

A High Resolution Compact Scheme for Compressible Flows Involving Shocks and Turbulence

Akshay Subramaniam, Man Long Wong and
Sanjiva K. Lele



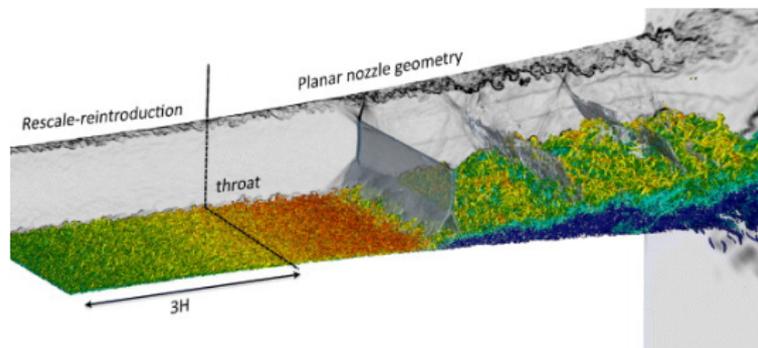
NASA AMS Seminar
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1. Introduction
2. Overview of the WCNS methodology
3. The WCHR scheme
 - Explicit interpolation
 - Explicit-compact interpolation
 - Nonlinear weights
 - Derivative scheme
 - Approximate dispersion relation
 - Extension to Euler equations
4. Results
 - 1D test problems
 - 2D test problems
 - 3D test problems
5. Implementation details
6. Conclusions

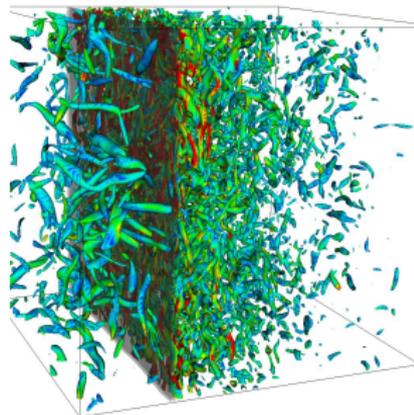
Outline

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Introduction



1



2

- Many practical problems involve shocks and turbulence
- Need minimally dissipative scheme to capture turbulence
- But enough to stabilize solutions at shocks and avoid spurious oscillations
- Conflicting requirements causes high sensitivity to numerical schemes

¹Britton J Olson and Sanjiva K Lele. "A mechanism for unsteady separation in over-expanded nozzle flow". In: *Physics of Fluids* 25.11 (2013), p. 110809.

²Johan Larsson and Sanjiva K Lele. "Direct numerical simulation of canonical shock/turbulence interaction". In: *Physics of Fluids* 21.12 (2009), p. 126101.

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Numerical method

- Consider a scalar conservation law in 1D

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

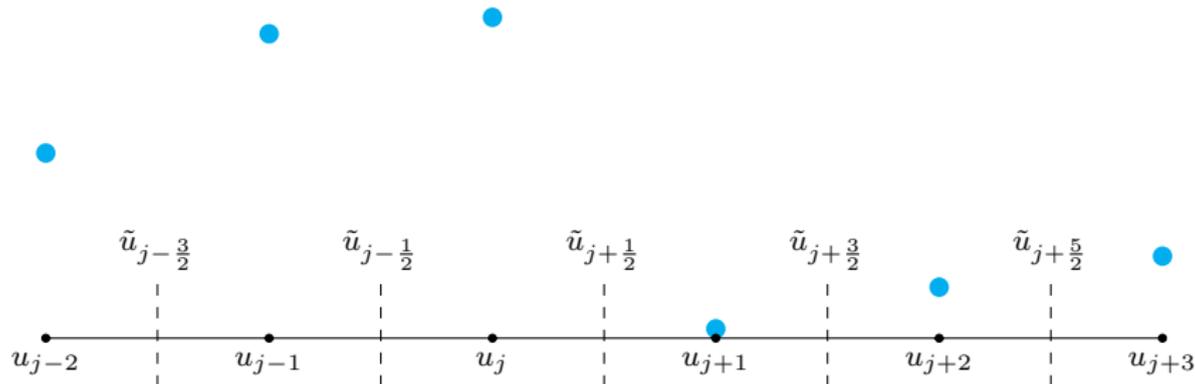
- Semi-discretize this equation on a grid with N points in the strong form

$$\frac{\partial u_j}{\partial t} + \frac{\partial f(u)}{\partial x} \Big|_j = 0$$

- Need a discrete approximation of the flux derivative

$$\frac{\partial f(u)}{\partial x} \Big|_j$$

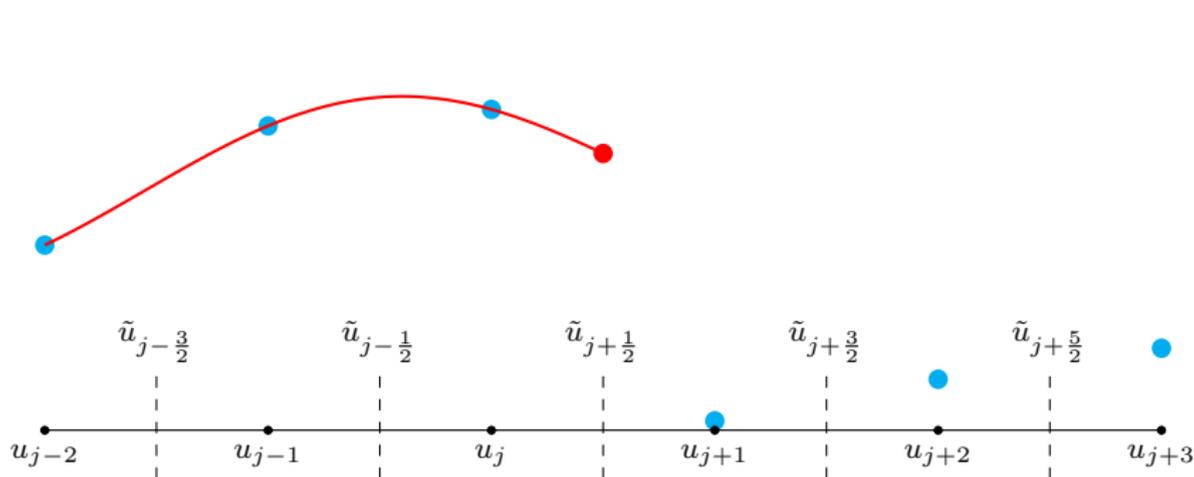
Weighted compact nonlinear scheme (WCNS) ^{3 4}



³Xiaogang Deng and Hanxin Zhang. "Developing high-order weighted compact nonlinear schemes". In: *Journal of Computational Physics* 165.1 (2000), pp. 22–44.

⁴Shuhai Zhang, Shufen Jiang, and Chi-Wang Shu. "Development of nonlinear weighted compact schemes with increasingly higher order accuracy". In: *Journal of Computational Physics* 227.15 (2008), pp. 7294–7321.

Weighted compact nonlinear scheme (WCNS) ³ ⁴

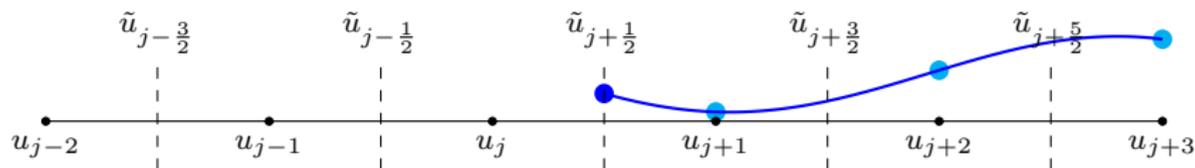


Left-biased interpolation

³Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

⁴Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".

Weighted compact nonlinear scheme (WCNS) ³ ⁴

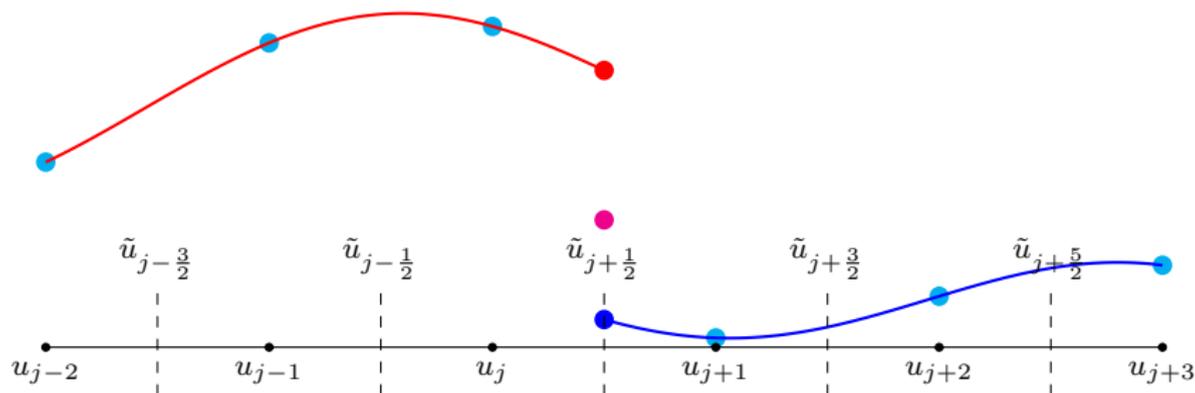


Right-biased interpolation

³Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

⁴Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".

