Gaussian processes for high order finite volume methods

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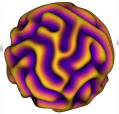

Goal

Solve the compressible Euler equations (2D)

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

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

accurately and robustly

Finite volume considerations

- Handles shocks naturally
- Discretely conservative
- Agreeable with AMR
- Non-trivial to take beyond 2^{nd} order accuracy

Finite volume formulation

Integrate over $D_{i,j} = \left[x_{i-1/2}, x_{i+1/2}\right] \times \left[y_{j-1/2}, y_{j+1/2}\right]$ and normalize

$$\int\limits_{D_{i,j}} \frac{\partial \mathbf{U}}{\partial t} dV = -\int\limits_{D_{i,j}} \nabla \cdot \underline{\underline{\mathbf{F}}} dV$$

$$\frac{\partial \langle \mathbf{U} \rangle_{i,j}}{\partial t} = -\frac{1}{\Delta x \Delta y} \int\limits_{\partial D_{i,j}} \underline{\underline{\mathbf{F}}} \cdot \hat{\mathbf{n}} dS$$

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

where

$$\langle h \rangle_{i,j} = \frac{1}{\Delta x \Delta y} \int\limits_{D_{i,j}} h dV \qquad \langle h \rangle_{i\pm 1/2,j} = \frac{1}{\Delta y} \int\limits_{y_{j-1/2}}^{y_{j+1/2}} h(x_{i\pm 1/2}, y) dy$$

Accuracy requirement

Numerical flux

$$\langle \mathbf{F} \rangle_{i\pm 1/2,j} = \frac{1}{\Delta y} \int\limits_{y_{j-1/2}}^{y_{j+1/2}} \mathbf{F}(\mathbf{U}(x_{i\pm 1/2}, y))dy$$

$$\approx \frac{1}{\Delta y} \int\limits_{y_{j-1/2}}^{y_{j+1/2}} \hat{\mathbf{F}}\left(\mathbf{U}^{-}_{i\pm 1/2}(y), \mathbf{U}^{+}_{i\pm 1/2}(y)\right) dy$$

Two barriers to high order in multiple dimensions

- Integral must be done accurately
- Numerical flux is defined *pointwise*, thus need accurate *pointwise* values of $\mathbf{U}^{\pm}_{i\pm 1/2}$

Polynomial reconstruction

Given the stencil $\{\langle \mathbf{U}\rangle_{i-r,j},\cdots,\langle \mathbf{U}\rangle_{i,j},\cdots,\langle \mathbf{U}\rangle_{i+r,j}\}$, there is a unique polynomial $\mathbf{Q}(x)$ of degree $p=2r$ satisfying:

$$\frac{1}{\Delta x}\int_{x_{i+s-1/2}}^{x_{i+s+1/2}} \mathbf{Q}(x)dx = \langle \mathbf{U}\rangle_{i+s,j}, \quad s=-r,\dots,r$$

which yields the approximation

$$\langle \mathbf{U}\rangle_{i\pm 1/2,j} = \mathbf{Q}(x_{i\pm 1/2}) + \mathcal{O}(\Delta x^{p+1})$$

Just plug it in, what could go wrong?

First note

$$\mathbf{U}(x_{i\pm 1/2}, y_j) = \langle \mathbf{U}\rangle_{i\pm 1/2,j} + \mathcal{O}(\Delta x^{p+1}) + \mathcal{O}(\Delta y^2),$$

and

Special cases

If $\mathbf{F}(\mathbf{U}) = \mathbf{A}\mathbf{U}$ then,

$$\begin{aligned}
\langle \mathbf{F} \rangle_{i\pm 1/2,j} &= \frac{1}{\Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} \mathbf{A}\mathbf{U}\left(x_{i\pm 1/2}, y\right) dy \\
&= \mathbf{A}\langle \mathbf{U} \rangle_{i\pm 1/2,j} \\
&= \mathbf{A}\mathbf{Q}(x_{i\pm 1/2}) + \mathcal{O}(\Delta x^{p+1}).
\end{aligned}$$

Linear benchmarks

Consider the Euler equations on $[0,1]^2$ with periodic boundaries and the initial condition:

$$\begin{pmatrix} \rho \\ u \\ v \\ p \end{pmatrix} = \begin{pmatrix} 1 + e^{-50(x+y-2)^2} + e^{-50(x+y-1)^2} + e^{-50(x+y)^2} \\ 1 \\ 1 \\ 1/\gamma \end{pmatrix}.$$

run to a final time of $T = 1/2$.

