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Sandia National Laboratories

High-Order Implicit-Explicit Multi-Block Method for Hyperbolic PDEs

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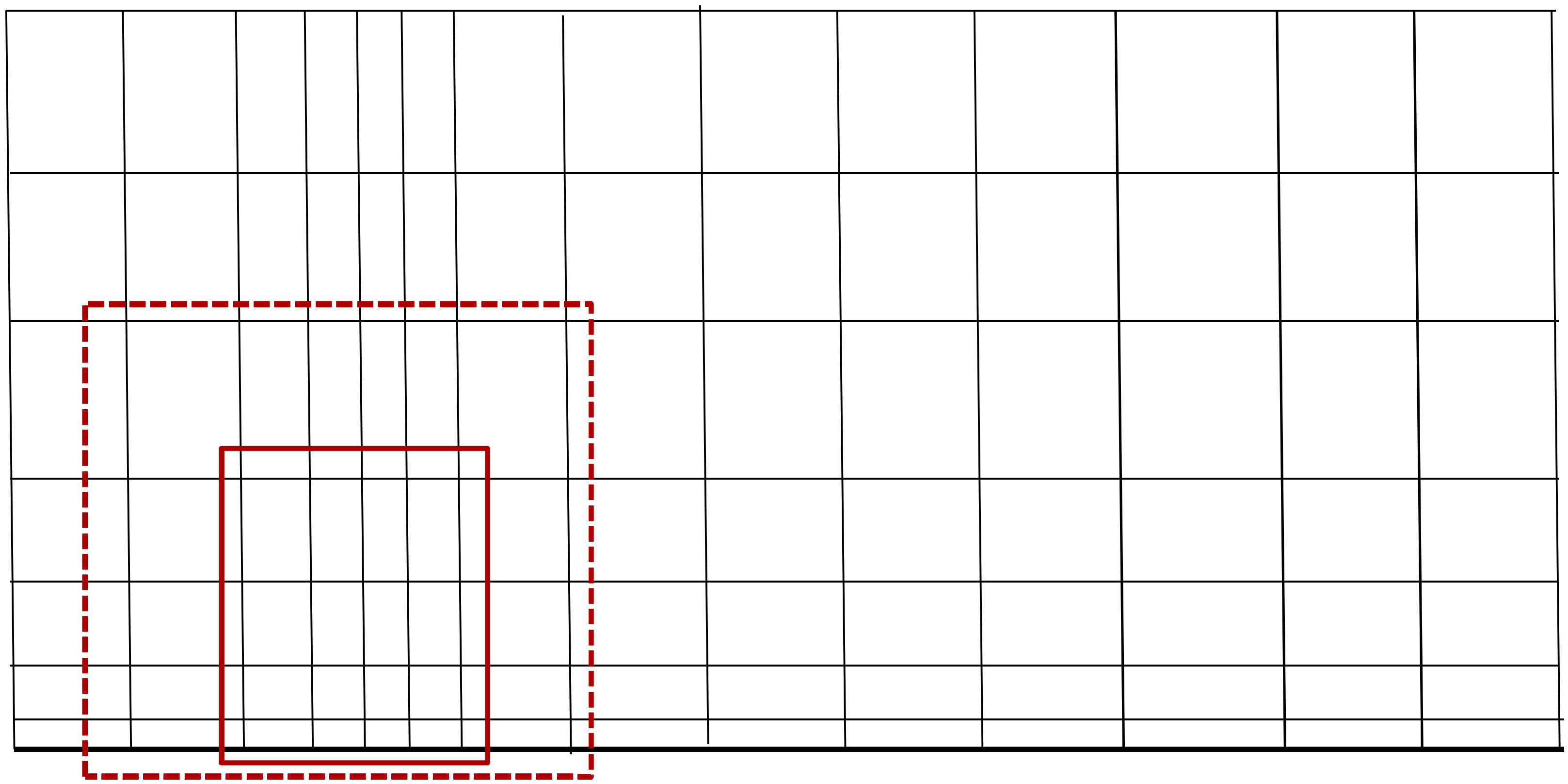
An Exploratory Effort

