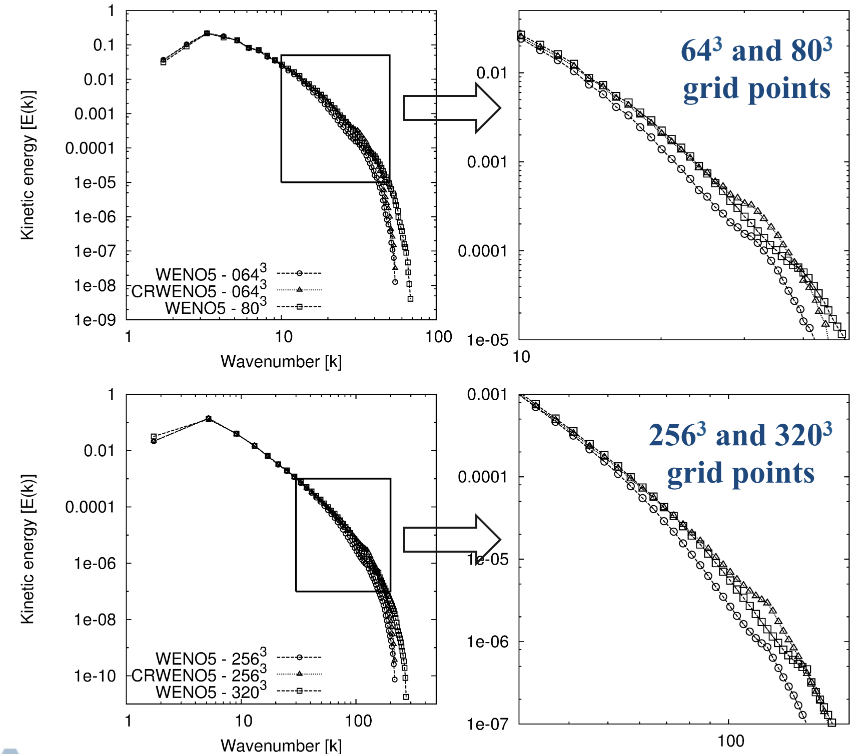


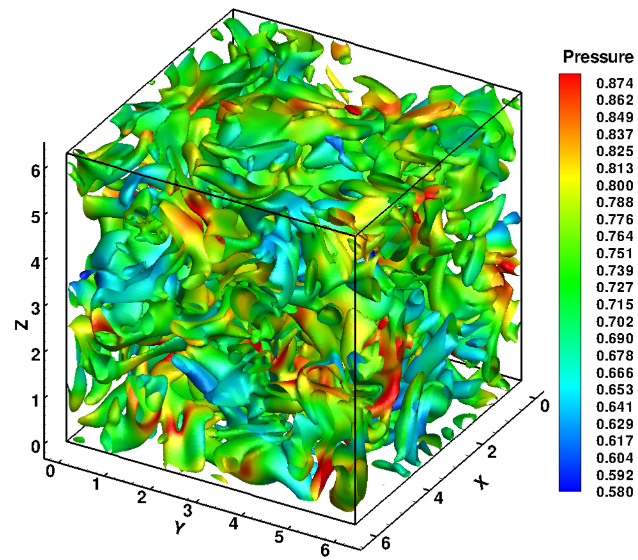


Scalability Results for Benchmark Flow Problems

Implicit LES of Isotropic Turbulence Decay

- Benchmark turbulent flow problem characterized by energy transfer from large to small length scales
- Non-linear weights are not optimal and thus, the CRWENO5 and WENO5 schemes are not at their best accuracy





- Problem solved at two sets of grid resolutions – 64^3 & 80^3, and 256^3 & 320^3
- Solutions obtained with the 4-stage, 4th order RK scheme
- WENO5 gives **comparable resolution** as CRWENO5 on grids with **~ 1.25^3x** (~ 2x) more points.
- Scaling results obtained on ALCF/*Mira* (IBM BG/Q)

Scalability Results for Benchmark Flow Problems

Strong Scalability

Domain size: Cube of length 2π

CRWENO5 Grid: 256^3 (~ 16 million points)