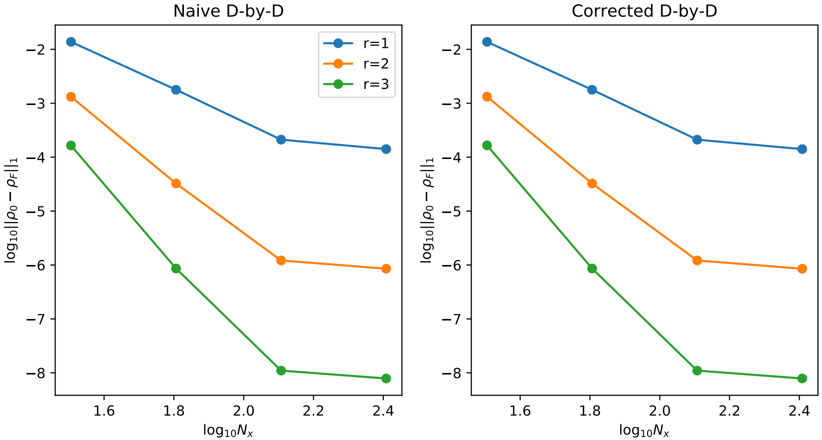

Figure: Modifications to retain non-linear accuracy don't matter for this benchmark.

Experimental convergence rates

	L_1	L_∞	L_1	L_∞
$r = 1$	2.29	2.32	2.29	2.32
$r = 2$	3.65	3.75	3.65	3.75
$r = 3$	4.94	5.08	4,94	5.08

Routes to high order

Expensive, but intuitive method

- Use multidimensional reconstruction to point values on faces directly
- Approximate flux integral with a Gauss rule
- $\Rightarrow$ Need multiple point values on each face, multiple calls to Riemann solver

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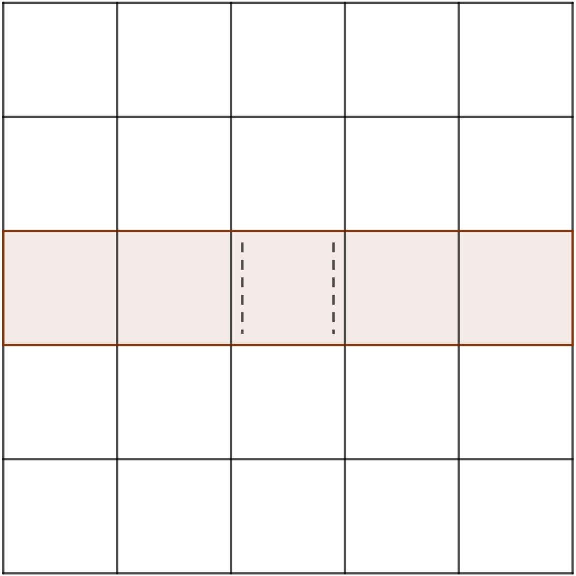
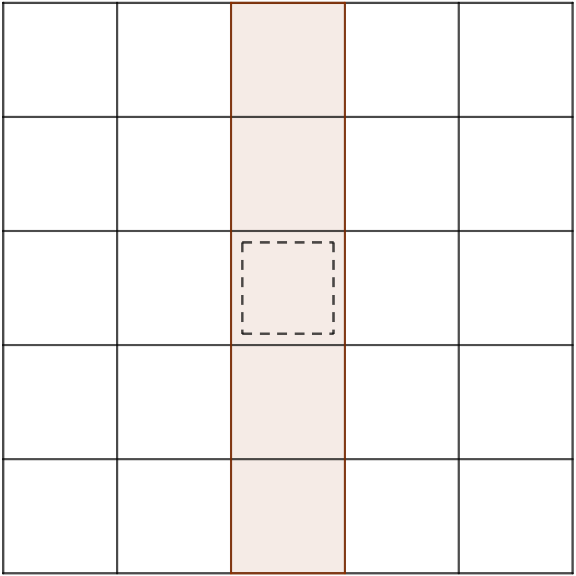
Modified dimension-by-dimension