Weighted compact nonlinear scheme (WCNS) ^{3 4}

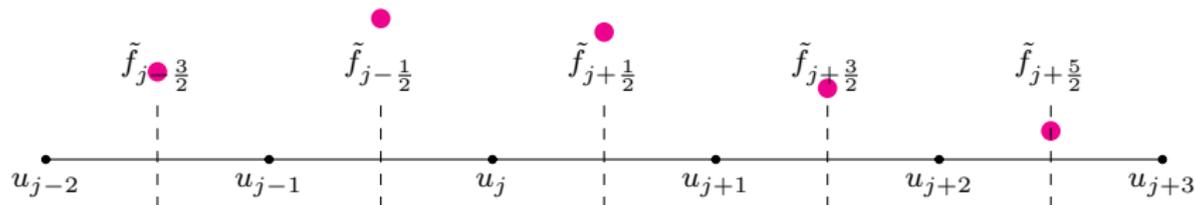


Riemann solver to get the interface flux

³Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

⁴Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".

Weighted compact nonlinear scheme (WCNS) ^{3 4}



Finite difference to get the flux derivative

³Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

⁴Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".

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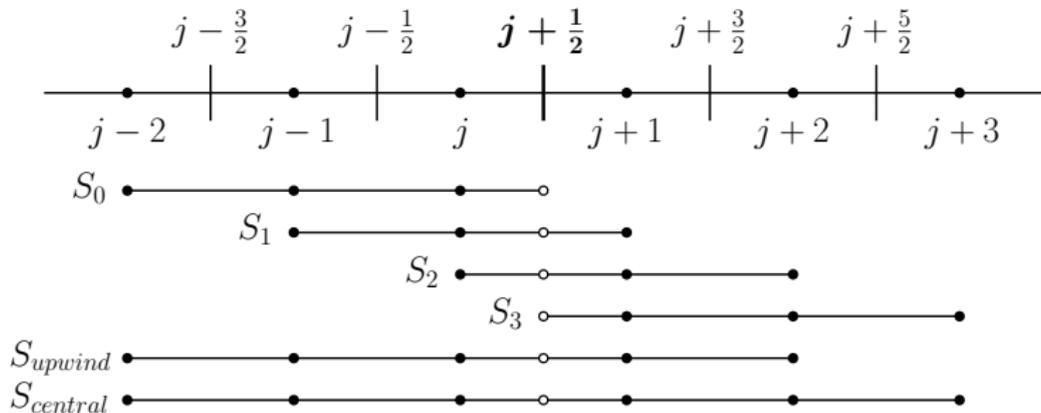
Interpolation

- Critical step since numerical dissipation is controlled by this step
- Typically the limiting step in determining the resolution of the scheme
- Nonlinear WENO style weighting to add dissipation in regions of discontinuities and under-resolved features

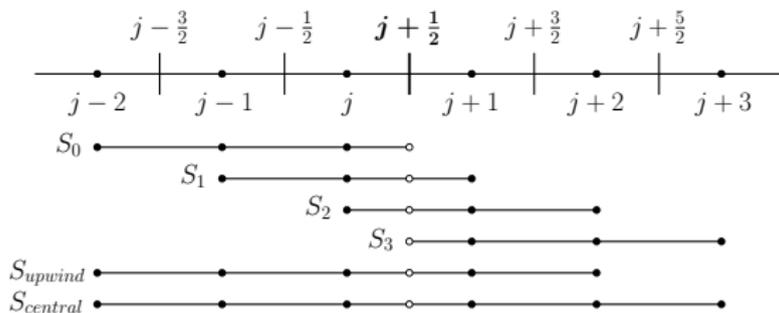
Interpolation

- Critical step since numerical dissipation is controlled by this step
- Typically the limiting step in determining the resolution of the scheme
- Nonlinear WENO style weighting to add dissipation in regions of discontinuities and under-resolved features
- Two types of interpolation
 - Explicit interpolation
 - Compact interpolation

Explicit interpolation (EI)



Explicit interpolation (EI)



$$EI_0 : \quad \tilde{u}_{j+\frac{1}{2}}^{(0)} = \frac{1}{8} (3u_{j-2} - 10u_{j-1} + 15u_j)$$

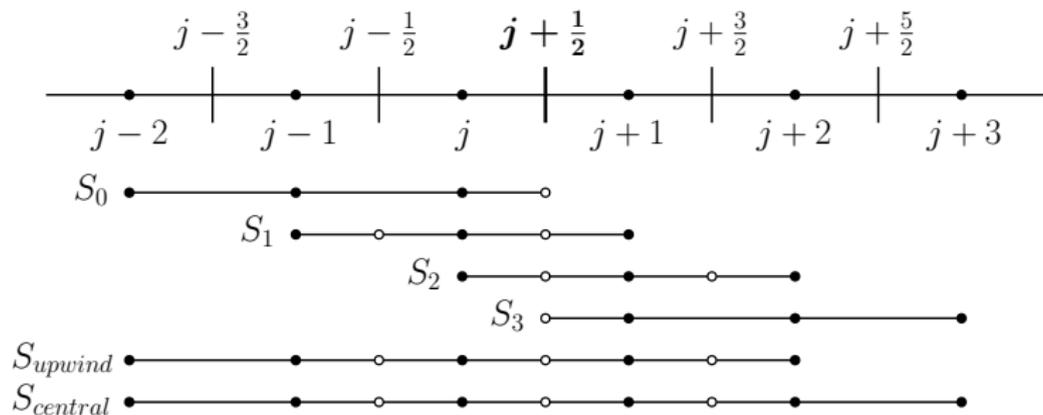
$$EI_1 : \quad \tilde{u}_{j+\frac{1}{2}}^{(1)} = \frac{1}{8} (-u_{j-1} + 6u_j + 3u_{j+1})$$

$$EI_2 : \quad \tilde{u}_{j+\frac{1}{2}}^{(2)} = \frac{1}{8} (3u_j + 6u_{j+1} - u_{j+2})$$

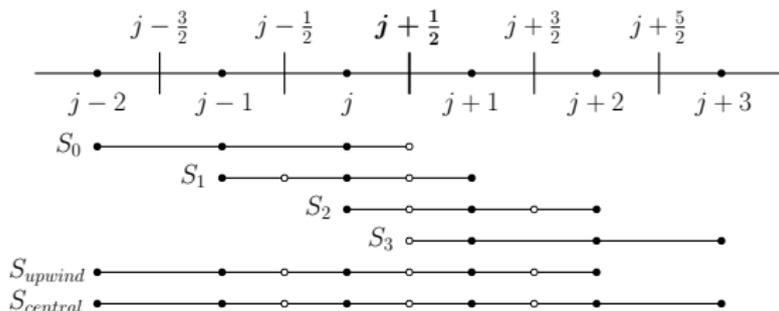
$$EI_3 : \quad \tilde{u}_{j+\frac{1}{2}}^{(3)} = \frac{1}{8} (15u_{j+1} - 10u_{j+2} + 3u_{j+3})$$

$$EI_{\text{upwind}} = \sum_{k=0}^2 d_k^{\text{upwind}} EI_k \quad (5^{\text{th}} \text{ order}); \quad EI_{\text{central}} = \sum_{k=0}^3 d_k^{\text{central}} EI_k \quad (6^{\text{th}} \text{ order})$$

Explicit-compact interpolation (ECI)



Explicit-compact interpolation (ECI)



$$ECI_0 : \quad \tilde{u}_{j+\frac{1}{2}}^{(0)} = \frac{3}{8}u_{j-2} - \frac{5}{4}u_{j-1} + \frac{15}{8}u_j$$

$$ECI_1 : \quad (1 - \xi) \tilde{u}_{j-\frac{1}{2}}^{(1)} + \xi \tilde{u}_{j+\frac{1}{2}}^{(1)} = \left(-\frac{\xi}{2} + \frac{3}{8}\right) u_{j-1} + \frac{3}{4}u_j + \left(\frac{\xi}{2} - \frac{1}{8}\right) u_{j+1}$$

$$ECI_2 : \quad \xi \tilde{u}_{j+\frac{1}{2}}^{(2)} + (1 - \xi) \tilde{u}_{j+\frac{3}{2}}^{(2)} = \left(\frac{\xi}{2} - \frac{1}{8}\right) u_j + \frac{3}{4}u_{j+1} + \left(-\frac{\xi}{2} + \frac{3}{8}\right) u_{j+2}$$

$$ECI_3 : \quad \tilde{u}_{j+\frac{1}{2}}^{(3)} = \frac{15}{8}u_{j+1} - \frac{5}{4}u_{j+2} + \frac{3}{8}u_{j+3}$$

