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Optimal Runge-Kutta Schemes for High-order Spatial and Temporal Discretizations

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June 23, 2015

Outline

- **Introduction**
- **Governing Equations**
  – Spatial Discretizations
  – Temporal Discretizations
- **Von Neumann Analysis (VNA)**
- **Computational Results**
  – One-dimensional Wave
  – Three-dimensional Vortex
- **Conclusions and Future Work**

Introduction

- High-order in space is now commonplace
- High-order in time… not so much…
- Is this sufficient? Is high-order in time needed?
- ***Limiting Fact:*** There are no *A*-stable backward-difference formula (BDF) methods with > *2nd* -order accuracy
- Thus, multistage methods, like Runge-Kutta (RK) methods, must be used for *3rd*- and higher-order
- Explicit RK methods are not amenable to stiff problems

Objective: **To find optimal diagonally-implicit Runge-Kutta time integrators for use with high-order spatial discretizations**

Governing Equations

- **Dual Time Stepping:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H} \qquad \mathbf{Q} = [\rho \quad \rho u_i \quad \rho e_0]^T$$

$$\mathbf{F}_i = [\rho u_i \quad \rho u_i u_j + p\delta_{ij} \quad u_i \rho h_0]^T \text{ where } h_0 = e_0 + \frac{p}{\rho}$$

- **Quasi-linear Form:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \underline{\mathbf{A}}\frac{\partial \mathbf{Q}}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H} \qquad \underline{\mathbf{A}} = \frac{\partial \mathbf{F}_i}{\partial \mathbf{Q}} = \underline{\mathbf{M \Lambda M}}^{-1}$$

$$\underline{\mathbf{\Lambda}} = diag\left\{u_i + c, u_i, u_i - c\right\}$$

- **Residual Form:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}_s(\mathbf{Q}) = 0 \quad where \quad \mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$

Spatial Discretizations

- **Central Differences with added artificial dissipation**
- **Central differences:**

$$\left.\frac{\partial \Upsilon_j}{\partial x_i}\right|_{II} = \frac{\Upsilon_{j+1} - \Upsilon_{j-1}}{2\Delta x_i}$$

$$\left.\frac{\partial \Upsilon_j}{\partial x_i}\right|_{IV} = \frac{-\Upsilon_{j+2} + 8\Upsilon_{j+1} - 8\Upsilon_{j-1} + \Upsilon_{j-2}}{12\Delta x_i}$$

$$\left.\frac{\partial \Upsilon_j}{\partial x_i}\right|_{VI} = \frac{\Upsilon_{j+3} - 9\Upsilon_{j+2} + 45\Upsilon_{j+1} - 45\Upsilon_{j-1} + 9\Upsilon_{j-2} - \Upsilon_{j-3}}{60\Delta x_i}$$

where Υ could be $\mathbf{F}_i$ or $\mathbf{Q}$ depending on the form of the equations

- **Scalar artificial dissipation:**

$$\mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \varepsilon_\eta \parallel \lambda \parallel \frac{\partial^\eta \mathbf{Q}}{\partial x_i^\eta} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$

where η is even and one more than the order of accuracy

$$\parallel \lambda \parallel = |u_i| + c \qquad \varepsilon_{II} = \frac{\Delta x_i}{2}, \quad \varepsilon_{IV} = -\frac{\Delta x_i^3}{12}, \quad \varepsilon_{VI} = \frac{\Delta x_i^5}{60}.$$

Temporal Discretizations

- **Runge-Kutta Methods:**

$$
\begin{array}{c|cccccc}
c_1 & a_{11} & a_{12} & a_{13} & \cdots & a_{1(s-1)} & a_{1s} \\
c_2 & a_{21} & a_{22} & a_{23} & \cdots & a_{2(s-1)} & a_{2s} \\
c_3 & a_{31} & a_{32} & a_{33} & \cdots & a_{3(s-1)} & a_{3s} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
c_{s-1} & a_{(s-1)1} & a_{(s-1)2} & a_{(s-1)3} & \cdots & a_{(s-1)(s-1)} & a_{(s-1)s} \\
c_s & a_{s1} & a_{s2} & a_s3 & \cdots & a_{s(s-1)} & a_{ss} \\
\hline
 & b_1 & b_2 & b_3 & \cdots & b_{s-1} & b_s \\
 & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_{s-1} & \hat{b}_s
\end{array}
$$

$$t^k = t^n + c_k \Delta t \qquad \mathbf{Q}^k = \mathbf{Q}^n - \Delta t \sum_{j=1}^{s} a_{kj} \mathbf{R}_s^j(\mathbf{Q}^j) \qquad k = 1, 2, \ldots, s$$