- Use 1D stencils to get accurate face-averaged states
- Reconstruct along faces to get accurate face-centered states
- Call Riemann solver once per interface
- Reconstruct face-average fluxes from face-centered fluxes

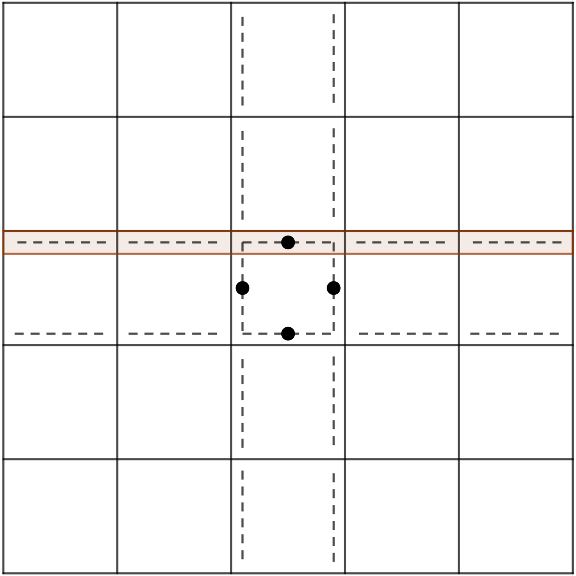
Modified dimension-by-dimension

Diagramatically





Modified dimension-by-dimension
Diagramatically



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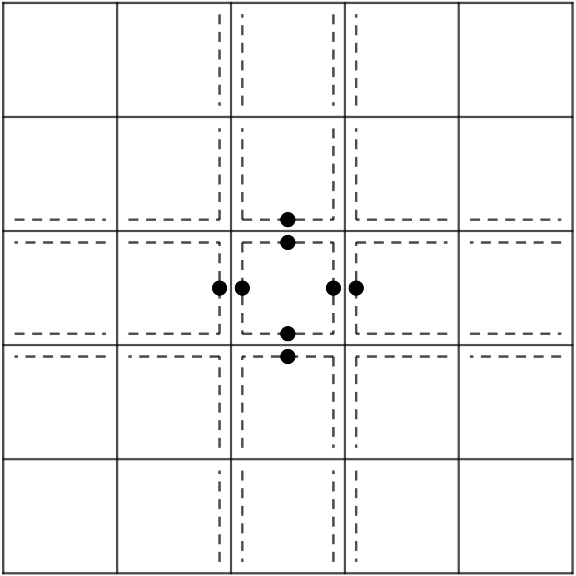

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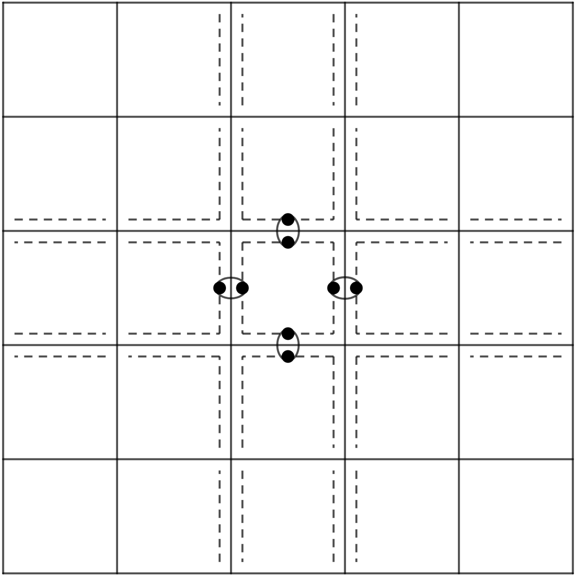

