High-Order Genuinely Multidimensional Finite Volume Methods via Kernel-Based WENO

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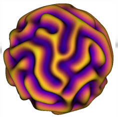

Introduction

Goal

Solve systems of hyperbolic conservation laws

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$$

with an *accurate* and *robust* finite volume method

$$\frac{\partial \langle \mathbf{U} \rangle_\Omega}{\partial t} + \frac{1}{||\Omega||} \int\limits_{\partial\Omega} \hat{\mathbf{F}} \left(\mathbf{U}^-(\mathbf{x}), \mathbf{U}^+(\mathbf{x}) \right) \cdot \mathbf{n} dx = \frac{1}{||\Omega||} \int\limits_{\Omega} \mathbf{S}(\mathbf{U}) d\boldsymbol{x}$$

in *multiple* dimensions.

Systems of interest

Compressible Euler equations

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{U}) + \frac{\partial}{\partial y}\mathbf{G}(\mathbf{U}) + \frac{\partial}{\partial z}\mathbf{H}(\mathbf{U}) = 0$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ u(E+p) \end{pmatrix} \quad \mathbf{G} = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v w \\ v(E+p) \end{pmatrix} \quad \mathbf{H} = \begin{pmatrix} \rho w \\ \rho u w \\ \rho v w \\ \rho w^2 + p \\ w(E+p) \end{pmatrix},$$

for a calorically ideal gas,

$$p = (\gamma - 1)\rho\epsilon, \quad \rho\epsilon = E - \frac{1}{2}\rho\mathbf{v}\cdot\mathbf{v}.$$

Systems of interest

Ideal GLM-MHD equations

$$
\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \\ B_x \\ B_y \\ B_z \\ \psi \end{pmatrix} \quad
\mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p_* - B_x^2 \\ \rho u v - B_x B_y \\ \rho u w - B_x B_z \\ F_E \\ C_h \psi \\ u B_y - v B_x \\ u B_z - w B_x \\ C_h B_x \end{pmatrix} \quad
\mathbf{S} = \begin{pmatrix} 0 \\ -B_x \nabla \cdot \mathbf{B} \\ -B_y \nabla \cdot \mathbf{B} \\ -B_z \nabla \cdot \mathbf{B} \\ -S_E \\ -u \nabla \cdot \mathbf{B} \\ -v \nabla \cdot \mathbf{B} \\ -w \nabla \cdot \mathbf{B} \\ -\mathbf{v} \cdot \nabla \psi \end{pmatrix},
$$

where,

$$
\begin{aligned}
p_* &= p_{\text{gas}} + p_{\text{mag}} \\
F_E &= u(E + p_g) + B_x \left(C_h \psi - \mathbf{v} \cdot \mathbf{B} \right) \\
S_E &= (\mathbf{v} \cdot \mathbf{B}) \nabla \cdot \mathbf{B} + \psi \mathbf{v} \cdot \nabla \psi
\end{aligned}
$$

Quick overview of FVM

Abstract formulation

Partition full domain Ω into *finite volumes* Ω_i such that $\Omega = \bigcup\limits_i \Omega_i$, and $\Omega_i \cap \Omega_j = \varnothing,\ i \neq j$. Denote

$$\langle \cdot \rangle_i = \frac{1}{||\Omega_i||} \int\limits_{\Omega_i} \cdot d\mathbf{x},$$

then for (systems of) hyperbolic conservation laws

$$\frac{\partial}{\partial t} \langle \mathbf{U} \rangle_i = -\frac{1}{||\Omega_i||} \oint\limits_{\partial \Omega_i} \hat{\mathbf{F}} \left(\mathbf{U}^-, \mathbf{U}^+ \right) \cdot \mathbf{n} ds$$

for numeric flux $\hat{\mathbf{F}}$, and states $\mathbf{U}^-$ and $\mathbf{U}^+$ inside and outside Ω_i.

Quick overview of FVM

Uniform 2D Cartesian grids

Let $\Omega_{i,j} = \left[x_i - \frac{\Delta x}{2}, x_i - \frac{\Delta x}{2}\right] \times \left[y_i - \frac{\Delta y}{2}, y_j - \frac{\Delta y}{2}\right]$, then

$$\frac{\partial}{\partial t}\langle \mathbf{U} \rangle_{i,j} = -\frac{1}{||\Omega_{i,j}||} \oint\limits_{\partial \Omega_{i,j}} \hat{\mathbf{F}}\left(\mathbf{U}^-, \mathbf{U}^+\right) \cdot \mathbf{n} ds$$

$$= -\frac{1}{\Delta x}\left(\langle \hat{\mathbf{F}} \rangle_{i+\frac{1}{2},j} - \langle \hat{\mathbf{F}} \rangle_{i-\frac{1}{2},j}\right) - \frac{1}{\Delta y}\left(\langle \hat{\mathbf{G}} \rangle_{i,j+\frac{1}{2}} - \langle \hat{\mathbf{G}} \rangle_{i,j-\frac{1}{2}}\right)$$

where half-indices indicate integration over faces.

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where half-indices indicate integration over faces.

Two barriers to high order in multiple dimensions

- Face integral must be done accurately
- Numerical flux is defined *pointwise*, thus need accurate *pointwise* values of $\mathbf{U}$ on faces

Accurate construction of Riemann states

Multidimensional concerns

Issues with polynomials

- Matching stencils to multivariate polynomial spaces is hard
- Forming valid substencils for WENO is even harder
- Dimension-by-dimension approaches do work, but get messy

[1] Omitting many technical details

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Kernel based interpolation/recovery

Each SPD *kernel* $K : \Omega \times \Omega \to \mathbb{R}$, induces a *reproducing kernel Hilbert space*[1], $\mathcal{H}$, consisting of

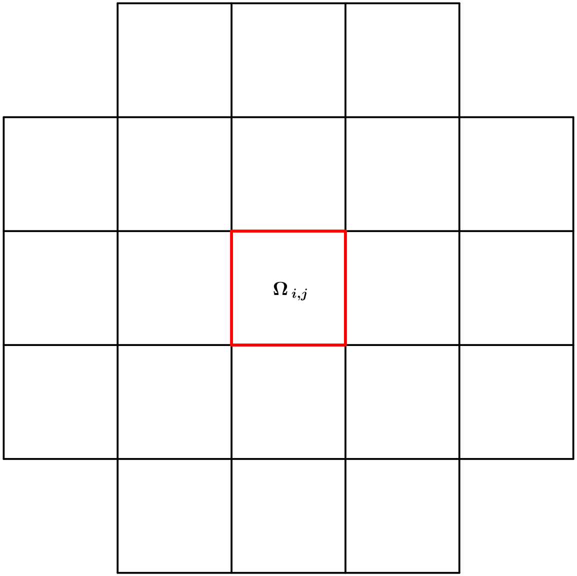
$$f(x) = \sum_i a_i K(x, x_i)$$

$$\sum_i \sum_j a_i a_j K(x_i, x_j) < \infty$$

For this talk: $K(x, y) = e^{-\frac{||x-y||^2}{2\ell^2}}$.