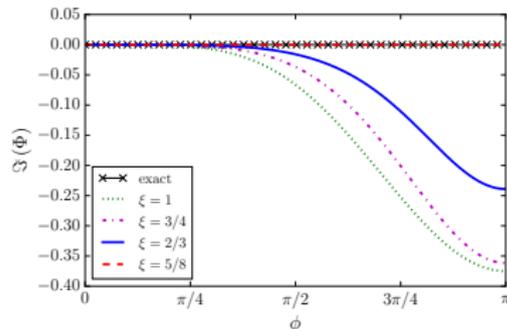
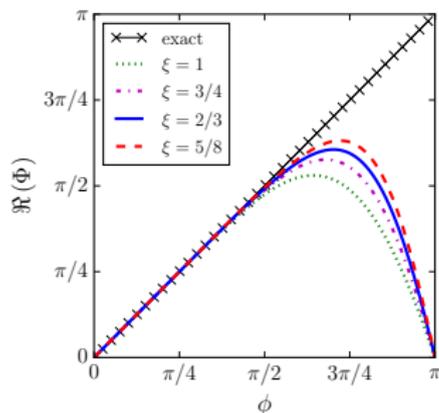
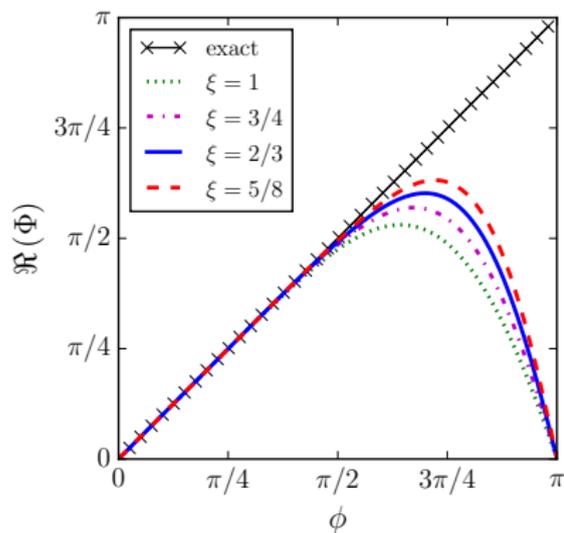
$$ECI_{\text{upwind}} = \sum_{k=0}^2 d_k^{\text{upwind}} ECI_k \quad (5^{\text{th}} \text{ order}); \quad ECI_{\text{central}} = \sum_{k=0}^3 d_k^{\text{central}} ECI_k \quad (6^{\text{th}} \text{ order})$$

Dispersion relation

Based on linear advection and exact derivatives

- Upwind-biased linear scheme

- Central linear scheme



Nonlinear weighting

- Adaptively add dissipation by using non-linear weighting of the candidate stencils
- We use the LD nonlinear weights⁵

$$\omega_k = \begin{cases} \sigma \omega_k^{\text{upwind}} + (1 - \sigma) \omega_k^{\text{central}}, & \text{if } R_\tau > \alpha_{RL}^\tau, \\ \omega_k^{\text{central}}, & \text{otherwise} \end{cases}, \quad k = 0, 1, 2, 3$$

⁵Man Long Wong and Sanjiva K Lele. "High-order localized dissipation weighted compact nonlinear scheme for shock-and interface-capturing in compressible flows". In: *Journal of Computational Physics* 339 (2017), pp. 179–209.

Flux derivative schemes

- A general compact finite difference scheme:

$$\alpha f'_{j-1} + f'_j + \alpha f'_{j+1} = a \frac{\tilde{f}_{j+\frac{1}{2}} - \tilde{f}_{j-\frac{1}{2}}}{\Delta x} + b \frac{f_{j+1} - f_{j-1}}{2\Delta x} + c \frac{\tilde{f}_{j+\frac{3}{2}} - \tilde{f}_{j-\frac{3}{2}}}{3\Delta x} + d \frac{\tilde{f}_{j+\frac{5}{2}} - \tilde{f}_{j-\frac{5}{2}}}{5\Delta x}$$

- Sixth order finite difference forms:

- Explicit midpoint-to-node differencing (MD):

$$\alpha = 0, a = \frac{75}{64}, b = 0, c = -\frac{25}{128}, d = \frac{3}{128}$$

- Explicit midpoint-and-node-to-node differencing (MND):

$$\alpha = 0, a = \frac{3}{2}, b = -\frac{3}{5}, c = \frac{1}{10}, d = 0$$

- Compact midpoint-to-node differencing (CMD):

$$\alpha = \frac{9}{62}, a = \frac{63}{62}, b = 0, c = \frac{17}{62}, d = 0$$

Weighted compact high resolution (WCHR) scheme



- The WCHR6 scheme is a combination of
 - 6th order compact midpoint-to-node finite difference scheme (CMD)
 - 6th order explicit-compact interpolation (ECI)
 - Hybrid central-upwind LD nonlinear weights

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- Other explicit interpolation schemes used for comparison:

	JS ⁶ (EI)	Z ⁷ (EI)	LD ⁸ (EI)	LD (ECI)
MND (- - -)	MND-WCNS5-JS	MND-WCNS5-Z	MND-WCNS6-LD	-
CMD (———)	WCNS5-JS	WCNS5-Z	WCNS6-LD	WCHR6

⁸Guang-Shan Jiang and Chi-Wang Shu. "Efficient implementation of weighted ENO schemes". In: *Journal of computational physics* 126.1 (1996), pp. 202–228.

⁸Rafael Borges et al. "An improved weighted essentially non-oscillatory scheme for hyperbolic conservation laws". In: *Journal of Computational Physics* 227.6 (2008), pp. 3191–3211.

⁸Wong and Lele, "High-order localized dissipation weighted compact nonlinear scheme for shock-and interface-capturing in compressible flows".

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CMD (———)	WCNS5-JS	WCNS5-Z	WCNS6-LD	WCHR6

- For all the test problems, only the schemes with the compact finite difference scheme (CMD) are used to highlight the importance of the compact interpolation
- $\xi = 2/3$ is used for all the cases with ECI

⁸Jiang and Shu, "Efficient implementation of weighted ENO schemes".

⁸Borges et al., "An improved weighted essentially non-oscillatory scheme for hyperbolic conservation laws".

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Approximate dispersion relation



- The dispersion relation plots earlier are for the linear schemes
- Characterizing the dispersion relation is harder for the full non-linear scheme

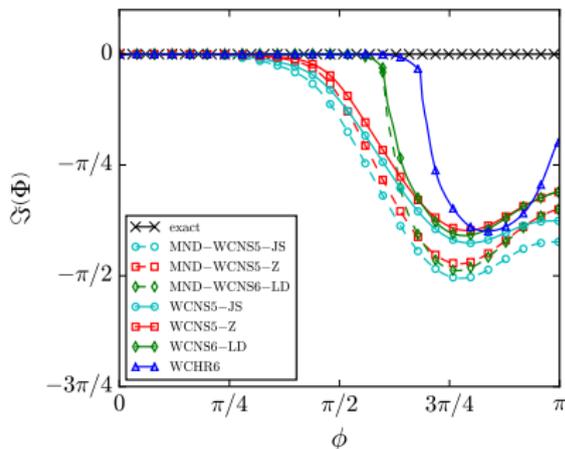
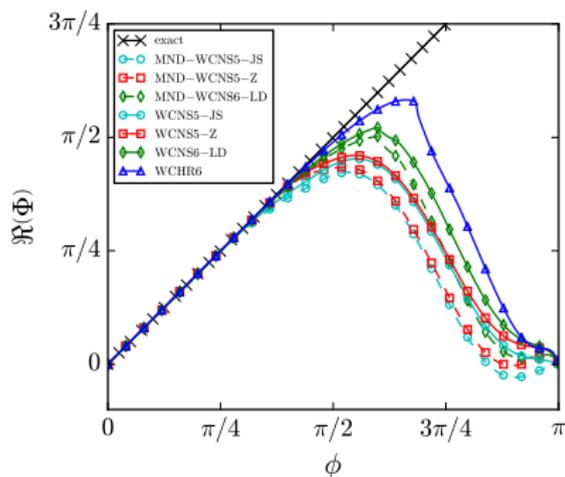
Approximate dispersion relation



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- Characterizing the dispersion relation is harder for the full non-linear scheme
- Can approximate the dispersion relation using the method proposed by Pirozzoli⁹
- Main idea is to numerically compute the dispersion relation for each wavenumber using a monochromatic wave with that wavelength

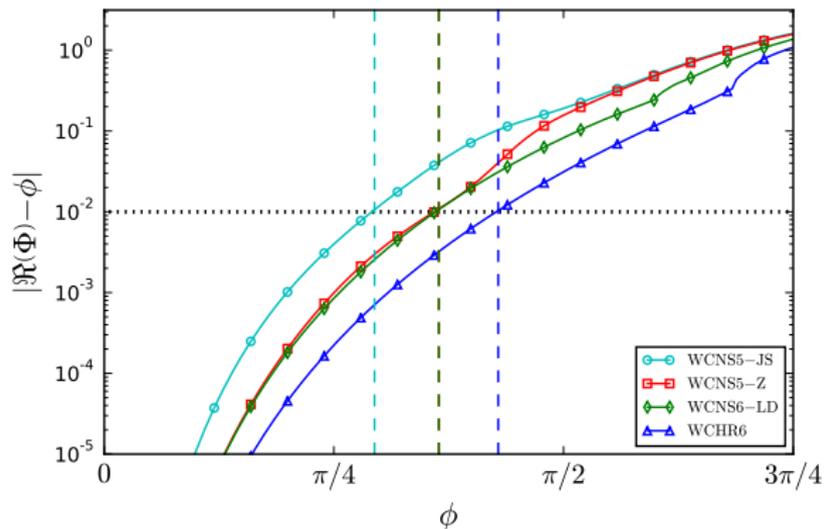
⁹Sergio Pirozzoli. "On the spectral properties of shock-capturing schemes". In: *Journal of Computational Physics* 219.2 (2006), pp. 489–497.