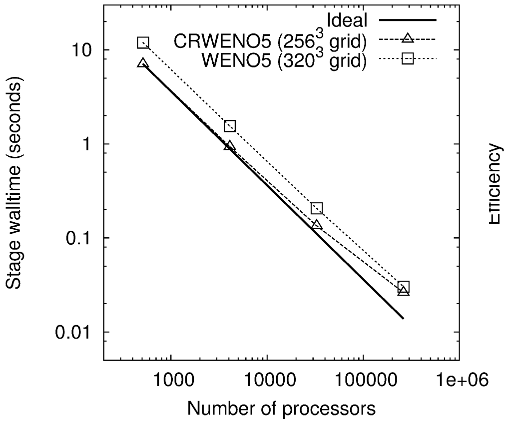
WENO5 Grid: 320^3 (~ 32 million points)

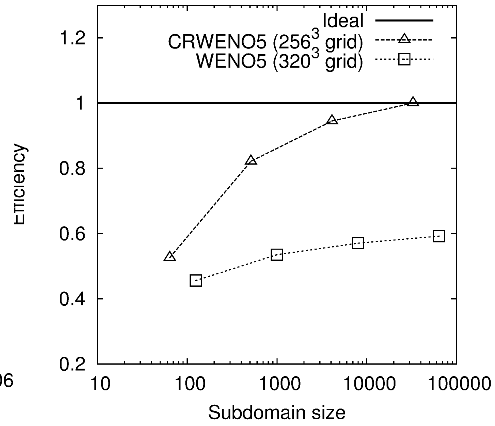
Number of processors:

8^3 (512) – Subdomain size 32^3 (40^3)

64^3 (262144) – Subdomain size 4^3 (5^3)

At very small subdomain sizes, CRWENO5 does not scale as well, yet absolute wall time (slightly) lower (higher efficiency)





Weak Scalability

Subdomain size: 4^3 (CRWENO5), 5^3 (WENO5)

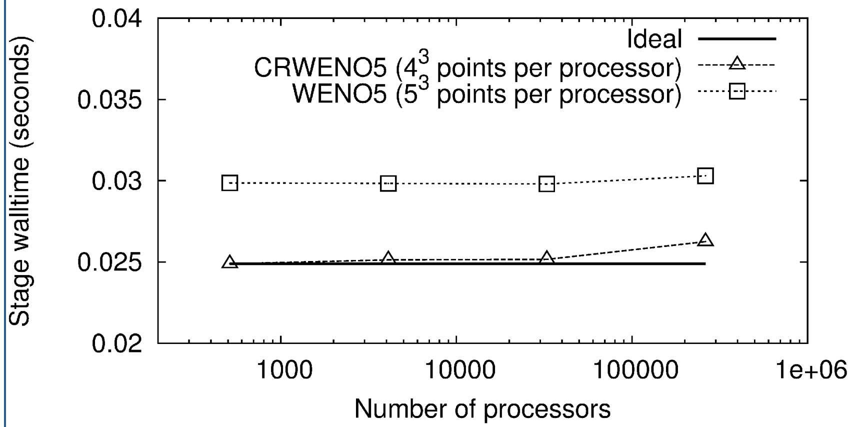
Domain: Cube of length 2π

CRWENO5 Grid (WENO5 grid is 1.25^3x):

From 32^3 points, 8^3 (512) processors

To 256^3 points, 64^3 (262144) processors

CRWENO5 scales well as global domain size and number of processors increase



Conclusions and Observations

Compressible Turbulent Flows

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

- **Compact-Reconstruction WENO Schemes**
  - Applies the WENO algorithm (solution-dependent interpolation) to compact schemes
  - **High spectral resolution** – Improved resolution of small length scales
  - **Non-oscillatory interpolation** across discontinuities and steep gradients
- **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

- **Near Future (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 the CRWENO5 scheme with ARKIMEX time-integration schemes (PETSc) and study the overall scalability
  - Implement this implementation of the CRWENO5 scheme in an existing, validated Navier-Stokes solver and apply to practical flow problems
- **Distant Future**
  - Use threads for further speedup and exploit the hybrid architecture of most HPC platforms
  - Study the scalability on non-BG/Q platforms, with more noisy communication networks

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