[1] Omitting many technical details

An exemplary stencil: $R = 2$



Kernel-based interpolation

Let $\{\boldsymbol{x}_i\} \subset \Omega$ be distinct, and $\mathbf{f}_i = f(\boldsymbol{x}_i)$ known.
Seek an interpolant of the form:

$$\widetilde{f}(\boldsymbol{x}) = \sum_{j=1}^{N} a_j K(\boldsymbol{x}, \boldsymbol{x}_j)$$

then enforcing that $\widetilde{f}(\boldsymbol{x}_i) = \mathbf{f}_i$, requires that $\mathbf{a}$ satisfy

$$\mathbf{K}\mathbf{a} = \mathbf{f}, \quad \mathrm{K}_{i,j} = K(\boldsymbol{x}_i, \boldsymbol{x}_j).$$

Properties of kernel-based interpolation

- $K(\boldsymbol{x}, \boldsymbol{x}_j) \in \mathcal{H}$, hence $\widetilde{f} \in \mathcal{H}$
- $(f - \widetilde{f}) \perp_{\mathcal{H}} \operatorname{span}(K(\boldsymbol{x}, \boldsymbol{x}_j))$
- The matrix $\mathbf{K}$ is SPD if the kernel K is

Kernel-based generalized interpolation

Symmetric form

Let $\{\lambda_i\} \subset \mathcal{H}'$ be linearly independent, and $\mathbf{g}_i = \lambda_i f$ known.
Seek an interpolant of the form:

$$\widetilde{f}(x) = \sum_{j=1}^{N} a_j \lambda_j^{(y)} K(x, y)$$

then enforcing that $\lambda_i^{(x)} \widetilde{f}(x) = \mathbf{g}_i$, requires that $\mathbf{a}$ satisfy

$$\mathbf{Ca} = \mathbf{g}, \quad \mathrm{C}_{i,j} = \lambda_i^{(x)} \lambda_j^{(y)} K(x, y).$$

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Relationship to regular interpolation

- $\lambda_j^{(y)} K(x,y) \in \mathcal{H}_A$, hence $\widetilde{f} \in \mathcal{H}_A$
- $(f - \widetilde{f}) \perp_{\mathcal{H}_A} \operatorname{span}\left(\lambda_j^{(y)} K(x,y)\right)$
- Point evaluation functionals, $\lambda_j = \delta_{x_j}$, gives previous result
- The matrix $\mathbf{C}$ is still SPD so long as K is

Kernel-based generalized interpolation
Asymmetric form with polynomial constraints

Additionally let $\{\boldsymbol{\alpha}_k : |\boldsymbol{\alpha}_k| \leq D\}$ be a set of multi-indices.

Seek an interpolant of the form:

$$\widetilde{f}(x) = \sum_{j=1}^{N} a_j K(x, x_j) + \sum_{|\boldsymbol{\alpha}_k| \leq D} b_k \boldsymbol{x}^{\boldsymbol{\alpha}_k}$$

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then enforcing that $\lambda_i^{(x)} \widetilde{f}(x) = \mathbf{g}_i$, requires that $\mathbf{a}$ and $\mathbf{b}$ satisfy

$$\mathbf{Qa} + \mathbf{Pb} = \mathbf{g}, \quad \mathrm{Q}_{i,j} = \lambda_i^{(x)} K(x, x_j), \; \mathrm{P}_{i,j} = \lambda_i^{(x)} \boldsymbol{x}^{\boldsymbol{\alpha}_k}.$$

To be exact for all $\boldsymbol{x}^{\boldsymbol{\alpha}_k}$ we also need $\mathbf{P}^T \mathbf{a} = \mathbf{0}$, so ultimately solve

$$\begin{bmatrix} \mathbf{Q} & \mathbf{P} \\ \mathbf{P}^T & \mathbf{0} \end{bmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ \mathbf{0} \end{pmatrix}$$

Precomputing reconstruction vectors
Asymmetric form

We can solve

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then evaluate the resulting interpolant at $\boldsymbol{x}^*$

$$\widetilde{f}(\boldsymbol{x}^*) = \sum_{j=1}^{N} a_j K(\boldsymbol{x}^*, \boldsymbol{x}_j) + \sum_{|\boldsymbol{\alpha}_k| \leq D} b_k (\boldsymbol{x}^*)^{\boldsymbol{\alpha}_k} = \mathbf{T}^T \mathbf{a} + \mathbf{S}^T \mathbf{b}.$$

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Hence the *reconstruction vector* can be precomputed from

$$\begin{bmatrix} \mathbf{Q}^T & \mathbf{P} \\ \mathbf{P}^T & \mathbf{0} \end{bmatrix} \begin{pmatrix} \mathbf{r} \\ \mathbf{w} \end{pmatrix} = \begin{pmatrix} \mathbf{T} \\ \mathbf{S} \end{pmatrix},$$

giving simply $\widetilde{f}(\boldsymbol{x}^*) = \mathbf{r}^T \mathbf{g}$.

Accurate flux integrals
Transverse corrections

- We can now obtain accurate point estimates of the solution
- Call an (approximate) Riemann solver to find pointwise fluxes
- But *where* should we do this?

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Find kernel-based interpolant through the fluxes and integrate it exactly. (Potentially interesting in 3D)

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Gaussian quadrature

Solve multiple Riemann problems per face, then do Gaussian quadrature.
Ultimately, Riemann solvers are not that expensive so this is the easiest (and most stable) option.

Taylor-Green vortex problem
Compressible Euler equations

Triply periodic vortex on $[0, 2\pi]^3$ that quickly becomes turbulent.