Approximate dispersion relation



- WCHR has highest resolution
- Since the linear version of scheme has higher resolution, more localized dissipation can be used

Dispersion error



Numerical schemes	Resolving efficiency
WCNS5-JS	0.291
WCNS5-Z	0.361
WCNS6-LD	0.361
WCHR6	0.426

- WCHR6 has highest resolving efficiency with a threshold of 10^{-2}

Extension to Euler equations



- In extending the scheme to the Euler equations, there are three choices
 1. Interpolate conservative variables
 2. Interpolate primitive variables
 3. Interpolate characteristic variables
- Interpolating characteristic variables is preferable in order to prevent the interaction of discontinuities in different characteristic fields
- Leads to more precise addition of numerical dissipation ¹⁰

¹⁰Eric Johnsen. "On the treatment of contact discontinuities using WENO schemes". In: *Journal of Computational Physics* 230.24 (2011), pp. 8665–8668.

Extension to Euler equations

- But characteristic interpolation requires solving a larger system
- Ensures consistency in transforming to and back from the characteristic space

$$\begin{aligned}
 & \alpha_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j-\frac{1}{2}} + \beta_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j+\frac{1}{2}} + \gamma_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j+\frac{3}{2}} = \\
 & \mathbf{a}_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j-1} + \mathbf{b}_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_j \\
 & + \mathbf{c}_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j+1} + \mathbf{d}_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j+2}
 \end{aligned}$$

Extension to Euler equations

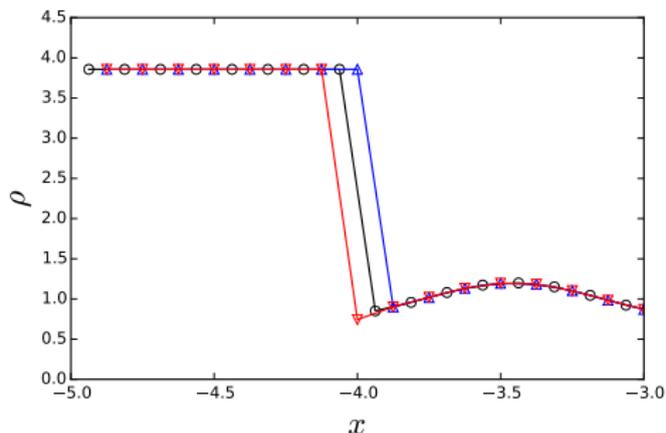
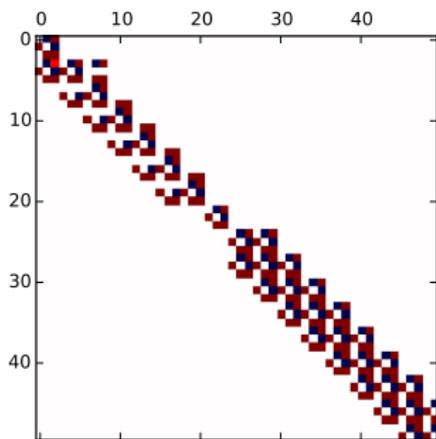
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 & \quad + \mathbf{c}_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j+1} + \mathbf{d}_{j+\frac{1}{2}} \mathbf{A}_{j+\frac{1}{2}}^{RL} \cdot \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}_{j+2}
 \end{aligned}$$

- Block-tridiagonal matrix in primitive variables instead of 3 independent tridiagonal systems in characteristic space

Characteristic based interpolation

- Need to do characteristic decomposition implicitly
- Block tri-diagonal system instead of 3 tri-diagonal systems



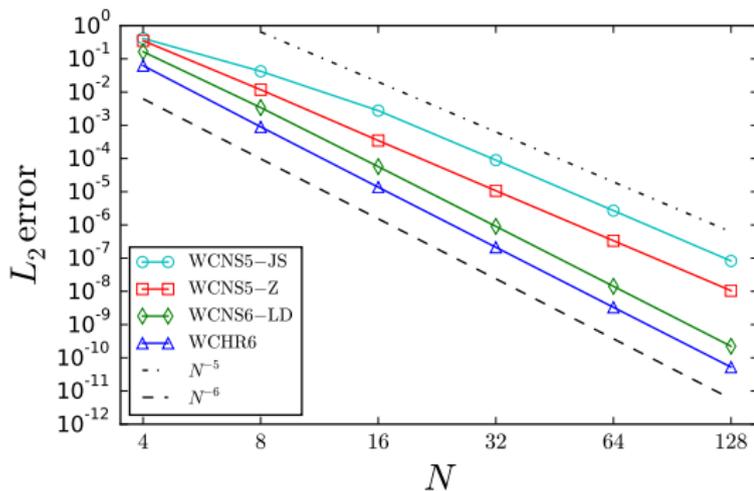
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Advection of a sinusoidal entropy wave

- Advection of a sinusoidal entropy wave in a periodic domain $x \in [0.0, 1.0)$ with initial conditions

$$(\rho, u, p) = (1 + 0.5 \sin(\pi x), 1, 1)$$



- WCHR6 is 6th order accurate.
- WCHR6 has ≈ 5 times smaller error than WCNS6-LD.

Advection of a broadband entropy disturbance



- Density of uniform flow disturbed by a broadband signal

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{pmatrix} 1 + \delta \sum_{k=1}^{N/2} (E_\rho(k))^{1/2} \sin(2\pi k(x + \psi_k)) \\ 1 \\ 1 \end{pmatrix}$$

- Broadband of density disturbances with power spectral density

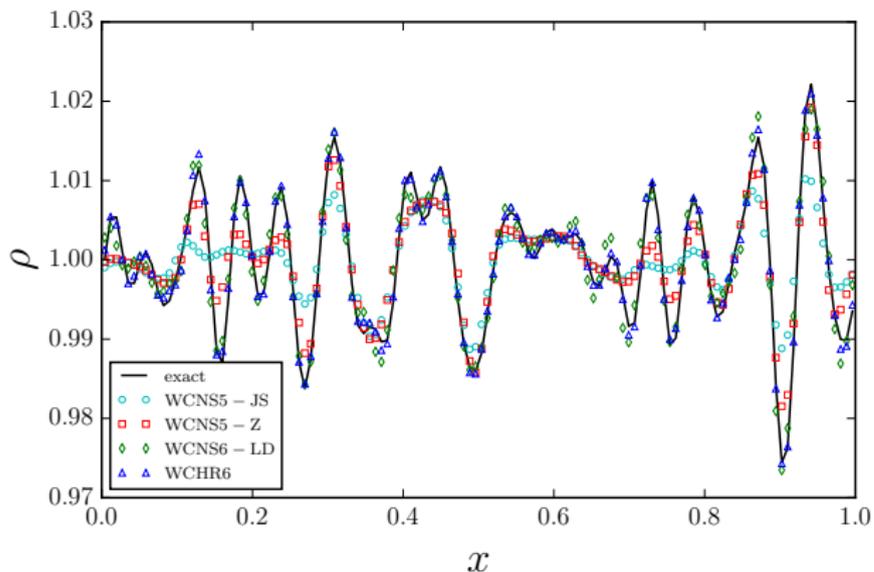
$$E(k) = \left(\frac{k}{k_0}\right)^4 \exp\left\{-2\left(\frac{k}{k_0}\right)^2\right\}$$

with $k_0 = 10$

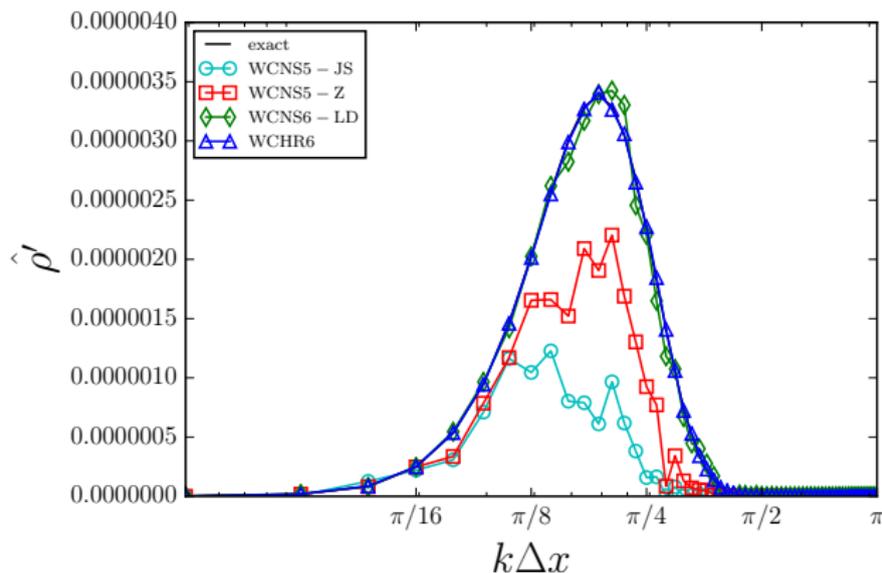
- The problem is solved using 128 points on a periodic domain $x \in [0.0, 1.0)$