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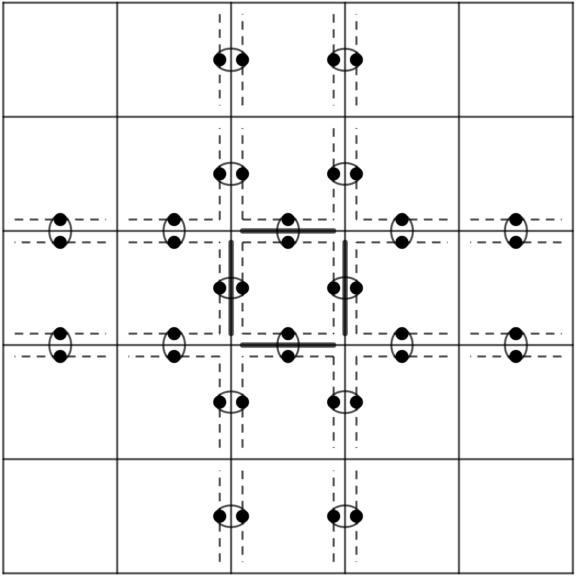

Why Gaussian processes?

They generalize very well

- Dimension agnostic
- Order agnostic
- (Un)Structured grid agnostic
- Flexible stencil choices
- Directly incorporate problem physics

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Downsides of Gaussian processes (subjective)

- Ill-conditioning problems
- Less intuitive
- Almost too flexible, lot's of choices to investigate
- The buzzword factor is high

Definition

For a domain D, a Gaussian process is given by a distribution over a function space:

$$f(\mathbf{x}) \sim \mathcal{N}\left(\mathbf{0}, K(\mathbf{x}, \mathbf{x}'; \ell)\right),$$

such that for $\mathbf{y} \in D$, $f(\mathbf{y})$ belongs to a multivariate normal distribution:

$$f(\mathbf{y}) \sim \mathcal{N}\left(\mathbf{0}, \mathbf{K}\right)$$
$$\mathbf{K}_{ij} = K(y_i, y_j; \ell),$$

for some correlation (kernel) function K. Defined here as:

$$K(\mathbf{x}, \mathbf{y}; \ell) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2\ell^2}}$$

Gaussian process interpolation

Posterior distribution

The Gaussian process conditioned on some given data, $f(\mathbf{y}_k) = \mathbf{q}$ at some locations $\mathbf{y}_k \in D$, goes as:

$$\left(f(\mathbf{x})\,|\,f(\mathbf{y}) = \mathbf{q}\right) \sim \mathcal{N}\left(\mu_{\mathbf{y}}, K_{\mathbf{y}}\right)$$
$$\mu_{\mathbf{y}} = K\left(\mathbf{x}, \mathbf{y}; \ell\right) \mathbf{K}^{-1}\mathbf{q}$$
$$K_y = K(\mathbf{x}, \mathbf{x}'; \ell) - K(\mathbf{x}, \mathbf{y}; \ell)\mathbf{K}^{-1}K(\mathbf{y}, \mathbf{x}'; \ell).$$

All functions described by this process interpolate the data.

Gaussian process interpolation

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All functions described by this process interpolate the data.

Mean is the most likely interpolant

To predict $f(\mathbf{x}^*)$ for some $\mathbf{x}^* \in D$ evaluate the mean: $f(\mathbf{x}^*) \approx \mu_{\mathbf{y}}(\mathbf{x}^*)$. Compactly:

$$\begin{aligned} f(\mathbf{x}^*) &\approx K\left(\mathbf{x}^*, \mathbf{y}; \ell\right)\mathbf{K}^{-1}\mathbf{q} \\ &\approx \mathbf{w}_*^{\mathrm{T}}\mathbf{q}\end{aligned}$$

Dealing with cell/face averaged values

We want to use GP to convert between data types. Define correlation matrix to match input data,

$$\mathbf{C}_{ij} = \frac{1}{||D_i||\,||D_j||} \int_{D_i} \int_{D_j} K(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$

and sample respecting the correlation between data types,

$$\mathbf{T}_i = \frac{1}{||D_i||} \int_{D_i} K(\mathbf{x}^*, \mathbf{x}) d\mathbf{x}$$

to find

$$f(\mathbf{x}^*) \approx \mathbf{T}^{\mathrm{T}} \mathbf{C}^{-1} \mathbf{g}$$

for known cell/face averages, $\mathbf{g}$

Converting point values back to average values

Very similar to interpolation, but with appropriate sample vector.
Defining:

$$\mathbf{K}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\mathbf{T}_i = \frac{1}{||D_i||} \int\limits_{D_*} K(\mathbf{x}_i, \mathbf{x}) d\mathbf{x}$$