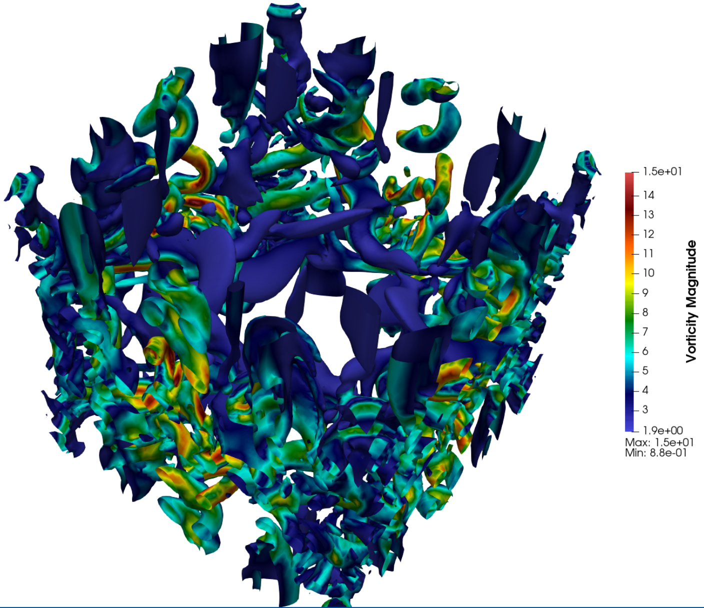
Initial conditions

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

Note: Without physical viscosity this problem is mostly of qualitative significance.

Taylor-Green vortex

$192 \times 192 \times 192$, Radius 2, $\ell = 24\Delta$



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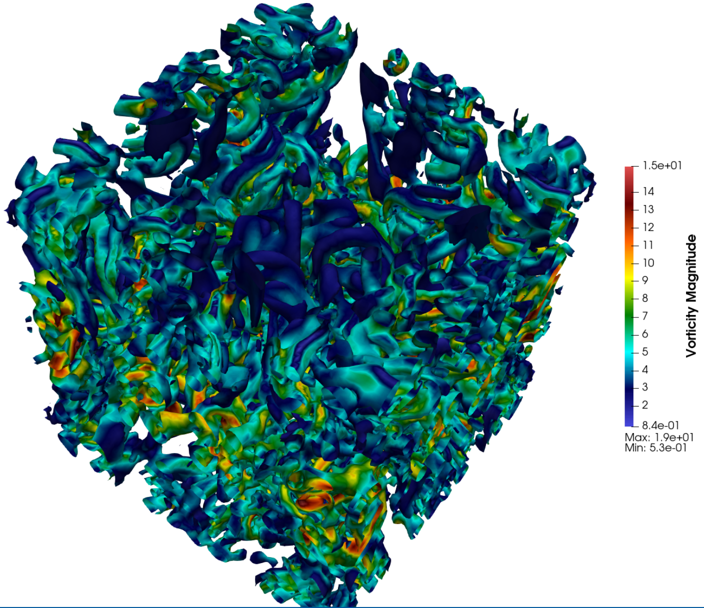

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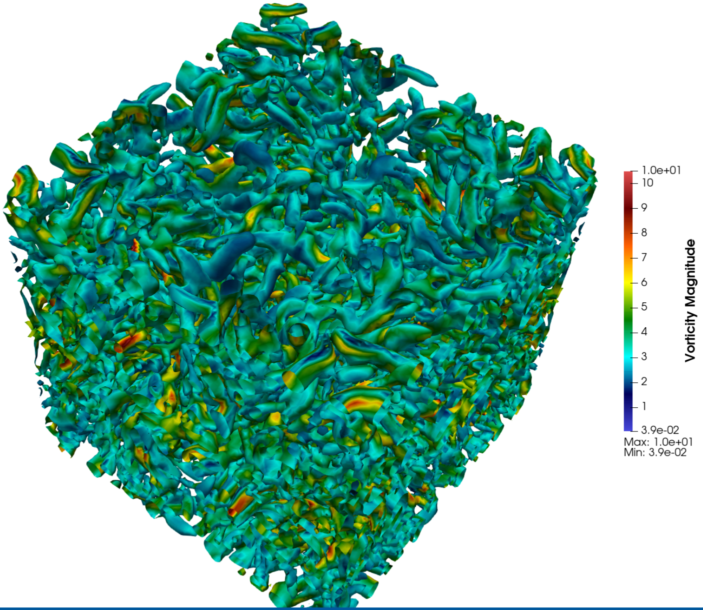

Dealing with shocks: WENO methods

Nonlinear reconstruction

The reconstruction presented is linear, i.e.

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WENO (weighted essentially non-oscillatory) methods

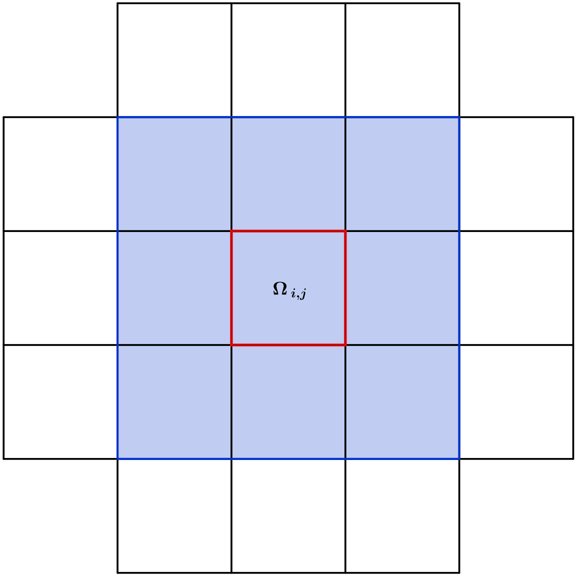
Break full stencil into substencils, use weighted combination of individual reconstructions

$$\widetilde{f}(\boldsymbol{x}^*) = \sum_{S_k \in \mathcal{S}_{i,j}} \omega_k \mathbf{r}_{(k)}^T \mathbf{g}_{(k)}$$

where $\mathcal{S}_{i,j}$ is set of substencils, and ω_k **depends** on the data in S_k.