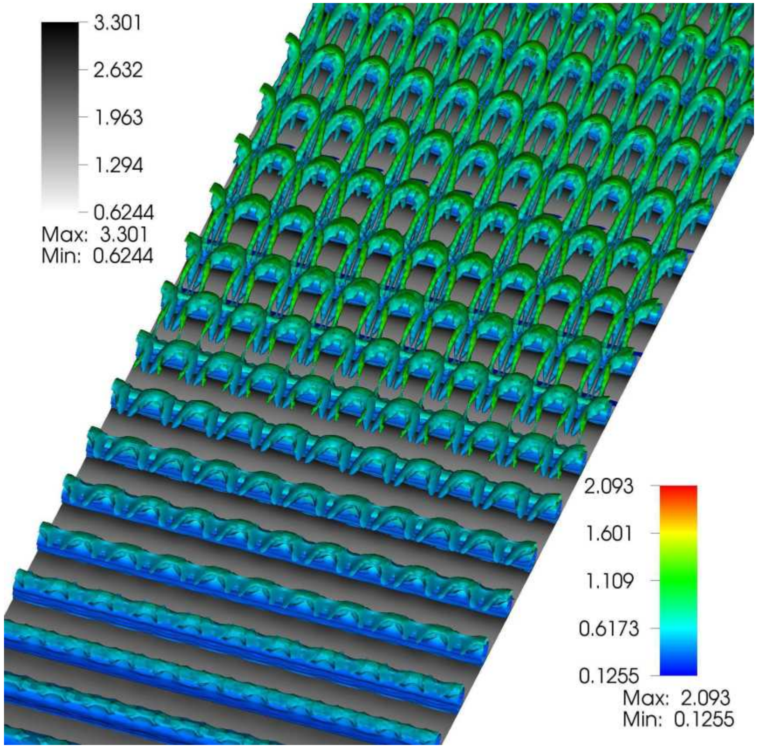


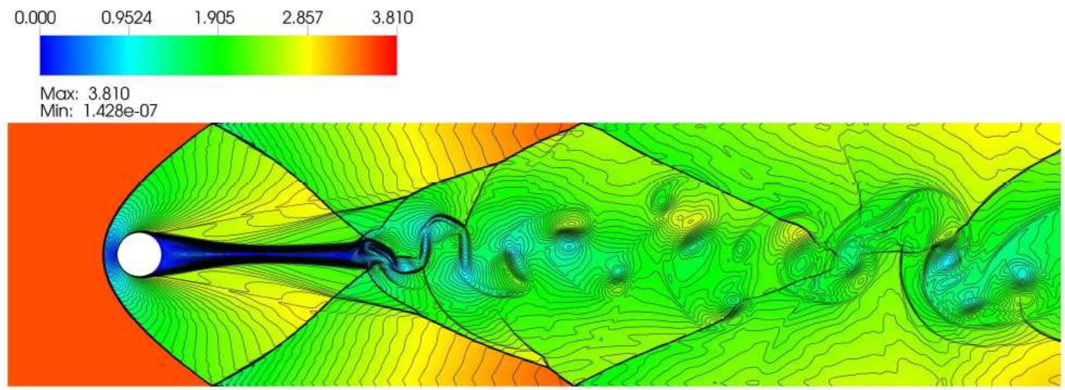
Use domain decomposition-like method to partition domains to isolate stiffness

Leverage IMEX generality to couple domains

Problems of Interest

This work focuses on model problems: $u_t + f(u)_x = \epsilon(Cu_x)_x$





Target Problems in DNS, LES, and Hybrid RANS/LES

- Time dependent problems
- Target maximum CFL or diffusion limit (DFL) ~ 10
- Need to accurately capture resolved vortex time scale

Spatial Discretization

$$\boldsymbol{u}_t + \mathrm{D}_x \boldsymbol{f}(\boldsymbol{u}) = \mathrm{D}_x^2(C)\boldsymbol{u} + \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{u_b})$$

Summation-by-parts finite difference method

$$\mathrm{D} = \mathrm{P}^{-1}\mathrm{Q} \qquad \mathrm{D}_{\mathrm{x}}^2(C) = \mathrm{P}^{-1}\left(\mathrm{B}C\mathrm{D} - \mathrm{D}^{\mathrm{T}}\mathrm{P}C\mathrm{D} - \mathrm{R}(C)\right)$$

Formal boundary closure on finite domain

Linearly Stable

High-Order Accurate

Use SAT penalty boundary conditions

IMEX Runge-Kutta Scheme

$$\boldsymbol{u}_t\Big|_t = \mathbf{F}(\boldsymbol{u}(t), t)$$

Additive Runge Kutta

$$\boldsymbol{u}^{(i)} = \boldsymbol{u}^{(n)} + \Delta t \sum_{k=1}^{n_{rk}} \sum_{j=1}^{s} a_{ij}^{(k)}\ \mathbf{F}^k\left(\boldsymbol{u}(t_j), t^{(n)} + c_j \Delta t\right)$$

$$\boldsymbol{u}^{(n+1)} = \boldsymbol{u}^{(n)} + \Delta t \sum_{k=1}^{n_{rk}} \sum_{j=1}^{s} b_j^{(k)}\ \mathbf{F}^k\left(\boldsymbol{u}^{(j)}, t^{(n)} + c_j \Delta t\right)$$

$$\hat{\boldsymbol{u}}^{(n+1)} = \boldsymbol{u}^{(n)} + \Delta t \sum_{k=1}^{n_{rk}} \sum_{j=1}^{s} \hat{b}_j^{(k)}\ \mathbf{F}^k\left(\boldsymbol{u}^{(j)}, t^{(n)} + c_j \Delta t\right)$$

IMEX Runge Kutta

$$c_j^{(IM)} = c_j^{(EX)}$$

$$b_j^{(IM)} = b_j^{(EX)}$$

$$\hat{b}_j^{(IM)} = \hat{b}_j^{(EX)}$$

Implicit uses ESDIRK Runge Kutta
Requires Nonlinear Solve

$$\boldsymbol{u}^{(i)} - \Delta t \mathbf{F}^{IM}\left(\boldsymbol{u}^{(i)}, t^n + c_j \Delta t\right) = \boldsymbol{u}^{(n)} + \Delta t \sum_{k=1}^{2} \sum_{j=1}^{i-1} a_{ij}^{(k)}\ \mathbf{F}^k\left(\boldsymbol{u}(t_j), t^{(n)} + c_j \Delta t\right)$$

Time Step Controller

Maximum CFL for Explicit Runge Kutta schemes may be greater than 1.