Advection of a broadband entropy disturbance

- The density field after one period:



Advection of a broadband entropy disturbance



- WCNS5-JS and WCNS5-Z have high dissipation errors
- WCNS6-LD has lower dissipation, but still distorts the spectrum
- WCHR6 has the least dissipation and spectral distortion

Sod shock-tube problem

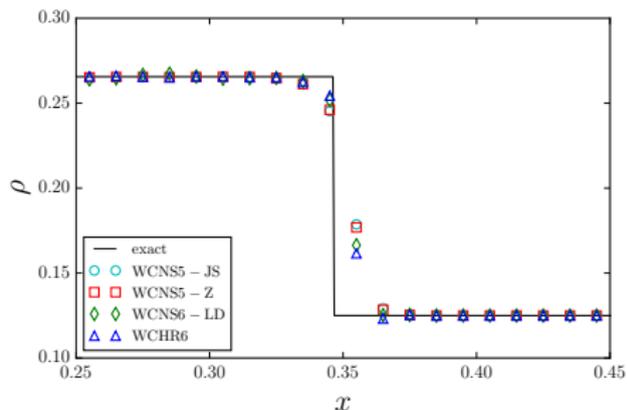
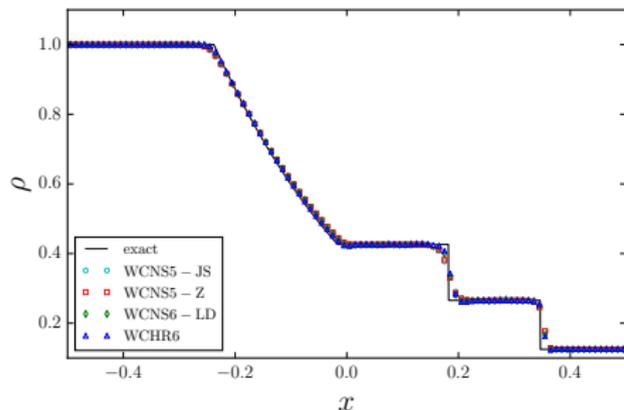


- The Sod shock-tube problem has an initial pressure and density discontinuity given by

$$(\rho, u, p) = \begin{cases} (1, 0, 1), & x < 0 \\ (0.125, 0, 0.1), & x \geq 0 \end{cases}$$

- The problem is solved using 100 points on a domain $x \in [-0.5, 0.5]$

Sod shock-tube problem



- All scheme can capture the shock well. WCNS6-LD and WCHR6 have sharpest gradients.

Shu-Osher problem



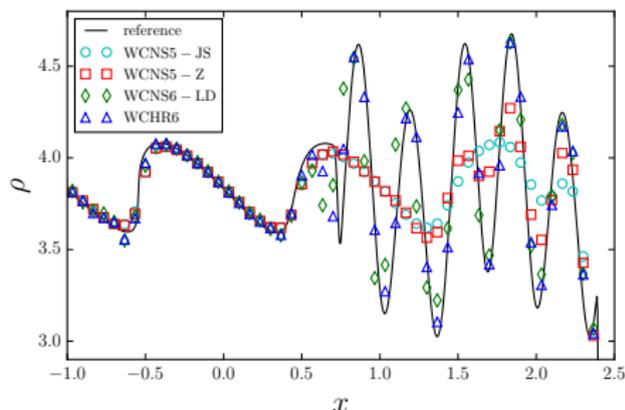
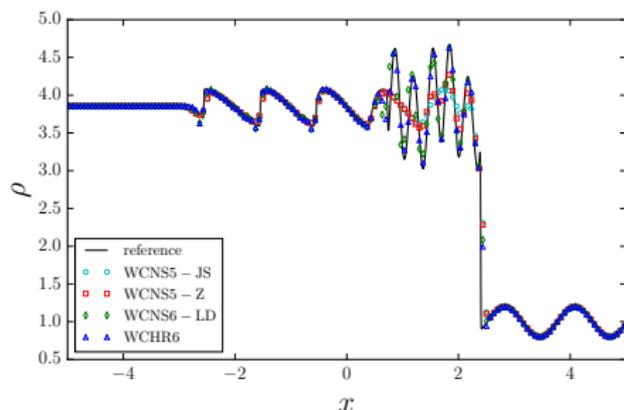
- This problem involves the interaction of a Mach 3 shock wave with an entropy wave. Initial conditions are

$$(\rho, u, p) = \begin{cases} (27/7, 4\sqrt{35}/9, 31/3), & x < -4 \\ (1 + 0.2 \sin(5x), 0, 1), & x \geq -4 \end{cases}$$

- The problem is solved using 150 points on a domain $x \in [-5, 5]$

Shu-Osher problem

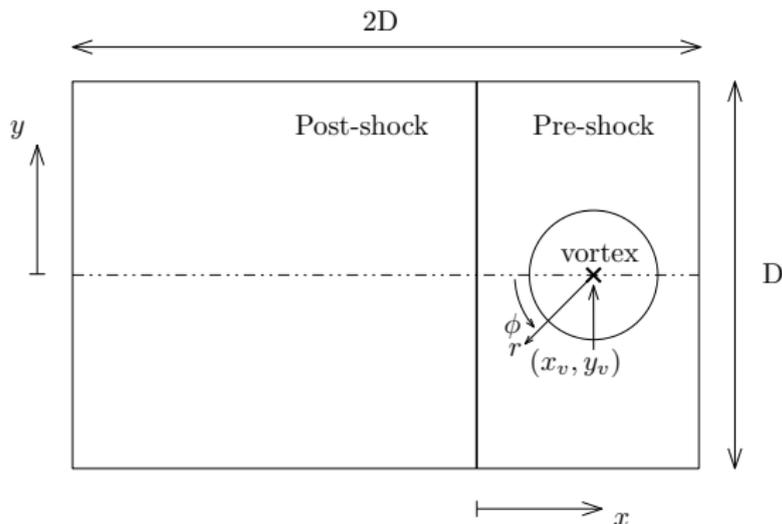
- With 150 points



- WCNS5-JS and WCNS5-Z (upwind-biased schemes) have much larger dissipation errors
- WCNS6-LD has larger dispersion error than WCHR6

Shock-vortex interaction

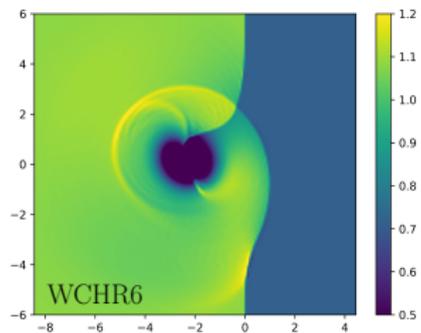
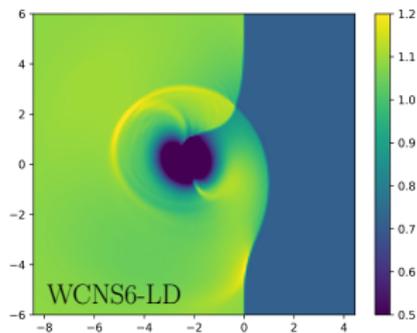
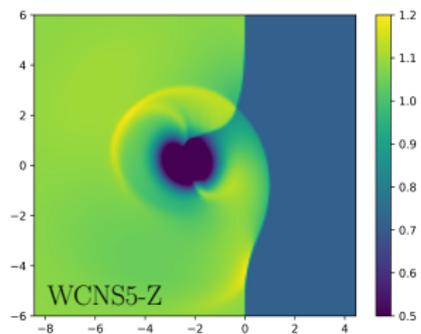
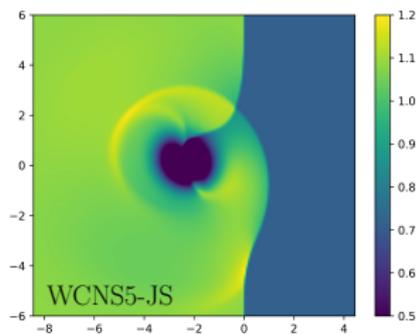
- A Mach 1.2 shock interaction with a strong vortex of vortex Mach number $M_v = 1$
- Domain size is chosen to be $[-D, D) \times [-D/2, D/2)$, where $D = 40$
- Periodic boundary conditions used in both x and y directions
- A 2D grid with 1024×512