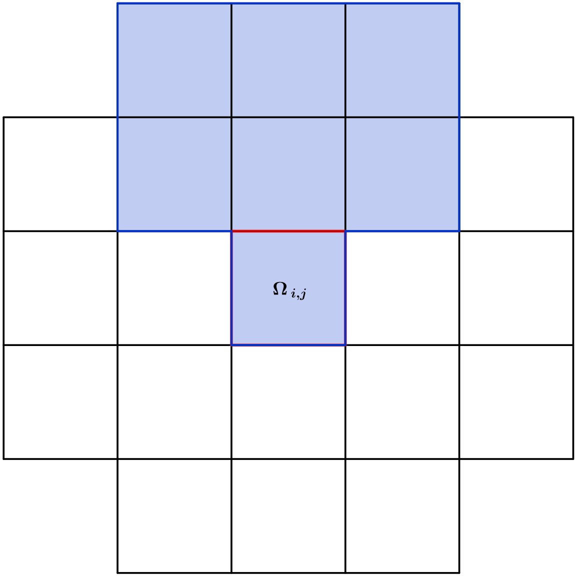
S_1: Central substencil

Substencils in the spirit of standard WENO



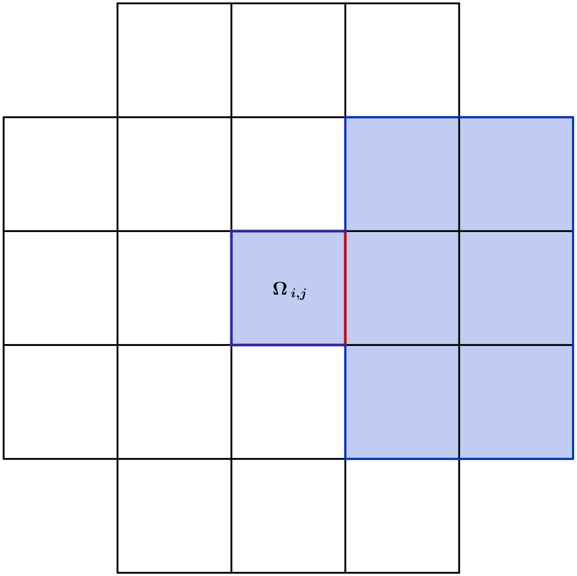
S_2: North substencil

Substencils in the spirit of standard WENO



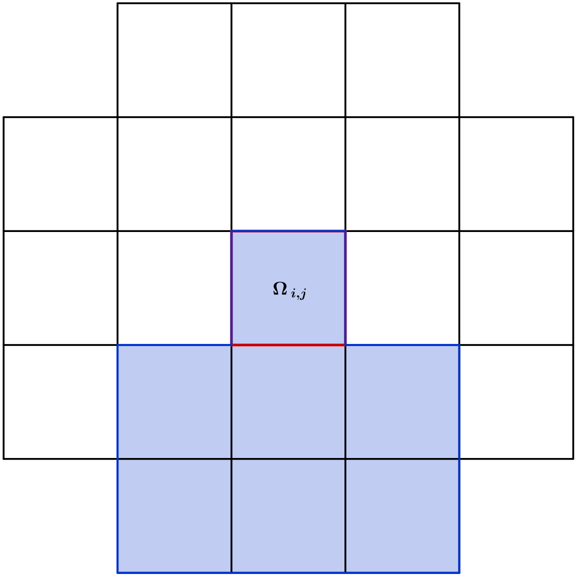
S_3: East substencil

Substencils in the spirit of standard WENO



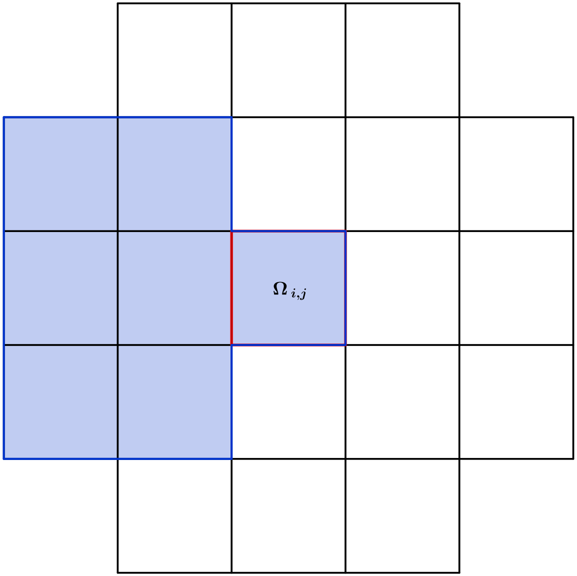
S_4: South substencil

Substencils in the spirit of standard WENO



S_5: West substencil

Substencils in the spirit of standard WENO



Optimal weights and standard WENO

The optimal linear weights γ_k minimize discrepancy in

$$\widetilde{f}(\boldsymbol{x}^*) \approx \sum_{k=1}^{5} \gamma_k \mathbf{r}_{(k)}^T \mathbf{g}_{(k)}$$

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Desired behavior of ω_k

- For smooth data $\omega_k \approx \gamma_k$ on all substencils
- For rough data $\omega_k \approx 0$ on rough substencils

This is obtained by use of *smoothness indicators*.

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Special cases: Polynomial reconstruction

For *some* polynomial degrees on *some* (sub)stencil choices, equality can be obtained (e.g. classical WENO5).

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Adaptive order WENO

Let S_0 correspond to the full stencil, and include it explicitly:

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Now we can choose γ_k solely to ensure stability, e.g.

$$\begin{aligned}\gamma_0 &= C_h,\\ \gamma_1 &= (1-C_h)C_l,\\ \gamma_2 = \gamma_3 = \gamma_4 = \gamma_5 &= \frac{(1-C_h)*(1-C_l)}{4},\end{aligned}$$

where $0 < C_h, C_l < 1$, e.g. $C_h = C_l = 0.8$.

Smoothness indicators
The last numerical ingredient

The smoothness of the solution on each substencil can be measured by

$$\beta_k = \sum_{|\alpha|=1}^{2} \sum_q w_q \left(\left. \frac{\partial^{|\alpha|} \widetilde{f}_k}{\partial \boldsymbol{x}^\alpha} \right|_{\boldsymbol{x}_q} \right)^2,$$

Then nonlinear weights are formed using a modified WENO-Z scheme

$$\tau = \left| \beta_0 - \frac{1}{4} \sum_{k=2}^{5} \beta_k \right|$$

$$\widetilde{\omega}_k = \gamma_k \left(1 + \left(\frac{\tau}{\beta_k + \epsilon} \right)^p \right)$$

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Observation: Mixed derivatives can be safely ignored.