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n - \Delta t \sum_{j=1}^{s} b_j \mathbf{R}_s^j(\mathbf{Q}^j) \qquad \hat{\mathbf{Q}}^{n+1} = \mathbf{Q}^n - \Delta t \sum_{j=1}^{s} \hat{b}_j \mathbf{R}_s^j(\mathbf{Q}^j)$$

$$\epsilon^{n+1} = \mathbf{Q}^{n+1} - \hat{\mathbf{Q}}^{n+1}$$

ESDIRK Methods

- **E**xplicit first stage **S**ingly-**D**iagonally **I**mplicit **R**unge-**K**utta
  - Stiffly accurate
  - Second-order stage accuracy
  - FSAL – **F**irst is the **S**ame **A**s **L**ast

$$
\begin{array}{c|cccccc}
c_1 = 0 & 0 & 0 & 0 & \dots & 0 & 0 \\
c_2 & a_{21} & \lambda & 0 & \dots & 0 & 0 \\
c_3 & a_{31} & a_{32} & \lambda & \dots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
c_{s-1} & a_{(s-1)1} & a_{(s-1)2} & a_{(s-1)3} & \dots & \lambda & 0 \\
c_s = 1 & b_1 & b_2 & b_3 & \dots & b_{s-1} & \lambda \\
\hline