Use temporal error estimate:

$$\delta = \|\boldsymbol{u} - \hat{\boldsymbol{u}}\| = C\Delta t^p$$

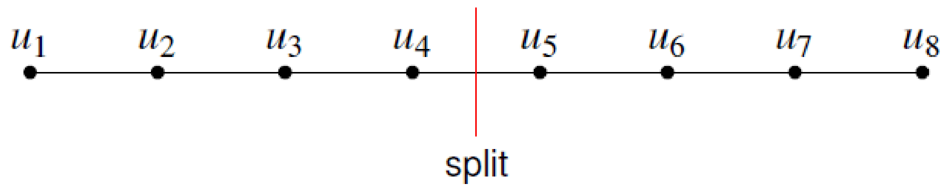
$$\frac{\delta^{(n+1)}}{\delta^{(n)}} = \left(\frac{\Delta t^{(n+1)}}{\Delta t^{(n)}}\right)^p$$

Set allowable time error, $\delta^{(n+1)} = \epsilon$

$$\Delta t^{(n+1)} = \Delta t^{(n)} \left(\frac{\epsilon}{\delta^{(n)}}\right)^{\frac{1}{p}}$$

Works for implicit and explicit.

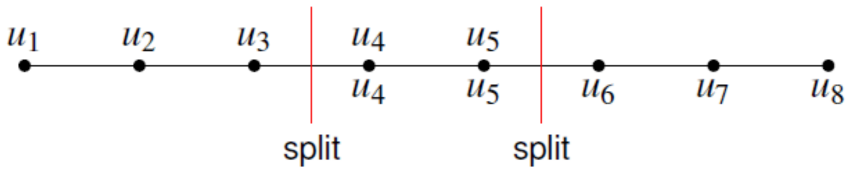
One-Dimensional Domain Partitioning



$$\begin{pmatrix} a_1 & c_1 & & & & & & \\ b_2 & a_2 & c_2 & & & & & \\ & b_3 & a_3 & c_3 & & & & \\ & & b_4 & a_4 & c_4 & & & \\ & & & b_5 & a_5 & c_5 & & \\ & & & & b_6 & a_6 & c_6 & \\ & & & & & b_7 & a_7 & c_7 \\ & & & & & & b_8 & a_8 \end{pmatrix} \cdot \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{pmatrix}$$

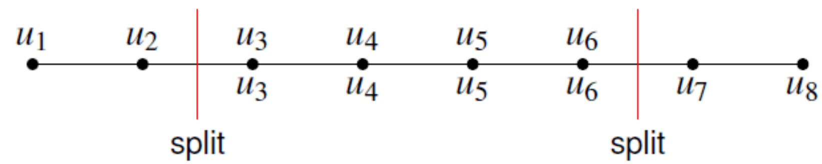
No Overlap

One-Dimensional Domain Partitioning



$$
\begin{pmatrix}
a_1 & c_1 & & & & & & & & \\
b_2 & a_2 & c_2 & & & & & & & \\
 & b_3 & a_3 & c_3 & & & & & & \\
 & & b_4 & a_4 & c_4 & & & & & \\
 & & & b_5 & a_5 & & & c_5 & & \\
 & & b_4 & & & a_4 & c_4 & & & \\
 & & & & & b_5 & a_5 & c_5 & & \\
 & & & & & & b_6 & a_6 & c_6 & \\
 & & & & & & & b_7 & a_7 & c_7 \\
 & & & & & & & & b_8 & a_8
\end{pmatrix}
\cdot
\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{pmatrix}
$$

Overlap = 1



$$
\begin{pmatrix}
a_1 & c_1 & & & & & & & & & & \\
b_2 & a_2 & c_2 & & & & & & & & & \\
 & b_3 & a_3 & c_3 & & & & & & & & \\
 & & b_4 & a_4 & c_4 & & & & & & & \\
 & & & b_5 & a_5 & c_5 & & & & & & \\
 & & & & b_6 & a_6 & & & & & c_6 & \\
 & b_3 & & & & & a_3 & c_3 & & & & \\
 & & & & & & b_4 & a_4 & c_4 & & & \\
 & & & & & & & b_5 & a_5 & c_5 & & \\
 & & & & & & & & b_6 & a_6 & c_6 & \\
 & & & & & & & & & b_7 & a_7 & c_7 \\
 & & & & & & & & & & b_8 & a_8
\end{pmatrix}
\cdot
\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{pmatrix}
$$