Reconstruction Variables
Linearized primitive variables

- The reconstruction scheme is defined for scalar data
- Must do reconstruction *componentwise*
- Reconstructing conservative variables directly is a bad idea

Note: Any linear combination of cell-averages is still a cell-average.

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Generic transformation

Fix some matrix Φ and set

$$\mathbf{W}_{i,j} = \mathbf{\Phi}\mathbf{U}_{i,j}, \quad \forall (i,j) \in \mathcal{S}_0,$$

reconstruct over $\mathbf{W}$ componentwise and map back with $\mathbf{\Phi}^*$.

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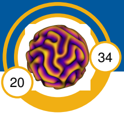
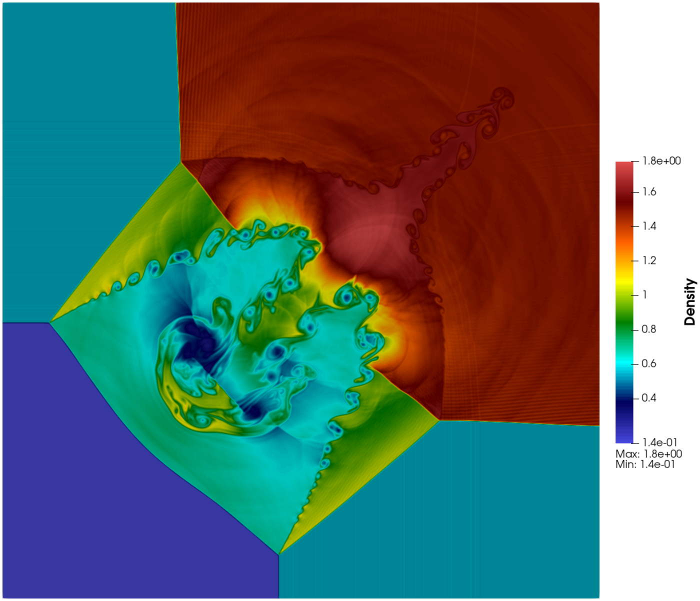
Specific transformations
- Decompose $\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\Big|_{\widetilde{\mathbf{U}}} = \mathbf{R}\mathbf{\Lambda}\mathbf{L}$, set $\mathbf{\Phi} = \mathbf{L}$ and $\mathbf{\Phi}^{-1} = \mathbf{R}$
  - These are characteristic variables (direction dependent!)
- Set $\mathbf{\Phi} = \frac{\partial \mathbf{V}}{\partial \mathbf{U}}\Big|_{\widetilde{\mathbf{U}}}$ and $\mathbf{\Phi}^{-1} = \frac{\partial \mathbf{U}}{\partial \mathbf{V}}\Big|_{\mathbf{V}(\widetilde{\mathbf{U}})}$
  - We've dubbed these *linearized primitive* variables

2D Riemann problem configuration 3

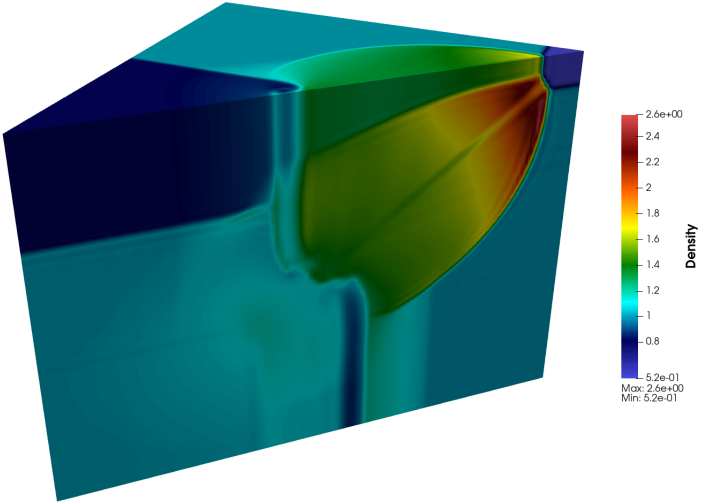
1024×1024, Radius 2, $\ell = 24\Delta$





3D Riemann problem configuration 1

$128 \times 128 \times 128$, Radius 2, $\ell = 24\Delta$



Positivity Preservation
When WENO fails

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- Only recourse is to mix in a first-order correction

Applying corrections

Replace Riemann states as $\mathbf{U}^* \leftarrow \mathbf{U}_{ctr} + \theta\left(\mathbf{U}^* - \mathbf{U}_{ctr}\right)$

- $\theta \in [0, 1]$, $\theta = 1$ for no correction
- Need to find largest θ that gives a valid state
- Must use the same θ for *all* Riemann states on a cell
- Trivial to make density valid, trickier for pressure
  - Ultimately θ will be a root of a quadratic with messy coefficients
- Set bounds on density and pressure using Balsara's self-adjusting limiter

Overview of RHS evaluation

Method-of-lines integrator

Evaluate all spatial terms on current state

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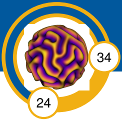
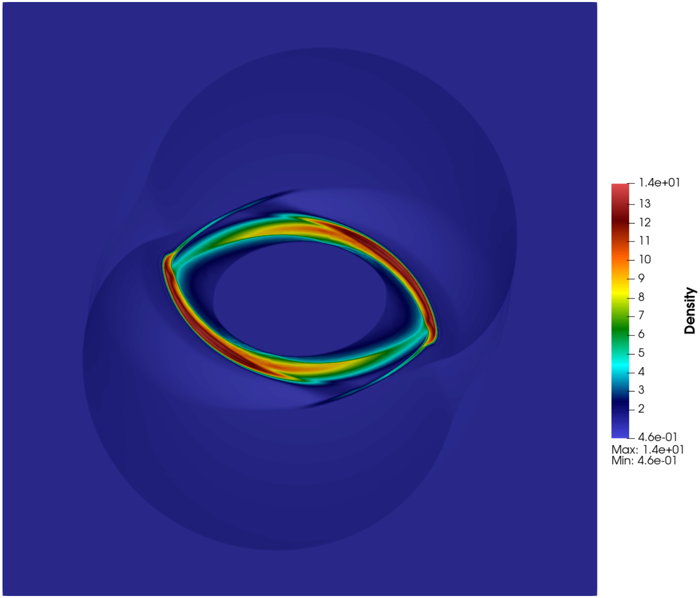
MHD Rotor