 & b_1 & b_2 & b_3 & \dots & b_{s-1} & \lambda \\
 & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \dots & \hat{b}_{s-1} & \hat{b}_s
\end{array}
$$

ESDIRK3 and 4

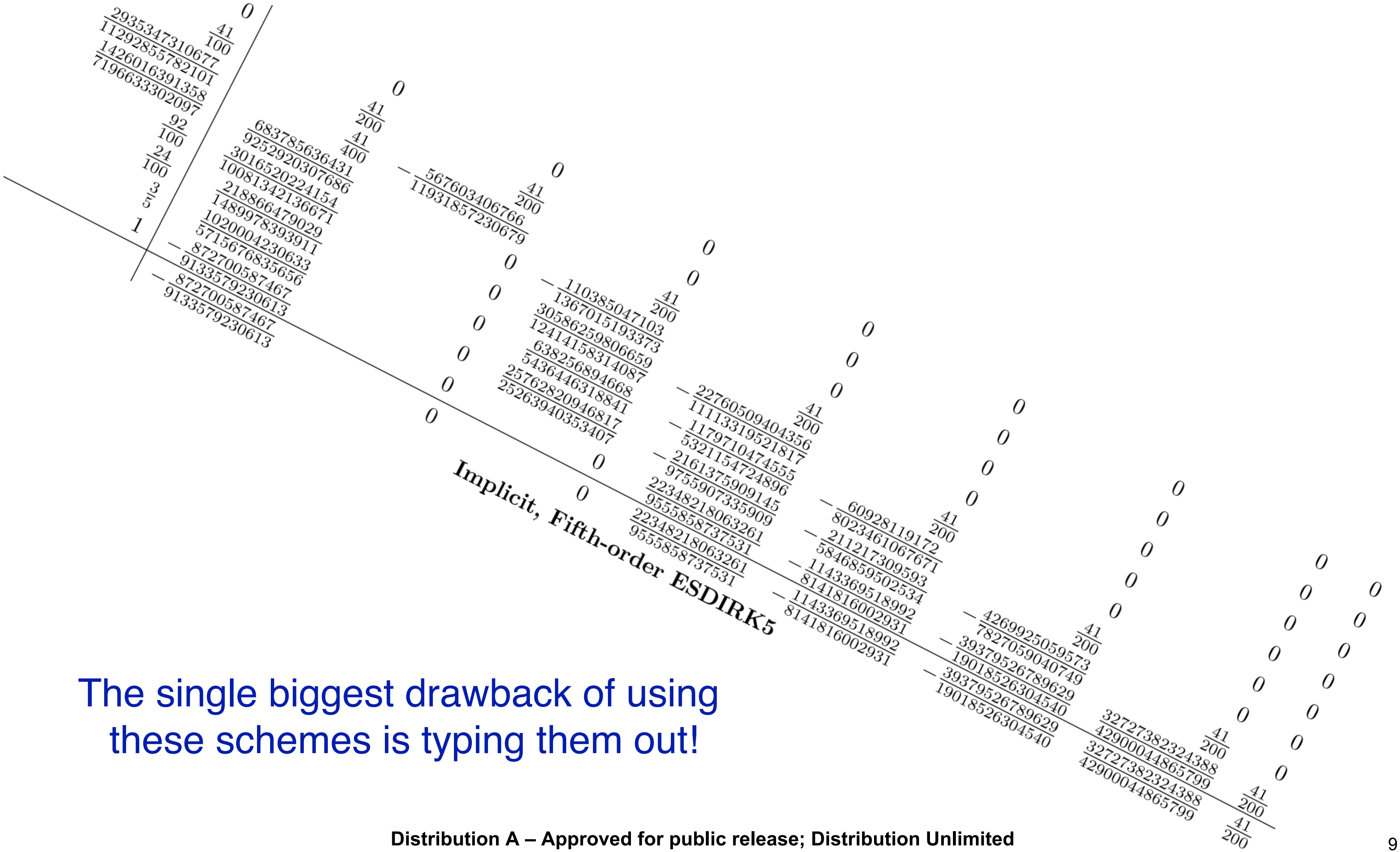
$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
\frac{1767732205903}{2027836641118} & \frac{1767732205903}{4055673282236} & \frac{1767732205903}{4055673282236} & 0 & 0 \\
\frac{3}{5} & \frac{2746238789719}{10658868560708} & -\frac{640167445237}{6845629431997} & \frac{1767732205903}{4055673282236} & 0 \\
1 & \frac{1471266399579}{7840856788654} & -\frac{4482444167858}{7529755066697} & \frac{11266239266428}{11593286722821} & \frac{1767732205903}{4055673282236} \\
\hline
 & \frac{1471266399579}{7840856788654} & -\frac{4482444167858}{7529755066697} & \frac{11266239266428}{11593286722821} & \frac{1767732205903}{4055673282236}
\end{array}
$$