Overlap = 2

One-Dimensional Test

$$u_t + f(u)_x = \mu u_{xx}$$

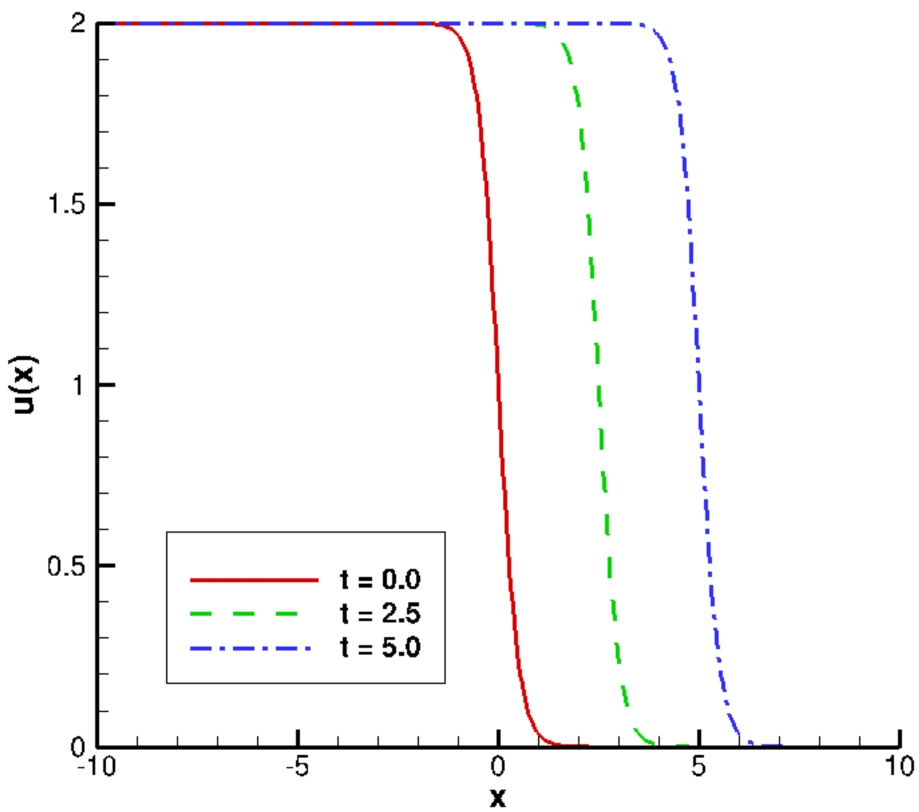
$$\boldsymbol{u}_t + \mathrm{D}_x \boldsymbol{f}(\boldsymbol{u}) = \mu \mathrm{D}_x^2 \boldsymbol{u} + \boldsymbol{g}_b$$

$$f(u) = \frac{u^2}{2}$$

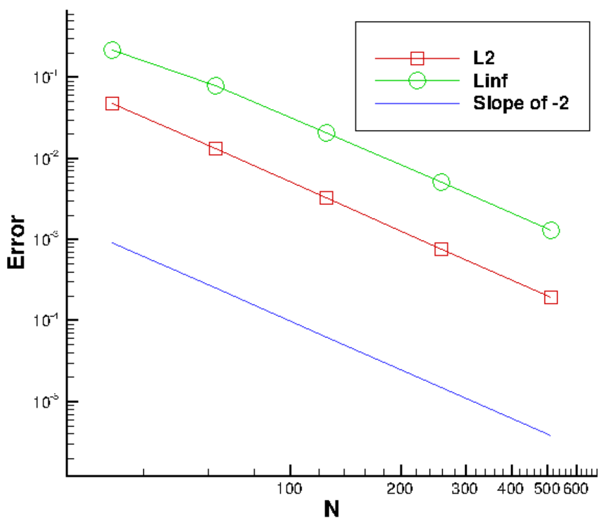
$$v(x,t) = 1 - \tanh\left(\frac{x - t - x0}{2\mu}\right),$$