1024×1024, Radius 2, $\ell = 24\Delta$





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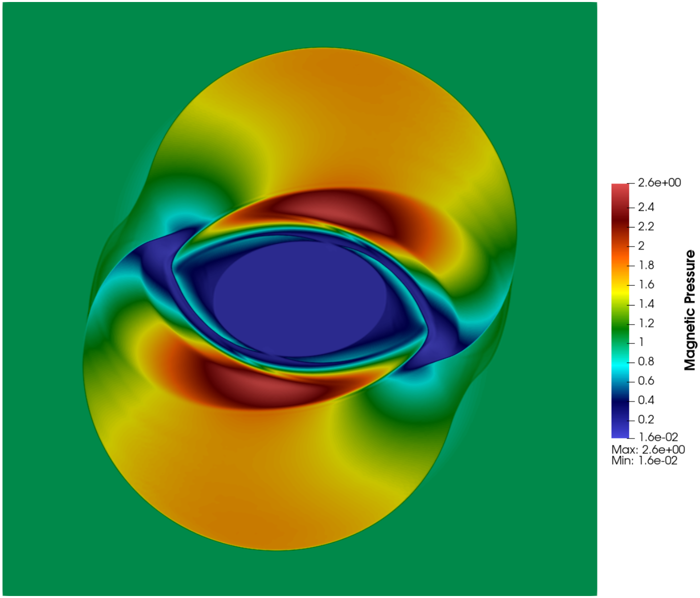
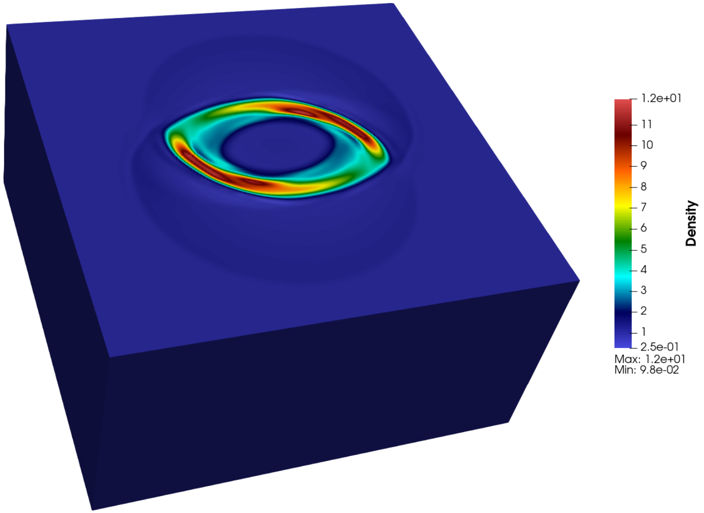


MHD Rotor

$192 \times 192 \times 192$, Radius 2, $\ell = 24\Delta$



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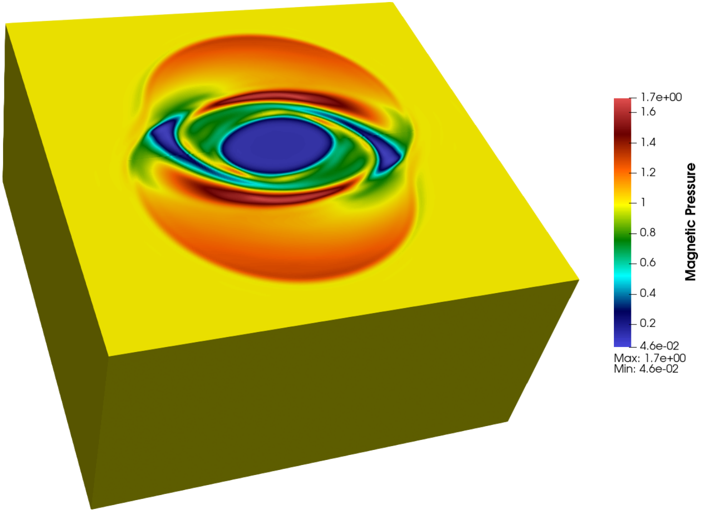

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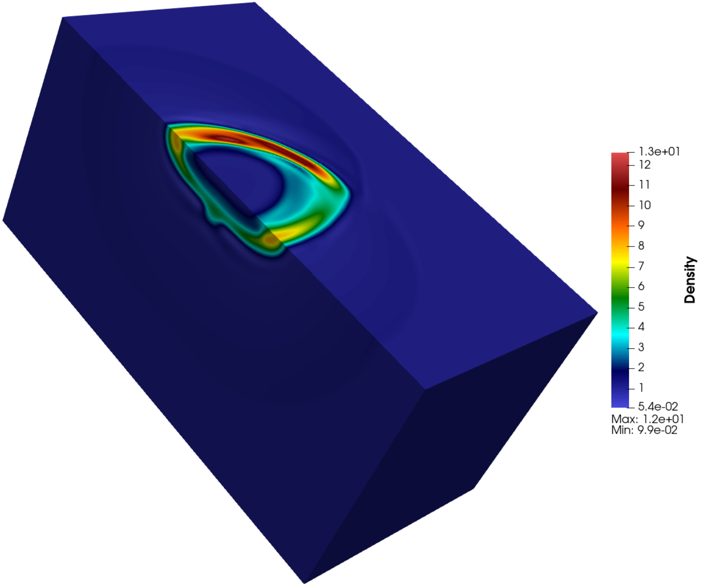