we find

$$\langle f(\mathbf{x}) \rangle_i \approx \mathbf{T}^{\mathrm{T}} \mathbf{K}^{-1} \mathbf{q}$$

from known point values $\mathbf{q}$

The isentropic vortex problem

A truly nonlinear benchmark problem

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

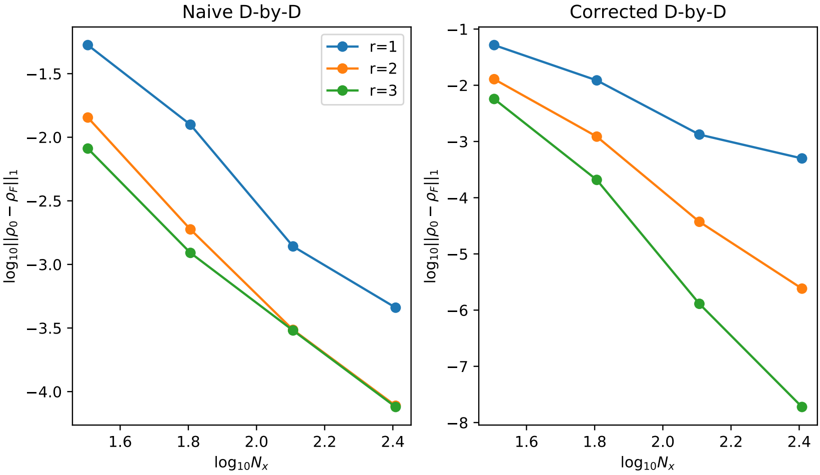
$$\begin{pmatrix} \rho \\ u \\ v \\ p \end{pmatrix} = \begin{pmatrix} T^{1/(\gamma-1)} \\ 1 - y\omega \\ 1 + x\omega \\ T^{\gamma/(\gamma-1)} \end{pmatrix}$$

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

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

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

The isentropic vortex problem



Experimental convergence rates

	L_1	L_∞	L_1	L_∞
$r=1$	2.38	2.22	2.33	2.21
$r=2$	2.53	2.95	4.22	4.08
$r=3$	2.23	2.37	6.19	6.16

Dealing with shocks – GP-WENO

Nonlinear GP reconstruction

The reconstruction presented is linear, i.e.

$$\langle \mathbf{U} \rangle_{i\pm 1/2,j} = \sum_{s=-r}^{r} w_k^{\pm} \langle \mathbf{U} \rangle_{i+s,j}$$

which is hopeless near discontinuities (Godunov)

WENO (weighted essentially non-oscillatory) methods

Idea: Break full stencil into substencils, reconstruct on each separately, use a weighted combination of these reconstructions

$$\langle \mathbf{U} \rangle_{i\pm 1/2,j;k} = \sum_{s=k-r-1}^{k-1} \langle \mathbf{U} \rangle_{i+s,j}$$

$$\langle \mathbf{U} \rangle_{i\pm 1/2,j;k} = \sum \omega_k^{\pm} \langle \mathbf{U} \rangle_{i\pm 1/2,j;k}$$

Optimal weights

For *smooth* data, $\omega_k^\pm$ should reduce to some optimal weights such that

$$\sum_{s=-r}^{r} w_s^\pm \langle \mathbf{U} \rangle_{i+s,j} \approx \sum \gamma_k^\pm \langle \mathbf{U} \rangle_{i\pm 1/2,j;k}$$

which can be found by solving the least squares problem (e.g. $r = 2$)

$$\begin{pmatrix} w_{1,1} & 0 & 0 \\ w_{2,1} & w_{1,2} & 0 \\ w_{3,1} & w_{2,2} & w_{1,3} \\ 0 & w_{3,2} & w_{2,3} \\ 0 & 0 & w_{3,3} \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{pmatrix}$$