$$x \in [-10,10], \qquad t \in [0,T]$$

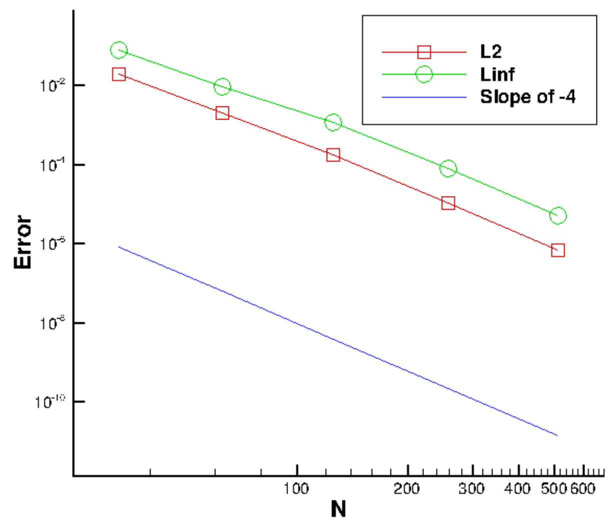
$$\mu = 0.25, \qquad x_0 = 0$$



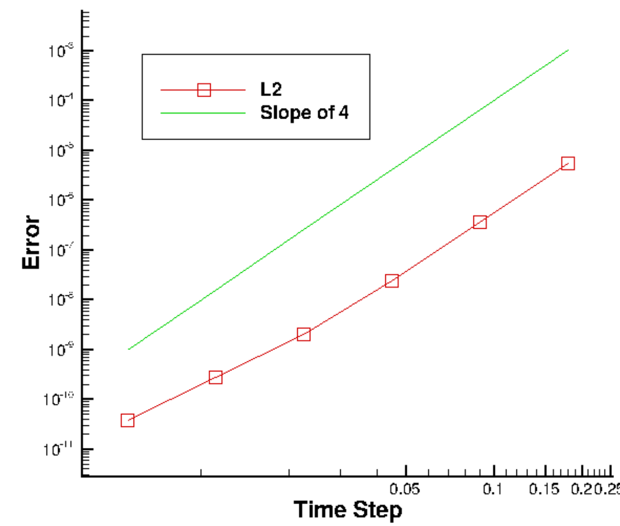
One-Dimensional Test: Accuracy



1-2-1
2nd Order Expected



2-4-2
4th Order Expected



6 Stage IMEX
4th Order Runge Kutta

One-Dimensional Test: Grid Refinement

N = 257

	SBP 1-2-1			SBP 2-4-2		
	CFL	DFL	Factor of Increase	CFL	DFL	Factor of Increase
Fully Explicit	0.64	1.03	1.00	0.46	0.74	1.00
IMEX, overlap = 0	3.60	5.78	5.60	2.49	4.00	5.39
IMEX, overlap = 1	12.85	20.64	20.00	10.20	16.39	22.06
IMEX, overlap = 2	13.78	22.13	21.44	10.25	16.47	22.17
IMEX, overlap = 5	13.90	22.33	21.64	10.25	16.47	22.17
IMEX, overlap = 10	13.90	22.33	21.64	10.25	16.47	22.17

N = 512

	SBP 1-2-1			SBP 2-4-2		
	CFL	DFL	Factor of Increase	CFL	DFL	Factor of Increase
Fully Explicit	0.31	0.98	1.00	0.20	0.66	1.00
IMEX, overlap = 0	1.48	4.75	4.83	1.08	3.44	5.25
IMEX, overlap = 1	12.39	39.65	40.33	9.22	29.49	45.00
IMEX, overlap = 2	12.80	40.96	41.67	9.22	29.49	45.00
IMEX, overlap = 5	12.75	40.80	41.50	9.22	29.49	45.00
IMEX, overlap = 10	12.80	40.96	41.67	9.22	29.49	45.00

N = 1013

	SBP 1-2-1			SBP 2-4-2		
	CFL	DFL	Factor of Increase	CFL	DFL	Factor of Increase
Fully Explicit	0.16	1.03	1.00	0.12	0.77	1.00
IMEX, overlap = 0	0.71	4.49	4.38	0.53	3.34	4.33
IMEX, overlap = 1	8.41	53.23	51.88	7.29	46.18	60.00
IMEX, overlap = 2	10.64	67.34	65.63	7.90	50.03	65.00
IMEX, overlap = 5	10.64	67.34	65.63	7.90	50.03	65.00
IMEX, overlap = 10	10.64	67.34	65.63	7.90	50.03	65.00

One-Dimensional Test: Effect of Viscosity

$\epsilon = 0.0625$

	SBP 1-2-1			SBP 2-4-2		
	CFL	DFL	Factor of Increase	CFL	DFL	Factor of Increase
Fully Explicit	1.20	0.94	1.00	1.00	0.74	1.00
IMEX, overlap = 0	9.88	7.91	8.22	6.71	5.37	6.72
IMEX, overlap = 1	14.03	11.22	11.67	11.21	8.97	11.23
IMEX, overlap = 2	13.93	11.14	11.59	11.11	8.89	11.13
IMEX, overlap = 5	13.77	11.02	11.46	10.91	8.72	10.92
IMEX, overlap = 10	14.08	11.26	11.72	10.96	8.77	10.97

$\epsilon = 0.125$

	SBP 1-2-1			SBP 2-4-2		
	CFL	DFL	Factor of Increase	CFL	DFL	Factor of Increase
Fully Explicit	0.61	0.98	1.00	0.46	0.74	1.00
IMEX, overlap = 0	3.48	5.57	5.67	2.46	3.93	5.33
IMEX, overlap = 1	13.21	21.14	21.50	10.19	16.30	22.11
IMEX, overlap = 2	13.77	22.04	22.42	10.24	16.38	22.22
IMEX, overlap = 5	13.88	22.20	22.58	10.24	16.38	22.22
IMEX, overlap = 10	13.93	22.28	22.67	10.24	16.38	22.22