Implicit, Third-order ESDIRK3

$$
\begin{array}{c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 \\
\frac{83}{250} & \frac{8611}{62500} & -\frac{1743}{31250} & \frac{1}{4} & 0 & 0 & 0 \\
\frac{31}{50} & \frac{5012029}{34652500} & -\frac{654441}{2922500} & \frac{174375}{388108} & \frac{1}{4} & 0 & 0 \\
\frac{17}{20} & \frac{15267082809}{155376265600} & -\frac{71443401}{120774400} & \frac{730878875}{902184768} & \frac{2285395}{8070912} & \frac{1}{4} & 0 \\
1 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} \\
\hline
 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4}
\end{array}
$$

Implicit, Fourth-order ESDIRK4

ESDIRK5

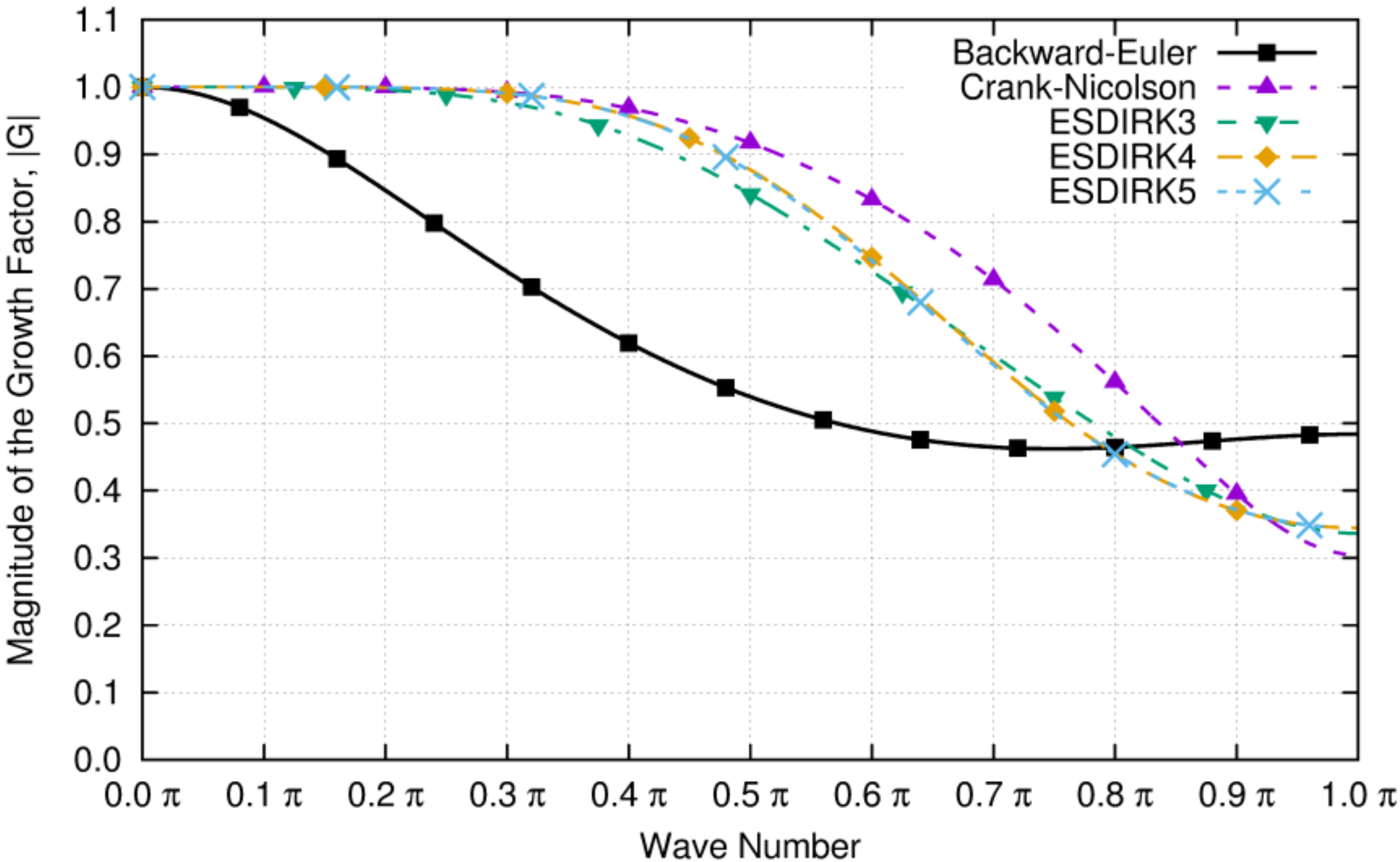


The single biggest drawback of using these schemes is typing them out!