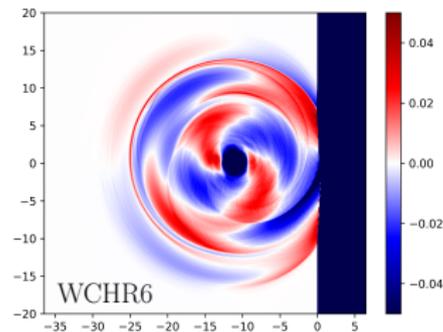
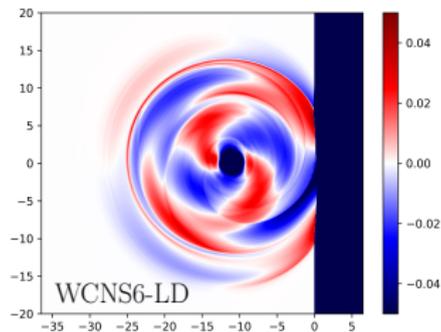
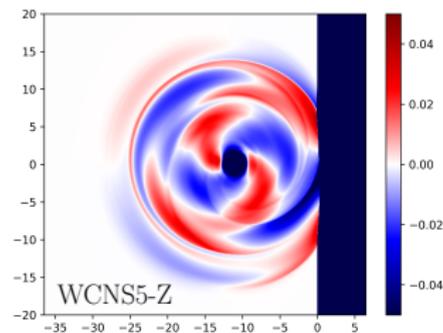
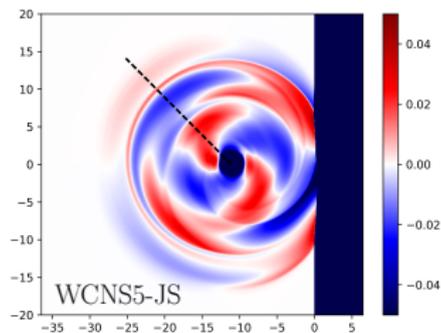


Shock-vortex interaction

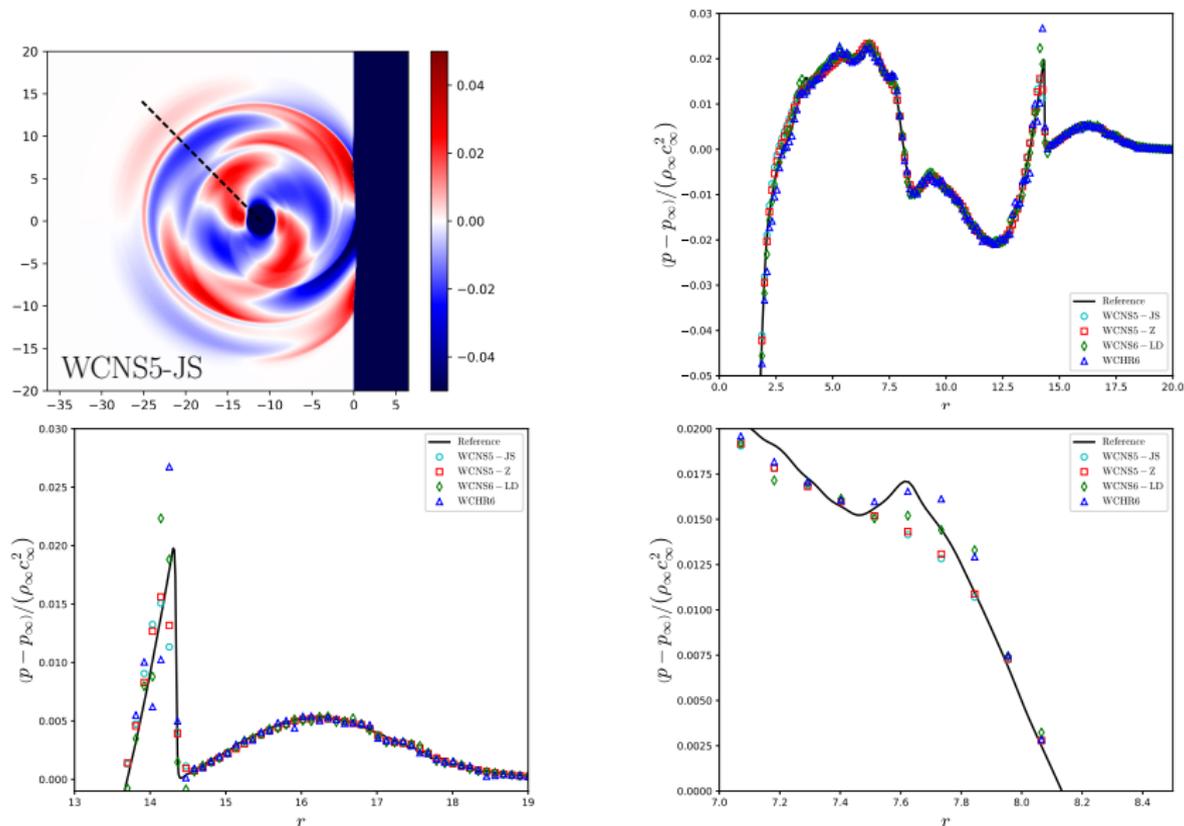
Density

$$(p - p_\infty) / (\rho_\infty c_\infty^2)$$

Pressure at $t = 6$ 

Sound pressure at $t = 16$ 

Sound pressure at radial direction



Taylor-Green Vortex

- Inviscid vortex breakdown in a periodic domain with size $[0, 2\pi]^3$
- The initial conditions are given by:

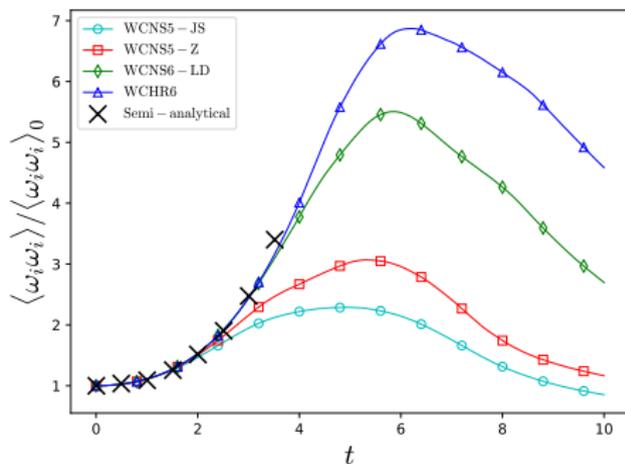
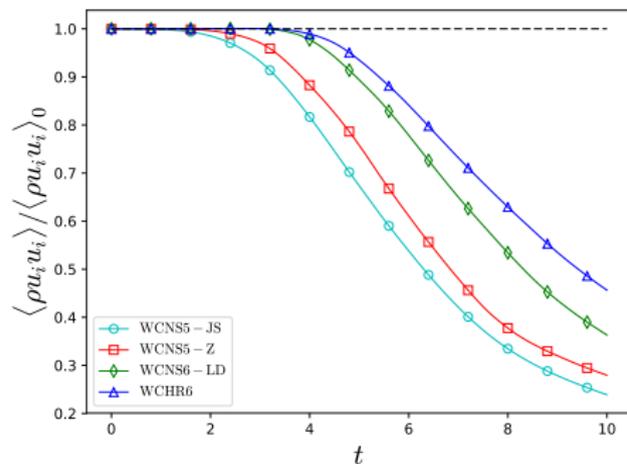
$$\begin{pmatrix} \rho \\ u \\ v \\ w \\ p \end{pmatrix} = \begin{pmatrix} 1 \\ \sin x \cos y \cos z \\ -\cos x \sin y \cos z \\ 0 \\ 100 + \frac{(\cos(2z) + 2)(\cos(2x) + \cos(2y)) - 2}{16} \end{pmatrix}$$

- Flow is essentially incompressible
- Grid resolutions of 32^3 and 64^3 are considered
- No sub-grid model is used in order to assess the dissipation characteristics of the scheme itself

Taylor-Green Vortex



- 32^3 problem



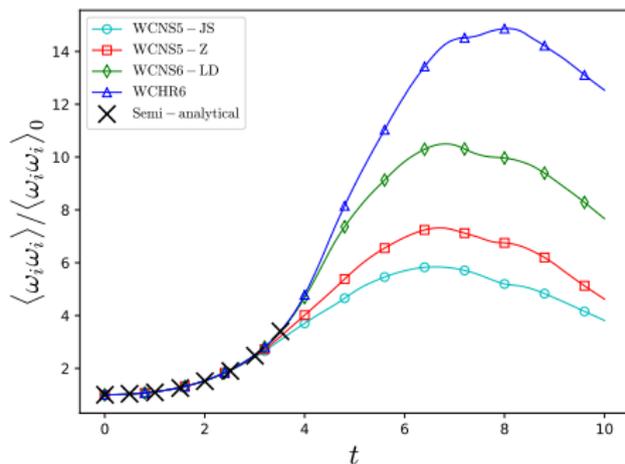
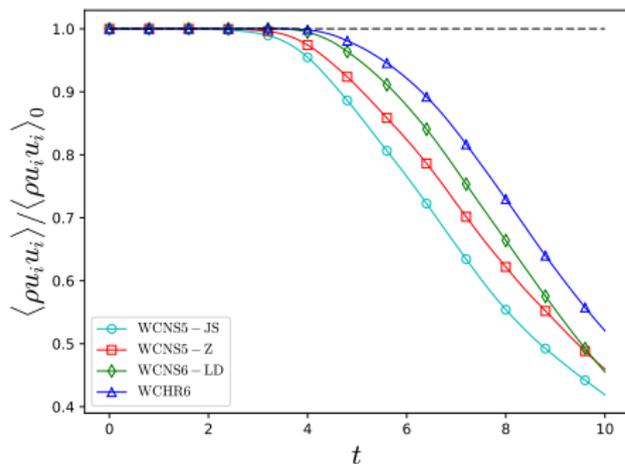
- WCHR is the least dissipative based on the TKE plot
- WCHR also has the most enstrophy and matches the semi-analytical result¹¹ for longer time

¹¹Marc E Brachet et al. "Small-scale structure of the Taylor-Green vortex". In: *Journal of Fluid Mechanics* 130 (1983), pp. 411-452.