$\epsilon = 0.25$

	SBP 1-2-1			SBP 2-4-2		
	CFL	DFL	Factor of Increase	CFL	DFL	Factor of Increase
Fully Explicit	0.31	0.98	1.00	0.20	0.66	1.00
IMEX, overlap = 0	1.48	4.75	4.83	1.08	3.44	5.25
IMEX, overlap = 1	12.39	39.65	40.33	9.22	29.49	45.00
IMEX, overlap = 2	12.80	40.96	41.67	9.22	29.49	45.00
IMEX, overlap = 5	12.75	40.80	41.50	9.22	29.49	45.00
IMEX, overlap = 10	12.80	40.96	41.67	9.22	29.49	45.00

Two-Dimensional Domain Partitioning

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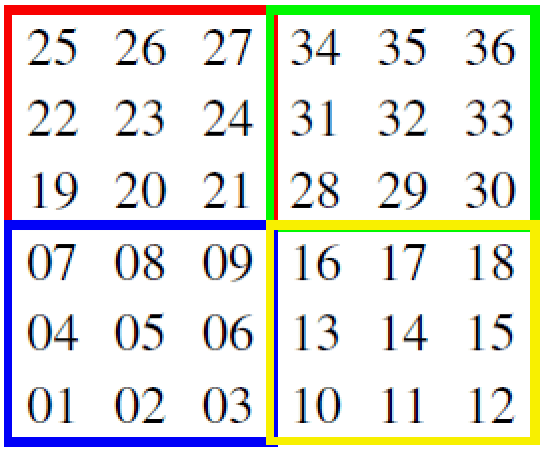
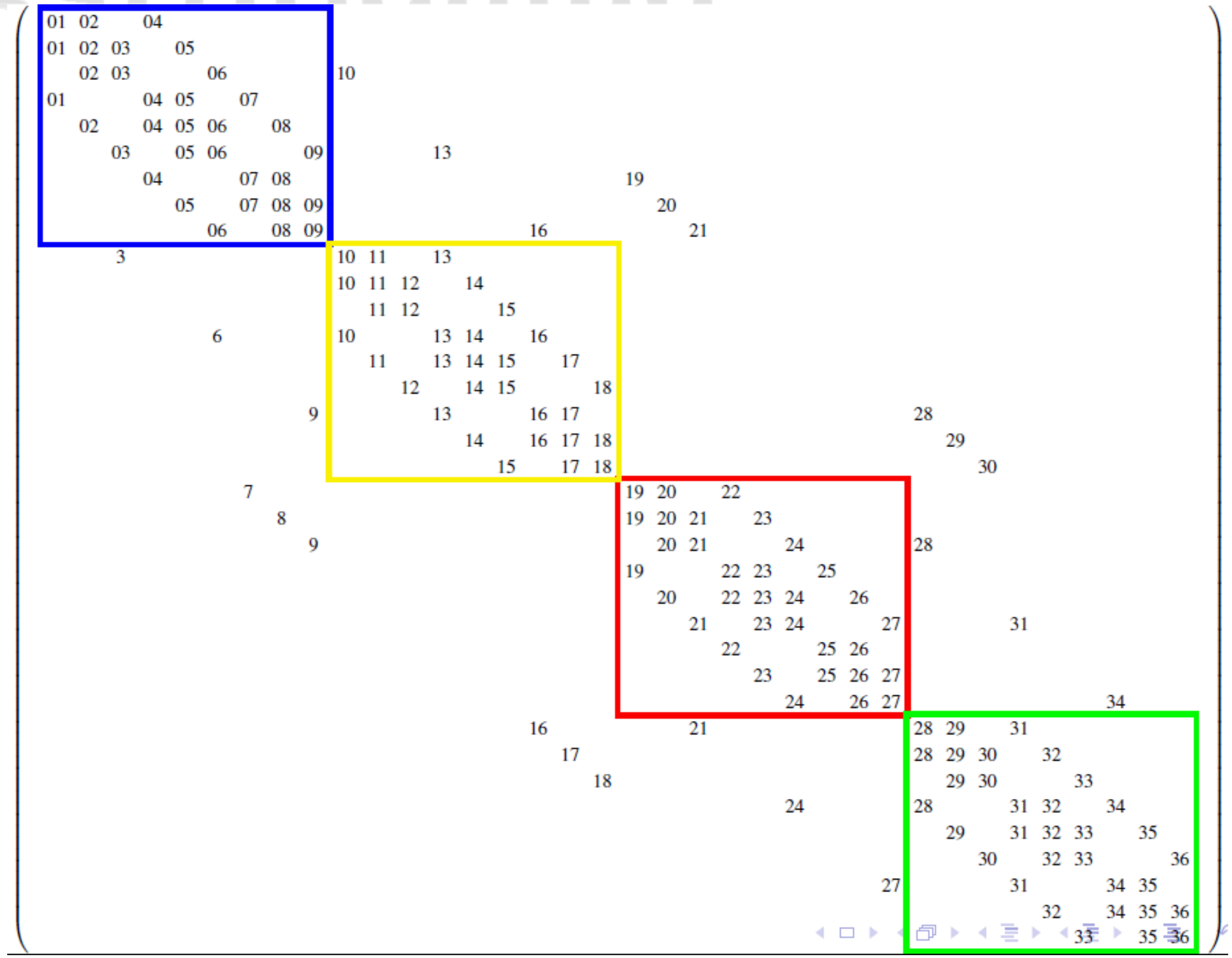