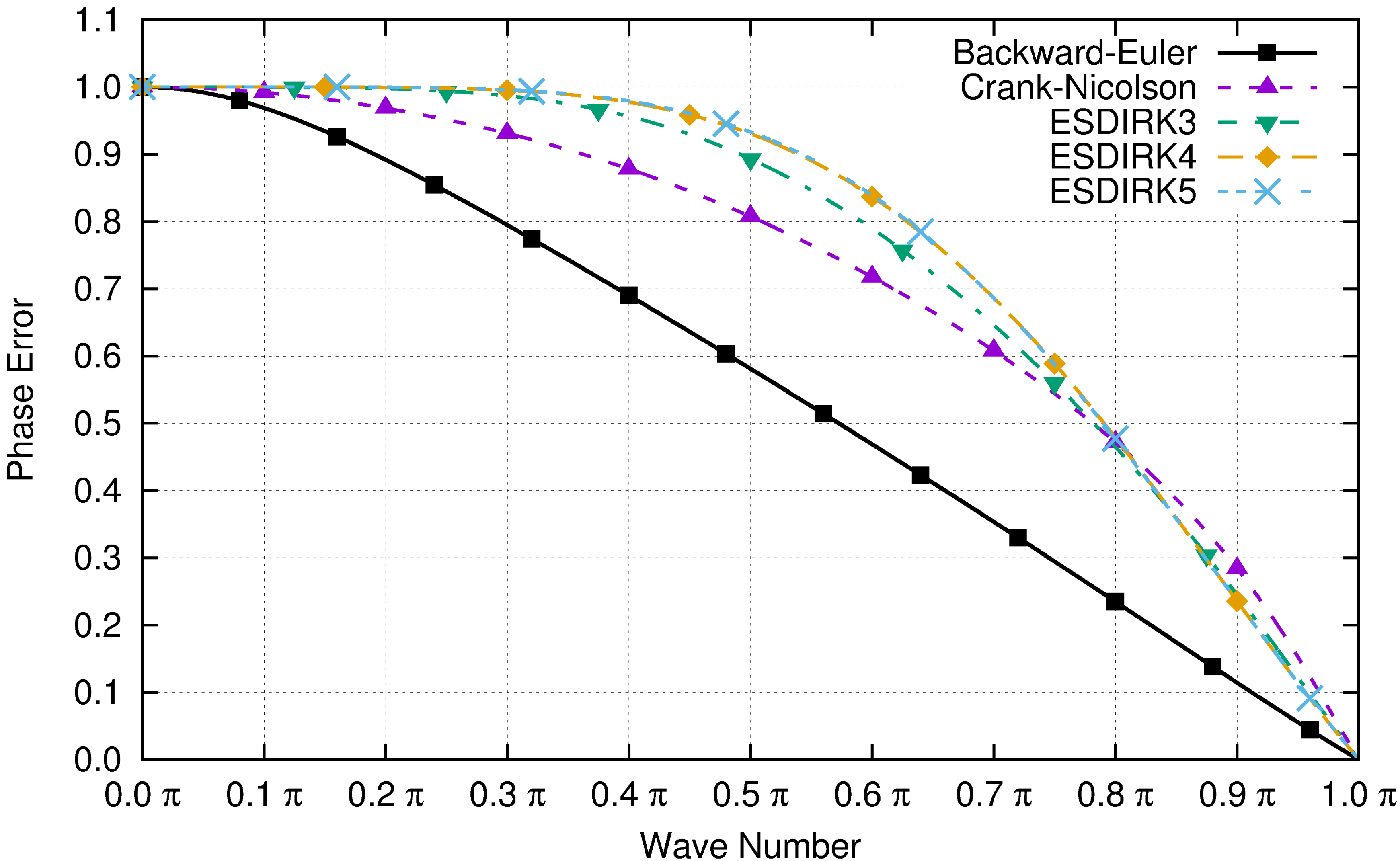
Von Neumann Analysis

- **Often used to study stability of schemes**
- **Von Neumann analysis is used to compare schemes for accuracy**
  - Dissipation error
  - Dispersion error
- **Assumes linear, periodic problems**
- **VNA theory and more results are in the associated paper**