Taylor-Green vortex



- 64^3 problem

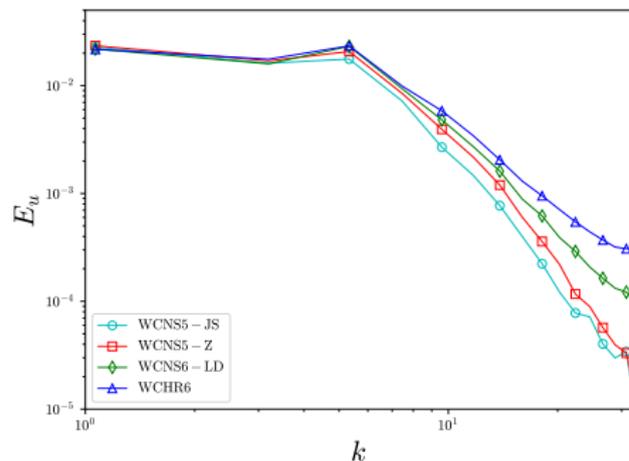


- On a 64^3 grid, WCHR captures much more of the enstrophy and is comparable to the LAD methods presented in Johnsen et. al.¹²

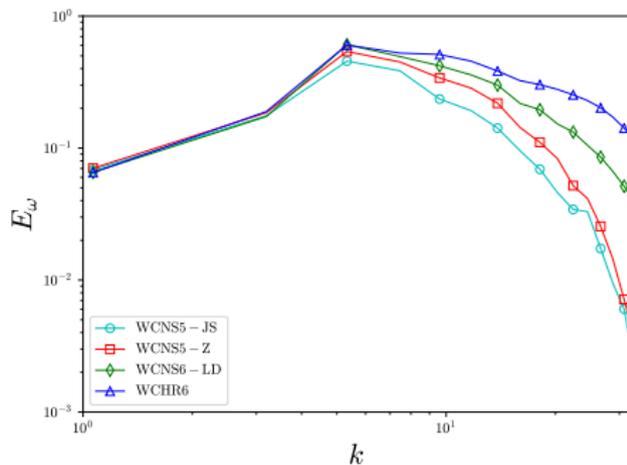
¹²Eric Johnsen et al. "Assessment of high-resolution methods for numerical simulations of compressible turbulence with shock waves". In: *Journal of Computational Physics* 229.4 (2010), pp. 1213–1237.

Taylor-Green vortex

- 64^3 , spectra at $t = 8$



Velocity energy spectrum



Vorticity energy spectrum

Compressible homogeneous isotropic turbulence



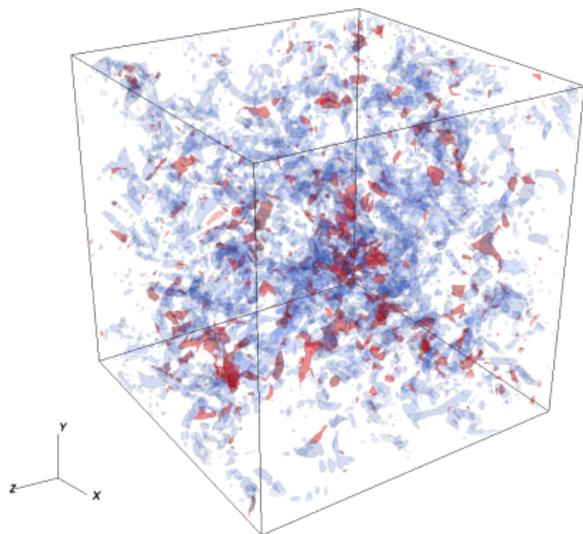
- Decaying compressible homogeneous isotropic turbulence

$$E(k) \propto k^4 \exp\left(-2\left(\frac{k}{k_0}\right)^2\right), \quad k_0 = 4$$

- Initial turbulent Mach number $M_t = 0.6$
- Initial Taylor Reynolds number $Re_\lambda = 100$
- High turbulent Mach number creates eddy shocklets in the domain ¹³
- Good test case to assess the numerical dissipation characteristics of different schemes
- No sub-grid model is used in order to assess the dissipation characteristics of the scheme itself
- Solved on a 64^3 grid

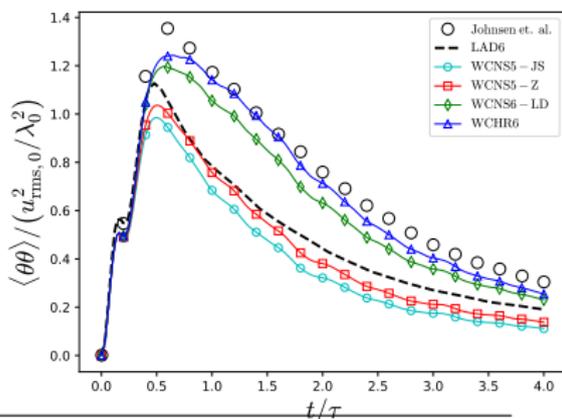
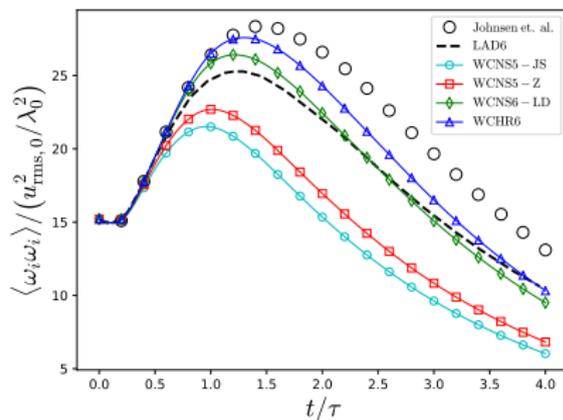
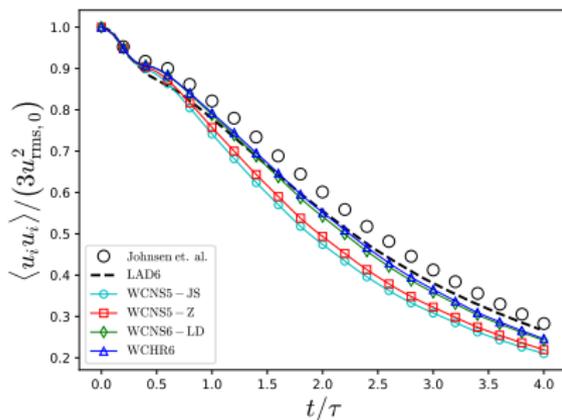
¹³Sangsan Lee, Sanjiva K Lele, and Parviz Moin. "Eddy shocklets in decaying compressible turbulence". In: *Physics of Fluids A: Fluid Dynamics* 3.4 (1991), pp. 657–664.

Compressible homogeneous isotropic turbulence



Numerical schlieren on a slice

1σ enstrophy contour (blue) and -3σ dilatation (red) contours at $t/\tau = 2$



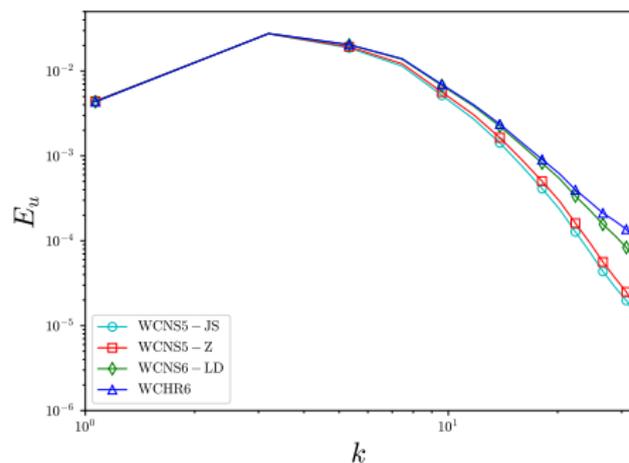
- Spectrally filtered DNS solution from Johnsen et. al.¹⁴ in open circles

¹⁴ Johnsen et al., "Assessment of high-resolution methods for numerical simulations of compressible turbulence with shock waves".