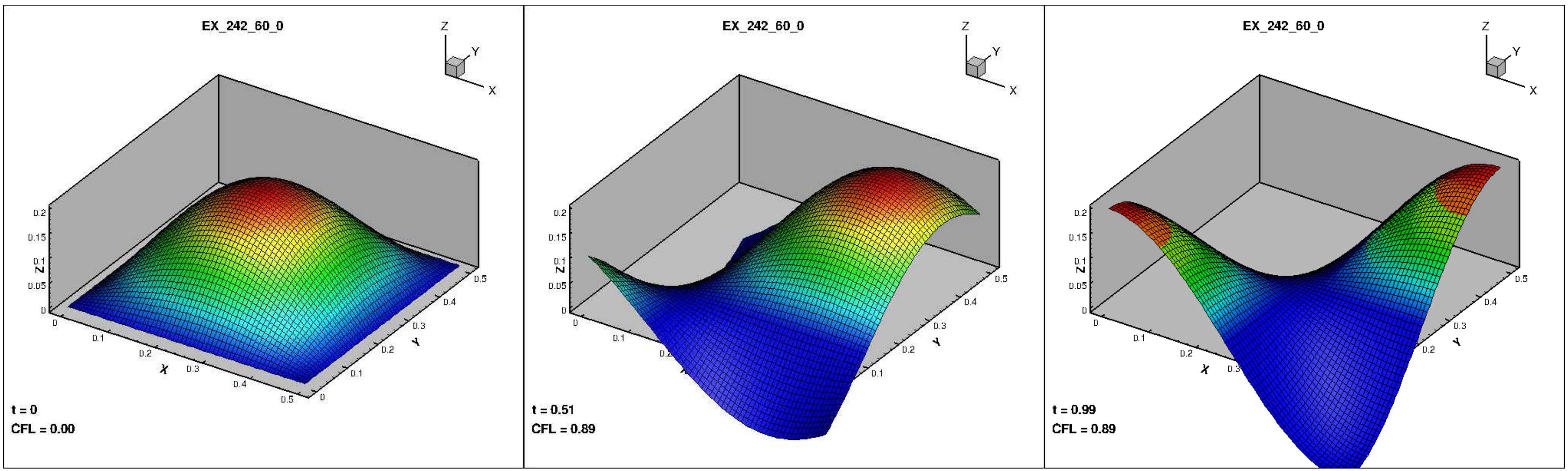


Apply reordering to increase matrix density

Two-Dimensional Test

$$u_t + Au_x + Bu_y = 0 \qquad \boldsymbol{u}_t + A\mathrm{D}_x\boldsymbol{u} + B\mathrm{D}_y\boldsymbol{u} = \boldsymbol{g}_b$$

$$v(x,y,t) = \sin\big(2\pi(x - At)\big)\sin\big(2\pi(y - Bt)\big),$$
$$x \in [0,0.5], y \in [0,0.5], t \in [0,T]$$