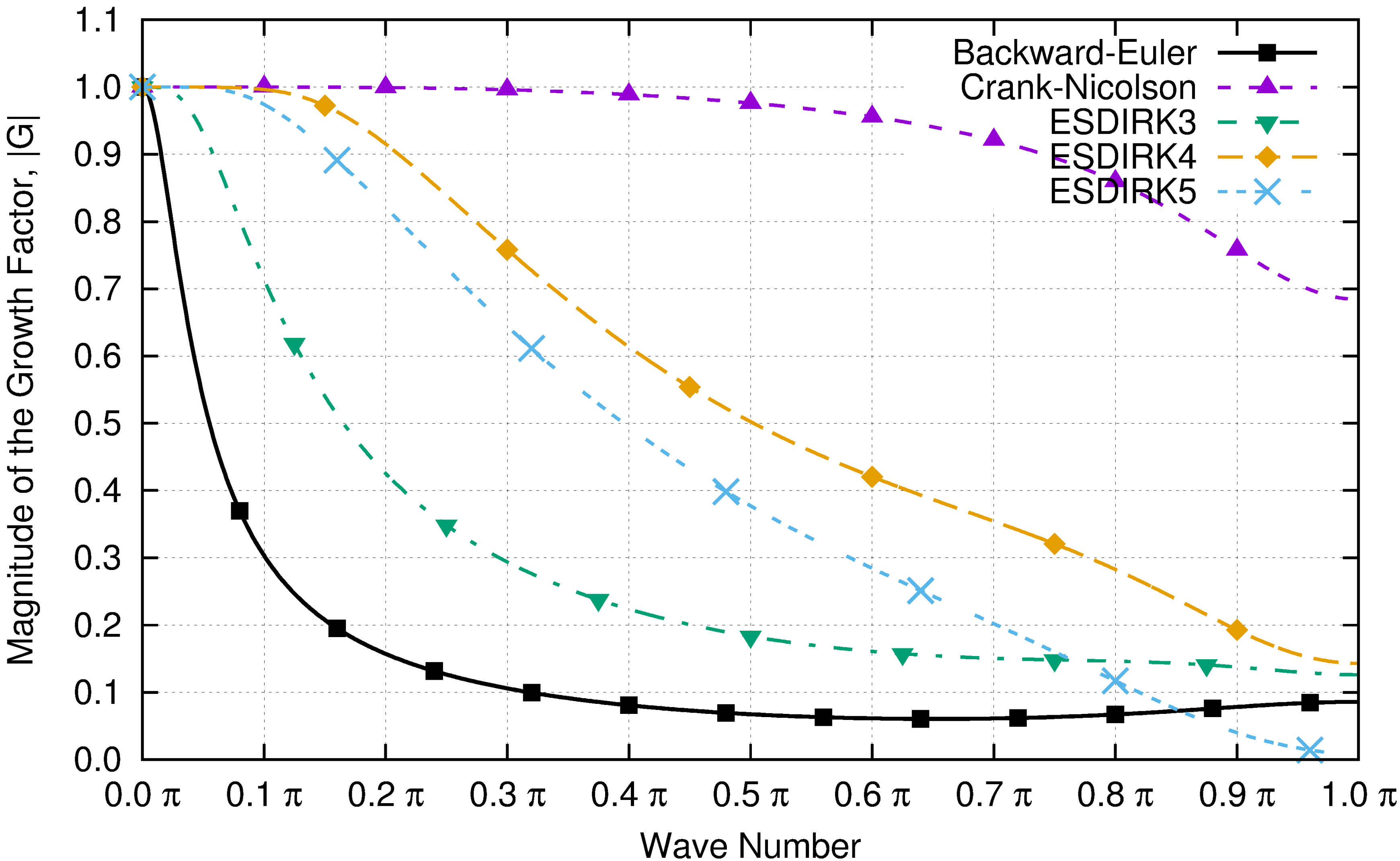
Dissipation, *CFL = 1.0*



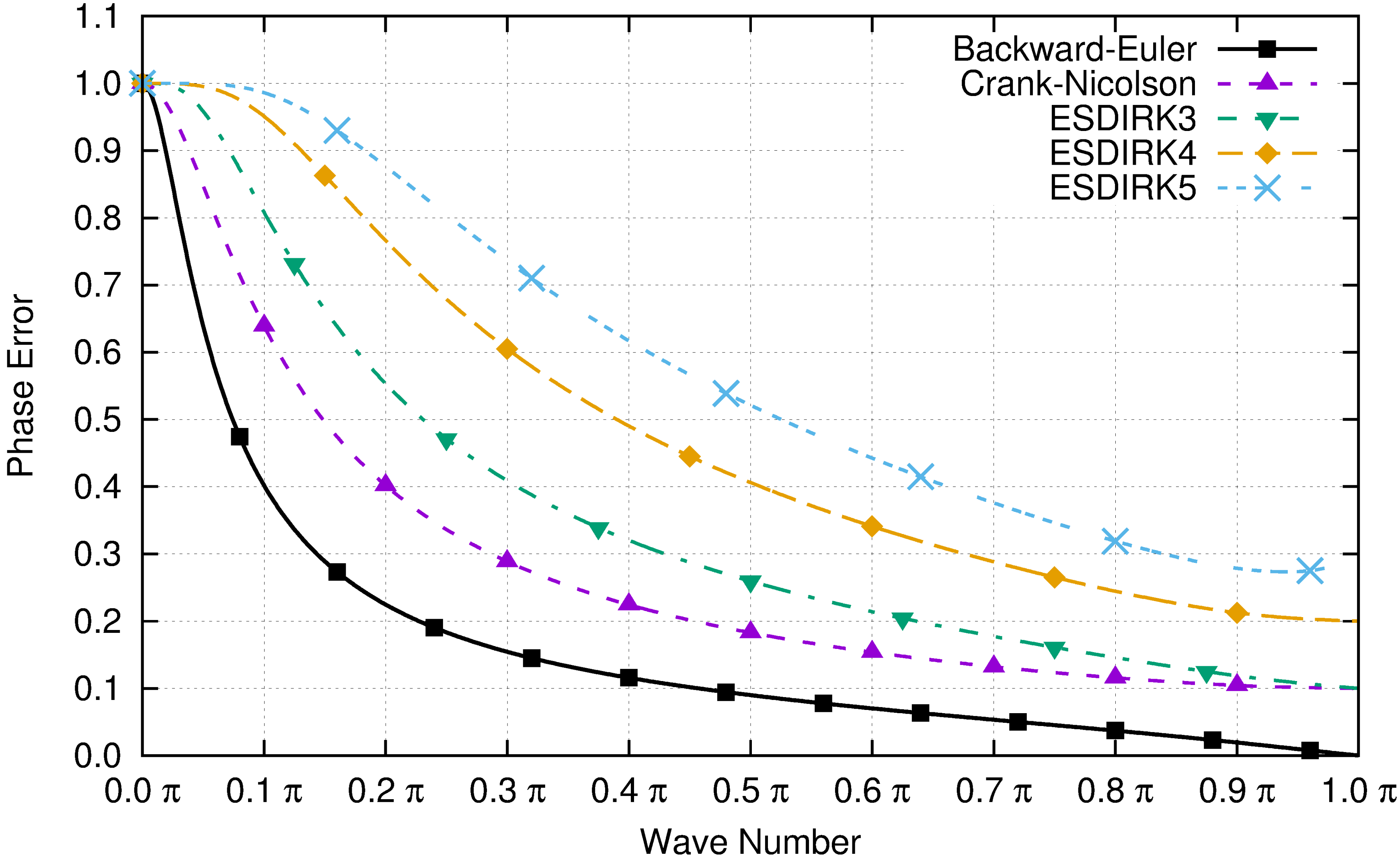
Dispersion, *CFL = 1.0*



Dissipation, *CFL = 10.0*



Dispersion, *CFL* = 10.0



1-D Acoustic Wave

- **Unperturbed Mach number of *0.5***

$$\rho_\infty = 8.7077 \times 10^{-1} \frac{kg}{m^3}$$