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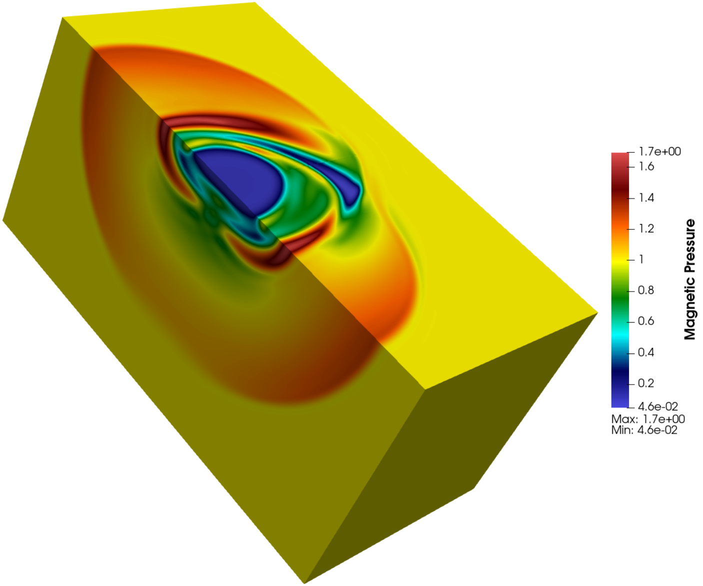
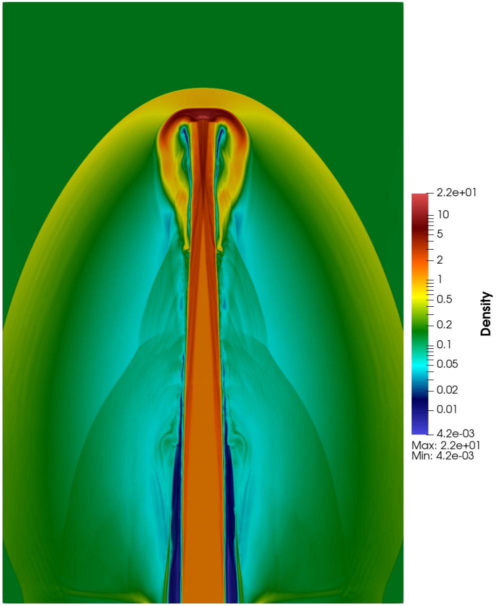


Magnetized Astrophysical Jet

1024×1536, Radius 2, $\ell = 24\Delta$



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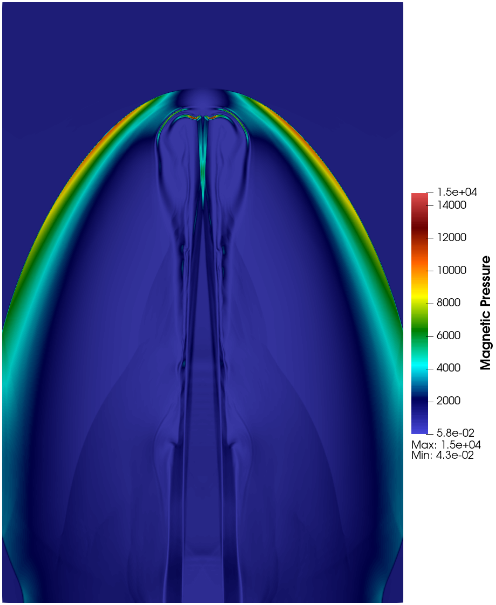
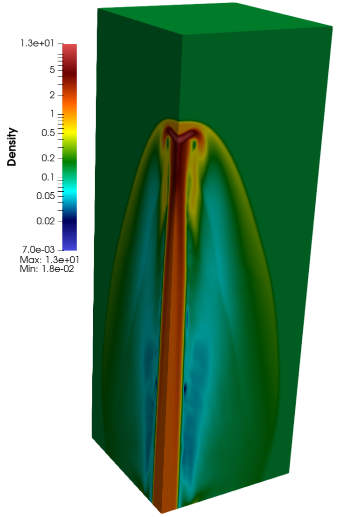
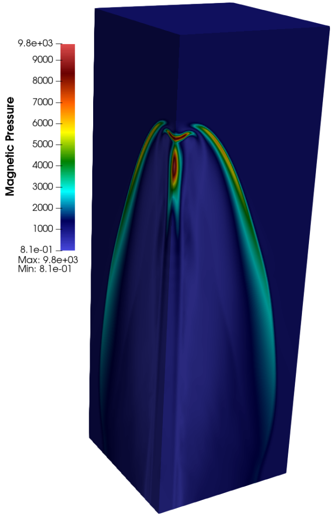


Magnetized Astrophysical Jet

$128 \times 384 \times 128$, Radius 2, $\ell = 24\Delta$





Expensive parts of RHS evaluation

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- Nonlinear reconstruction is only really needed near shocks
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Large time derivatives of pressure indicate shocks

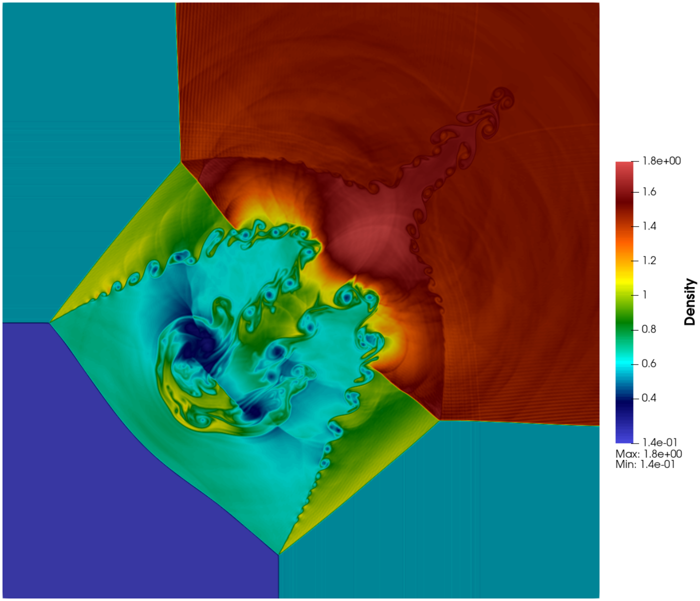
Only do WENO if:

$$\frac{\left|p^{(n)} - p^{(n-1)}\right|}{\min\left\{p^{(n)}, p^{(n-1)}\right\}} > C\Delta t,$$

for some C, typically $C \approx 10$. (Adapted from Alina Chertok's LSI)