Two-Dimensional Test: Accuracy

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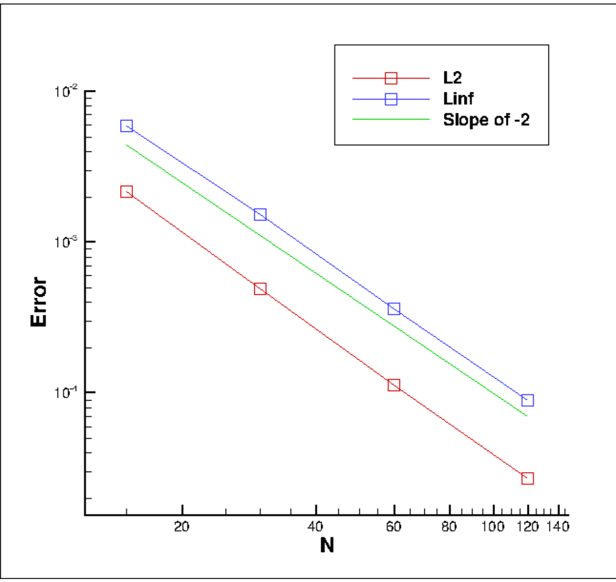
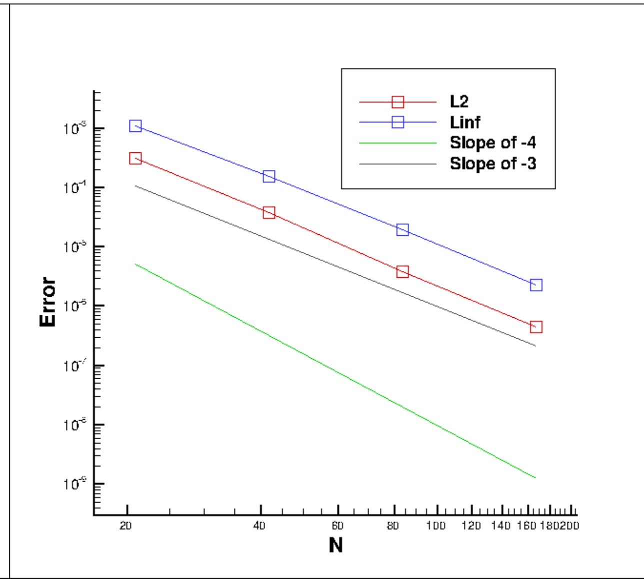
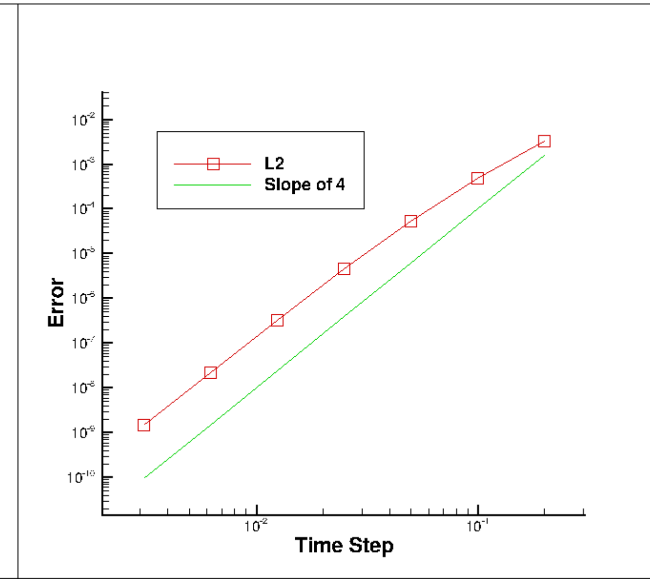


1-2-1
2^{nd} Order Expected



2-4-2
4^{th} Order Expected



6 Stage IMEX
4^{th} Order Runge Kutta

Two-Dimensional Test: Grid Refinement

N_x=30, N_y=30

	SBP 1-2-1		SBP 2-4-2	
	CFL	Factor of Increase	CFL	Factor of Increase
Fully Explicit	2.0	1.0	1.5	1.0
IMEX, overlap = 0	-	-	-	-
IMEX, overlap = 1	7.5	3.8	-	-
IMEX, overlap = 2	7.4	3.7	-	-
IMEX, overlap = 3	7.7	3.9	6.6	4.4
IMEX, overlap = 4	8.0	4.0	7.0	4.7

N_x=90, N_y=90

	SBP 1-2-1		SBP 2-4-2	
	CFL	Factor of Increase	CFL	Factor of Increase
Fully Explicit	2.0	1.0	1.5	1.0
IMEX, overlap = 6	-	-	-	-
IMEX, overlap = 7	15.7	7.9	-	-
IMEX, overlap = 8	15.8	7.9	-	-
IMEX, overlap = 9	16.0	8.0	14.3	9.5
IMEX, overlap = 10	16.1	8.1	14.4	9.6

N_x=60, N_y=60

	SBP 1-2-1		SBP 2-4-2	
	CFL	Factor of Increase	CFL	Factor of Increase
Fully Explicit	2.0	1.0	1.5	1.0
IMEX, overlap = 3	-	-	-	-
IMEX, overlap = 4	11.6	5.8	-	-
IMEX, overlap = 5	12.0	6.0	-	-
IMEX, overlap = 6	12.2	6.1	10.6	7.1
IMEX, overlap = 7	-	-	11.0	7.3
IMEX, overlap = 8	12.6	6.3	11.2	7.5
IMEX, overlap = 9	12.7	6.4	11.2	7.5

N_x=120, N_y=120

	SBP 1-2-1		SBP 2-4-2	
	CFL	Factor of Increase	CFL	Factor of Increase
Fully Explicit	2.0	1.0	1.5	1.0
IMEX, overlap = 6	-	-	-	-
IMEX, overlap = 7	18.5	9.3	-	-
IMEX, overlap = 8	-	-	-	-
IMEX, overlap = 9	19.0	9.5	-	-
IMEX, overlap = 10	19.2	9.6	-	-
IMEX, overlap = 11	19.5	9.8	17.2	11.5
IMEX, overlap = 12	19.5	9.8	17.7	11.8

Shortcomings and Future Work

- Need to compare simulation times
  - Problems examined were uniform grids
  - Need problems with scale separation
  - Stiffness needs to be isolated
  - Requires efficient linear solver for block size
- Need to implement in compressible Euler and Navier-Stokes
- Need to extend to 3D
- Evaluate other discretization types

Acknowledgement

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