$$\rho u_\infty = 1.7458 \times 10^{2} \frac{kg}{m^2 \cdot s}$$
$$T_\infty = 400K$$
$$R_\infty = 2.871 \times 10^{2} \frac{J}{kg \cdot K}$$
$$\gamma = 1.4$$

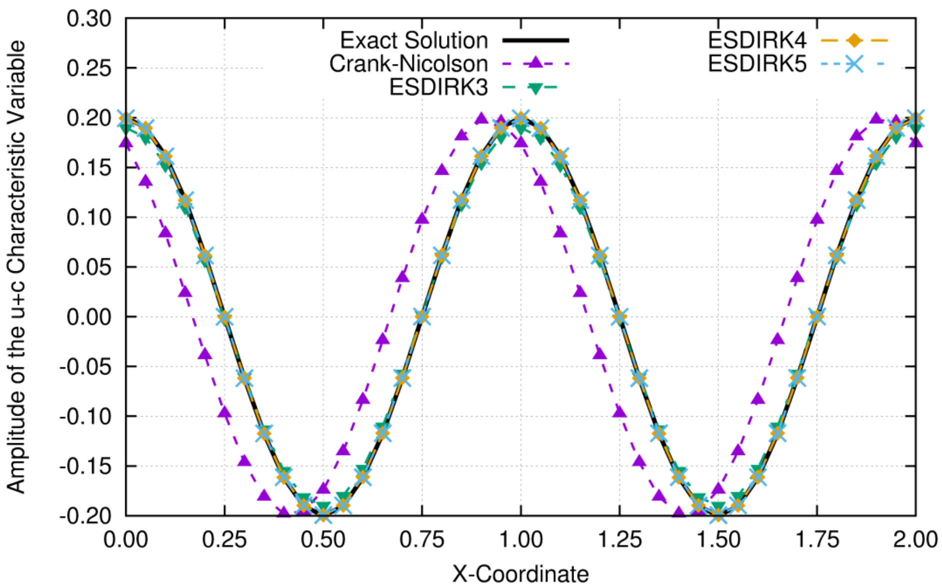
- **Perturbation wave - 20 points per wave resolution**