Smoothness indicators

Following Jiang and Shu, we can define

$$\omega_k = \frac{\widetilde{\omega}_k}{\sum \widetilde{\omega}_s} \qquad \widetilde{\omega}_k = \frac{\gamma_k}{(\epsilon + \beta_k)^p}$$

where β_k measures the smoothness of the data on the k^{th} sub-stencil

Likelihood measures smoothness

A GP with a SE kernel is good at representing smooth functions, thus the log-likelihood

$$\log L_k = -\frac{1}{2}\left(\log|\mathbf{K}_k| + \mathbf{q}^{\mathrm{T}}\mathbf{K}_k^{-1}\mathbf{q} + 2\log(2\pi)\right)$$

indicates how smooth the k^{th} sub-stencil is. Choosing

$$\beta_k = \mathbf{q}^{\mathrm{T}}\mathbf{K}_k^{-1}\mathbf{q}$$

works well for equispaced grids

Notes on (GP) WENO

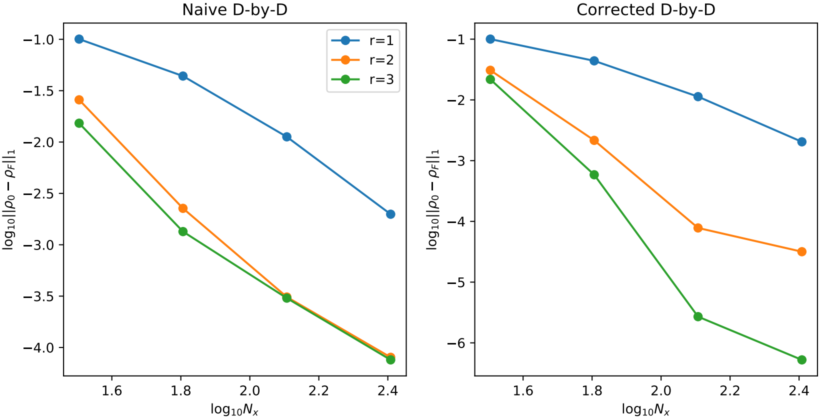
General WENO

- Transform to characteristic variables first
- Componentwise limiting works well enough, lower dissipation
- Lots of non-linear weights other than WENO-JS

GP-WENO

- Note $\mathbf{K}_k$ instead of $\mathbf{C}_k$ in formula for β_k
- Could use completely different types of stencils
- No need to derive new expressions for each order

The isentropic vortex – WENO active



Experimental convergence rates

	L_1	L_∞	L_1	L_∞
$r=1$	1.90	1.65	1.88	1.66
$r=2$	2.79	3.12	3.46	3.98
$r=3$	2.51	3.29	5.38	5.80

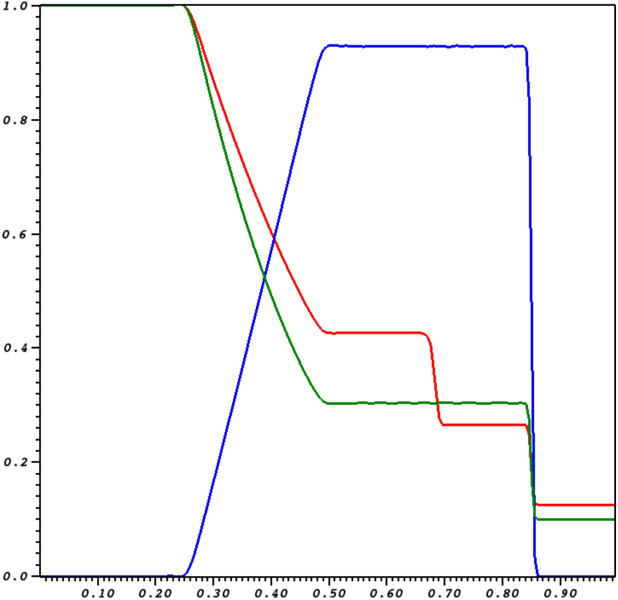
Sod shock tube

The standard Riemann problem

Euler equations on $[0,1]$ with inflow/outflow boundaries and initial condition

$$\begin{pmatrix}\rho\\ u\\ p\end{pmatrix} = \begin{cases}\begin{pmatrix}1 & 0 & 1\end{pmatrix}^{\mathrm{T}}, & x < 0.5\\ \begin{pmatrix}0.125 & 0 & 0.1\end{pmatrix}^{\mathrm{T}}, & x > 0.5\end{cases}$$