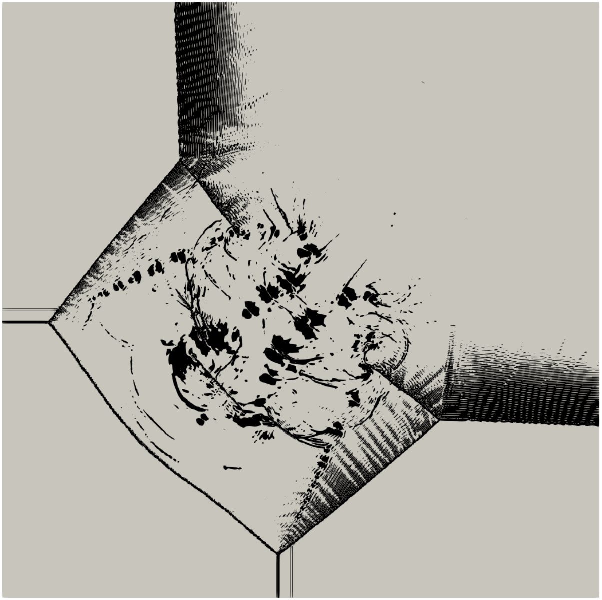
2D Riemann problem configuration 3

1024×1024, Radius 2, $\ell = 24\Delta$



2D Riemann problem configuration 3

WENO Map for $C = 10$



Accelerators and Heterogeneous Computing

The vast majority of the work to be done is the same for each cell.
$\Rightarrow$ Huge amounts of data parallelism.

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- Cache misses and memory latency are huge problem for all hardware choices
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- Supporting a variety of hardware is headache

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```
for (int i=0; i<nX; i++) {
  for (int j=0; j<nY; j++) {
    uNew(i,j) = f(uOld(i,j),
                  uOld(i+1,j),uOld(i-1,j),
                  uOld(i,j+1),uOld(i,j-1));
  }
}
```

Kokkos

Performance portability

- Data layout and parallel hardware are tightly coupled
- Provide a simple abstraction for launching parallel work
- Provide data structures that conform to the chosen architecture
  - These also need to account for *where* data is stored

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```
auto rng = MDRange<Cuda,Rank<2>>({0,0},{nX,nY});
parallel_for(``Kernel Name'',rng,
  KOKKOS_LAMBDA (const int i,const int j) {
    uNew(i,j) = f(uOld(i,j),
                   uOld(i+1,j),uOld(i-1,j),
                   uOld(i,j+1),uOld(i,j-1));
  });
```

Distributed memory parallelism

Communication points

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Final thoughts

Conclusion

- Kernel based reconstruction is very flexible
  - Easy to go straight from averages to point values
- There are many choices for reconstruction variables
- Effective positivity preservation is reasonably straightforward
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Next steps

- Evaluate MHD accuracy fully
- Continue on relativistic hydrodynamics
- Investigate HWENO methods
- Extend to AMR
- Incorporate physical viscosity

The isentropic vortex problem

A truly nonlinear benchmark problem

The Euler equations on $[-L,L]^2$ with periodic boundaries and initial condition

$$\begin{pmatrix}\rho\\ u\\ v\\ p\end{pmatrix} = \begin{pmatrix}T^{1/(\gamma-1)}\\ 1-y\omega\\ 1+x\omega\\ T^{\gamma/(\gamma-1)}\end{pmatrix}$$

$$T = 1 - \frac{\gamma-1}{8\gamma\pi^2}e^{1-x^2-y^2}$$

$$\omega = \frac{1}{2\pi}e^{(1-x^2-y^2)/2}$$

recover the initial condition at time $T_f = 2L$

The isentropic vortex problem

$\Omega = [-10, 10]^2$, $\ell = 2$

Grid	L_1 Error	L_1 Order	L_∞ Error	L_∞ Order
		$R = 2$		
50^2	$1.43e-1$	–	$2.29e-2$	–
100^2	$1.49e-2$	**3.27**	$4.49e-3$	**2.35**
200^2	$6.20e-4$	**4.58**	$9.52e-5$	**5.56**
400^2	$2.04e-5$	**4.93**	$3.24e-6$	**4.88**
		$R = 3$		
50^2	$8.37e-2$	–	$1.89e-2$	–
100^2	$2.36e-3$	**5.15**	$3.13e-4$	**5.91**
200^2	$3.18e-5$	**6.21**	$1.06e-5$	**4.89**
400^2	$2.72e-7$	**6.87**	$9.58e-8$	**6.78**
		$R = 4$		
50^2	$4.42e-2$	–	$9.31e-3$	–
100^2	$6.94e-4$	**5.99**	$2.34e-4$	**5.31**
200^2	$2.53e-6$	**8.10**	$1.11e-6$	**7.72**
400^2	$5.70e-9$	**8.80**	$2.30e-9$	**8.92**

Systems of interest

Special relativistic Euler equations

$$\mathbf{U} = \begin{pmatrix} D \\ S_x \\ S_y \\ S_z \\ \tau \end{pmatrix} = \begin{pmatrix} \rho W \\ \rho h W^2 u \\ \rho h W^2 v \\ \rho h W^2 w \\ \rho W (hW - 1) - p \end{pmatrix} \qquad \mathbf{F} = \begin{pmatrix} Du \\ S_x u + p \\ S_x v \\ S_x w \\ S_x - Du \end{pmatrix},$$

where,

$$\begin{aligned} W &= (1 - \mathbf{v} \cdot \mathbf{v})^{-1/2} \\ h &= 1 + \gamma e \\ e &= \frac{p}{(\gamma - 1)\rho} \end{aligned}$$

Stabilizing large ℓ

We need to compute

$$\mathbf{z}^T = \mathbf{w}^T \mathbf{C}^{(-1)},$$

where $\mathbf{C}$ and $\mathbf{w}$ both depend on ℓ.

- Large values of ℓ tend to give more accurate interpolants
- Large values of ℓ give horribly conditioned linear systems

Stable evaluation of prediction vectors

Consider $\epsilon = \ell^{-1}$, and allow complex ϵ. Then

- $z_i(\ell^{-1}) = \mathbf{w}^T \mathbf{C}^{(-1)} \mathbf{e}_i$ is holomorphic apart from isolated poles
- Evaluate $z_i(\ell^{-1})$ on a circle in $\mathbb{C}$ where computation is stable
- Back out an approximate Laurent expansion of $z_i(\ell^{-1})$
- Evaluate that Laurent expansion at the real $\epsilon = \ell^{-1}$ of interest