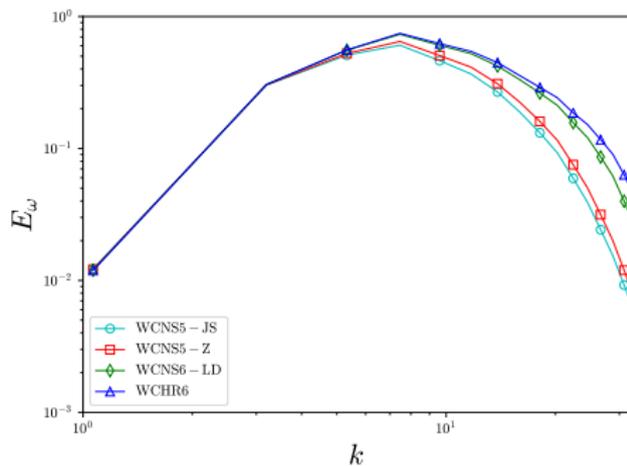
Compressible homogeneous isotropic turbulence



- Spectra at $t/\tau = 2$



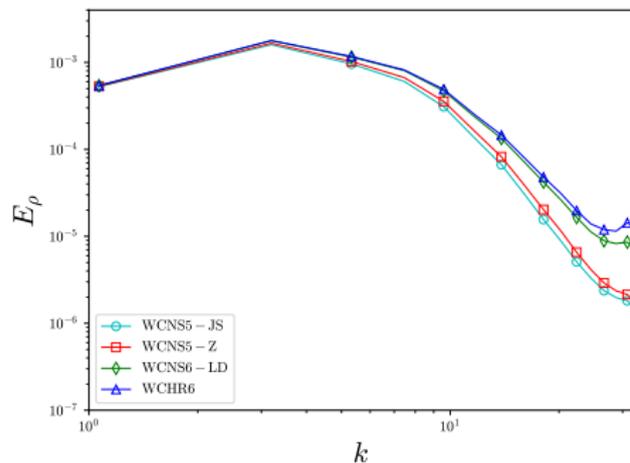
Velocity energy spectrum



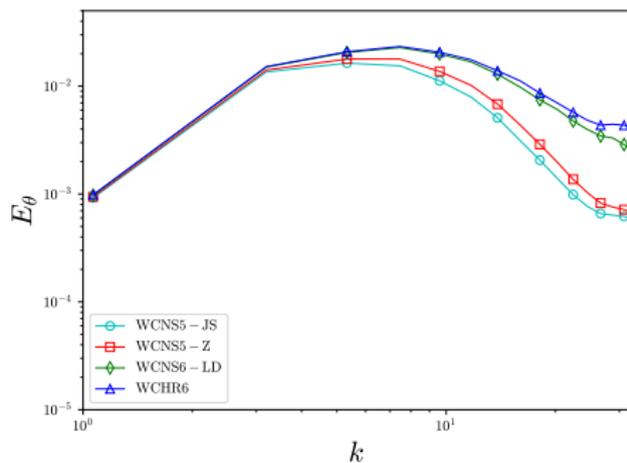
Vorticity energy spectrum

Compressible homogeneous isotropic turbulence

- Spectra at $t/\tau = 2$



Density energy spectrum



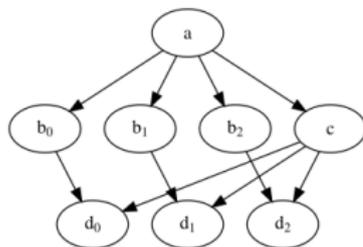
Dilatation energy spectrum

Outline

1. Introduction
2. Overview of the WCNS methodology
3. The WCHR scheme
 - Explicit interpolation
 - Explicit-compact interpolation
 - Nonlinear weights
 - Derivative scheme
 - Approximate dispersion relation
 - Extension to Euler equations
4. Results
 - 1D test problems
 - 2D test problems
 - 3D test problems
- 5. Implementation details**
6. Conclusions

Regent task based system

- Regent is a language for implicit dataflow parallelism
- Discovers dataflow parallelism in sequential code by computing a dependence graph over tasks



- Programmer only expresses the parallelism but does not explicitly implement any communication, etc.
- Data transfer between tasks is handled by the runtime system
- Works for node-node and CPU-GPU data transfers

Computational cost estimate

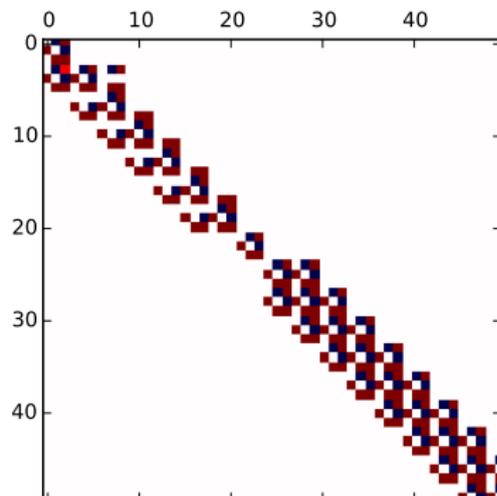
- For a 3D problem, the cost per grid point for the interpolation in one direction is given below

Operation Counts	EI char.	EI prim.	EI char.
Matrix solve	11	45	195
Interpolation RHS	55	55	55
Characteristic decomposition	66	0	66
Smoothness indicators	440	440	440
Nonlinear weights	630	720	720
Total	1202	1260	1476

- EI with characteristic decomposition is about 23% more expensive in terms of operation count

Block-tridiagonal solve

- The main bottleneck in performance is the block tridiagonal matrix system



- Use the SuperLU¹⁵ library to solve the block-tridiagonal matrix system
- Do symbolic factorization once and use sparsity pattern multiple times

¹⁵James W. Demmel et al. "A supernodal approach to sparse partial pivoting". In: *SIAM J. Matrix Analysis and Applications* 20.3 (1999), pp. 720–755.

- With SuperLU, the block tridiagonal solves take $\approx 80 - 90\%$ of the total wall clock time
- Not consistent with Flop count estimates from before
- Need to perform some data copies to be able to interface with SuperLU, but that still does not explain the high cost

Custom block-tridiagonal solver

- Consider a block tridiagonal matrix system $\mathbf{Ax} = \mathbf{b}$

$$\begin{pmatrix} \tilde{\beta}_1 & \tilde{\gamma}_1 & & & & \\ \tilde{\alpha}_2 & \tilde{\beta}_2 & \tilde{\gamma}_2 & & & \\ & & \ddots & & & \\ & & & \tilde{\alpha}_{N-1} & \tilde{\beta}_{N-1} & \tilde{\gamma}_{N-1} \\ & & & & \tilde{\alpha}_N & \tilde{\beta}_N \end{pmatrix} \begin{pmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \vdots \\ \tilde{x}_{N-1} \\ \tilde{x}_N \end{pmatrix} = \begin{pmatrix} \tilde{b}_1 \\ \tilde{b}_2 \\ \vdots \\ \tilde{b}_{N-1} \\ \tilde{b}_N \end{pmatrix}$$

- $\tilde{\alpha}_i$, $\tilde{\beta}_i$ and $\tilde{\gamma}_i$ are 5×5 matrices corresponding to the Jacobian of conserved variables w.r.t primitive variables
- \tilde{x}_i and \tilde{b}_i are 5×1 vector elements of the solution vector and the RHS vector respectively

Custom block-tridiagonal solver

- Speed up the block-tridiagonal solver performance using a custom solver
- The Jacobian matrix forming each block in the x interpolation is

$$\begin{pmatrix} 0 & -\frac{\rho c}{2} & 0 & 0 & \frac{1}{2} \\ 1 & 0 & 0 & 0 & -\frac{1}{c^2} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{\rho c}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

- Idea is to decouple v and w interpolations to get a 3×3 block tridiagonal system and 2 tridiagonal systems instead of a 5×5 block tridiagonal system
- Cost of each block inversion reduces from $\mathcal{O}(5^3)$ to $\mathcal{O}(3^3)$

Custom block-tridiagonal solver

- Use approach similar to the regular Thomas algorithm to derive a block-tridiagonal algorithm
- Forward elimination

$$\Delta_i = \left[\tilde{\beta}_i - \tilde{\alpha}_i \Delta_{i-1} \tilde{\gamma}_{i-1} \right]^{-1}$$

$$\hat{b}_i = b_i - \tilde{\alpha}_i \Delta_{i-1} \hat{b}_{i-1}$$

- Back substitution

$$x_i = -\Delta_i \left[-\hat{b}_i + \tilde{\gamma}_i x_{i+1} \right]$$

- Use Sherman-Morrison low rank correction for periodic problems

$$\left(A + UV^T \right)^{-1} = A^{-1} - A^{-1}U \left(I + V^T A^{-1}U \right)^{-1} V^T A^{-1}$$

- The custom algorithm was implemented in Regent without any specific optimizations
- $\sim 30\times$ speedup in the matrix solves
- $\sim 8\times$ speedup of the full interpolation algorithm
- For full 3D taylorgreen vortex on a 64^3 grid
 - Old implementation took $\sim 73s$ per time step
 - New implementation takes $\sim 15s$ per time step
 - HAMeRS¹⁶ (fully explicit scheme) takes $\sim 7.5s$ per time step
- Being within a factor of 2 compared to HAMeRS is quite good since no vectorization optimizations have been performed

¹⁶<https://fpal.stanford.edu/hamers>

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- WCHR6 has higher resolution than other WCNS's due better spectral properties of the nonlinear explicit-compact interpolation
- Computational cost in terms of operation count was shown to be only $\sim 23\%$ more than traditional WCNS's
- 1D and 2D problems show the robustness of WCHR6 in capturing shocks and high wavenumber features
- 3D problems highlight the minimal dissipation characteristic of the WCHR6 compared to other WCNS's
- Future work:
 - Develop consistent and stable boundary schemes
 - Analyze space-time characteristics of WCHR6
 - Parallel algorithms for the block tri-diagonal solve

Questions?