Sod shock tube



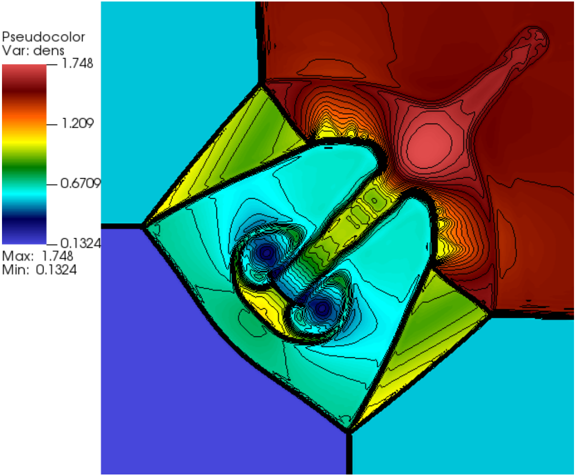
2D Riemann problem configuration 3

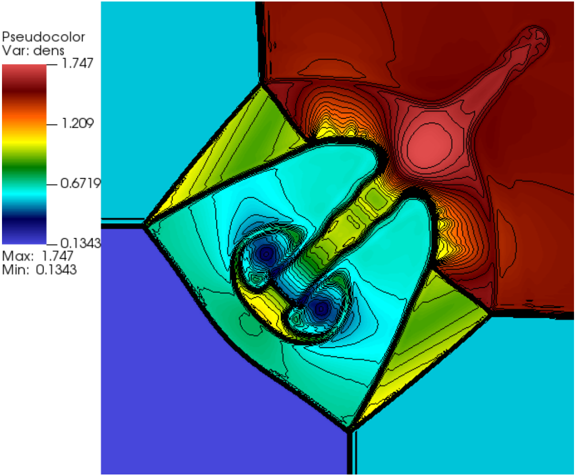
Euler equations on $[0,1]^2$ with outflow boundaries and initial condition

$$\begin{pmatrix}\rho_1\\u_1\\v_1\\p_1\end{pmatrix}=\begin{pmatrix}0.5323\\1.206\\0\\0.3\end{pmatrix}\qquad\begin{pmatrix}\rho_2\\u_2\\v_2\\p_2\end{pmatrix}=\begin{pmatrix}1.5\\0\\0\\1.5\end{pmatrix}$$

$$\begin{pmatrix}\rho_3\\u_3\\v_3\\p_3\end{pmatrix}=\begin{pmatrix}0.138\\1.206\\1.206\\0.029\end{pmatrix}\qquad\begin{pmatrix}\rho_4\\u_4\\v_4\\p_4\end{pmatrix}=\begin{pmatrix}0.5323\\0\\1.206\\0.3\end{pmatrix}$$

Without flux correction

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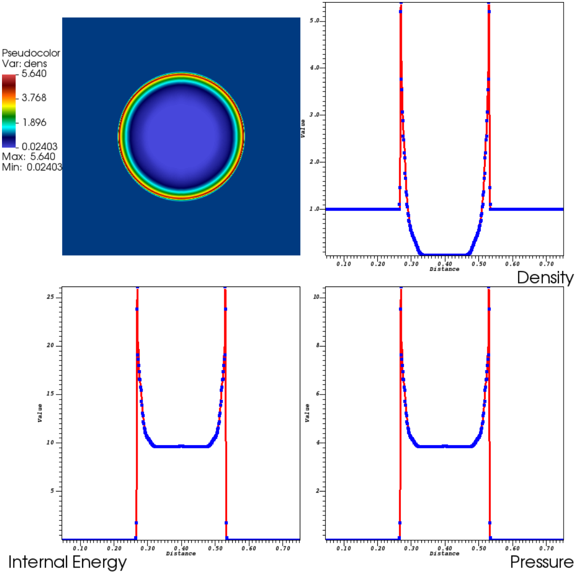
Min: 0.1343

Sedov blast problem



Final thoughts

Conclusion

- Naive use of 1D stencils in 2D yields 2^{nd} nonlinear accuracy
- A cheap modification to the reconstruction recovers accuracy (Buchmuller and Helzel)
- Gaussian process reconstruction is super flexible, same formulas for many orders
- GP yields simple, effective, smoothness indicators for WENO

Next steps

- Appropriate limiting for flux reconstruction
- Time stepping without RK
- Ideal MHD – Divergence free GP methods
- 3D problems

The isentropic vortex problem

L_∞