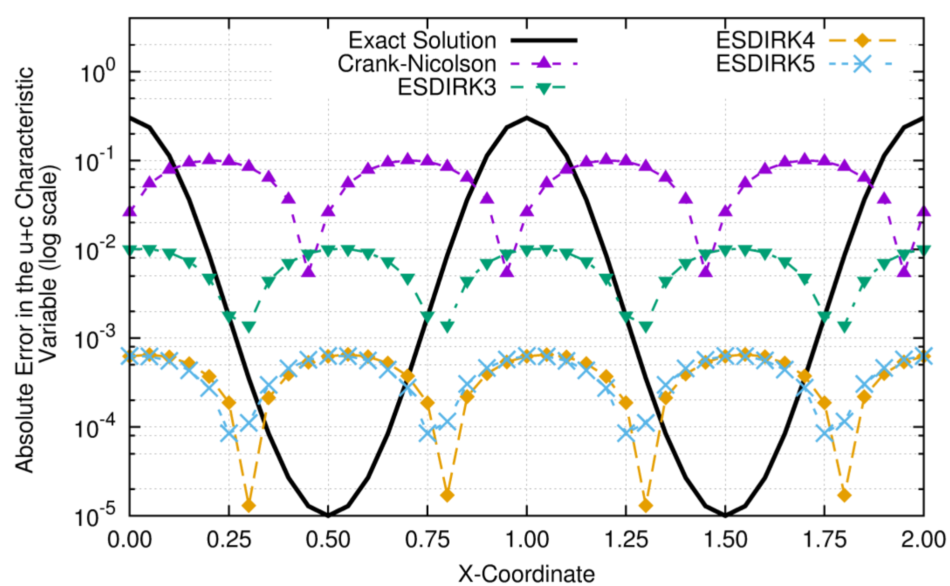
$$\begin{aligned} Q_o &= Q_\infty + M\delta\hat{Q}_{u,u\pm c} \\ \delta\hat{Q}_{u,u\pm c} &= \hat{\delta} \cdot \cos(kx) \end{aligned}$$
$$\text{where } \hat{\delta} = 0.01$$

- **More results in the paper**

1-D, *CFL* = *1.0*, 10 Periods

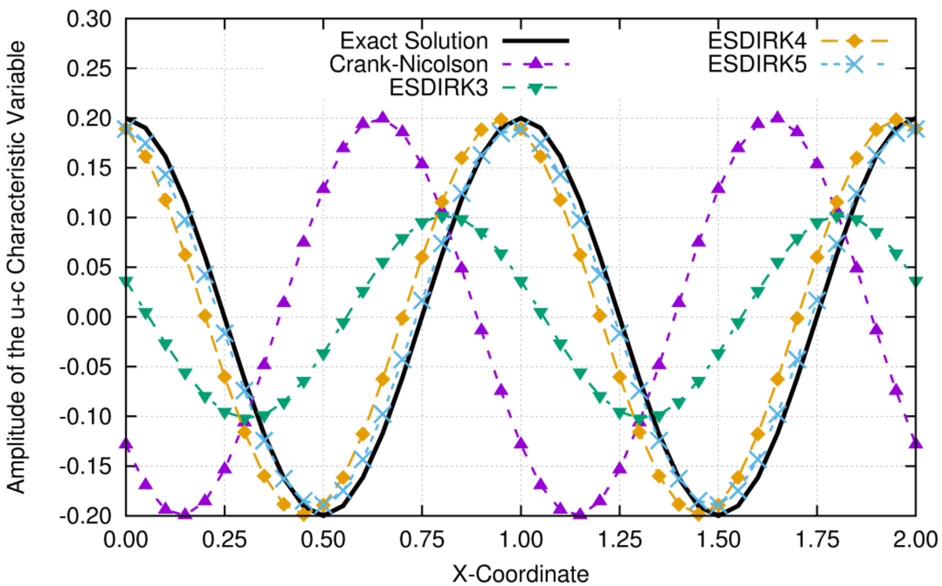
	Dissipation Error		Dispersion Error	
Scheme	VNA	Simulation	VNA	Simulation
Crank-N-colson	3.05×10^{-3}	1.00×10^{-2}	8.11×10^{-2}	8.11×10^{-2}
ESDIRK3	5.02×10^{-2}	5.02×10^{-2}	1.51×10^{-3}	1.53×10^{-3}
ESDIRK4	3.13×10^{-3}	3.13×10^{-3}	1.50×10^{-4}	1.58×10^{-4}
ESDIRK5	3.14×10^{-3}	3.14×10^{-3}	6.78×10^{-5}	6.90×10^{-5}

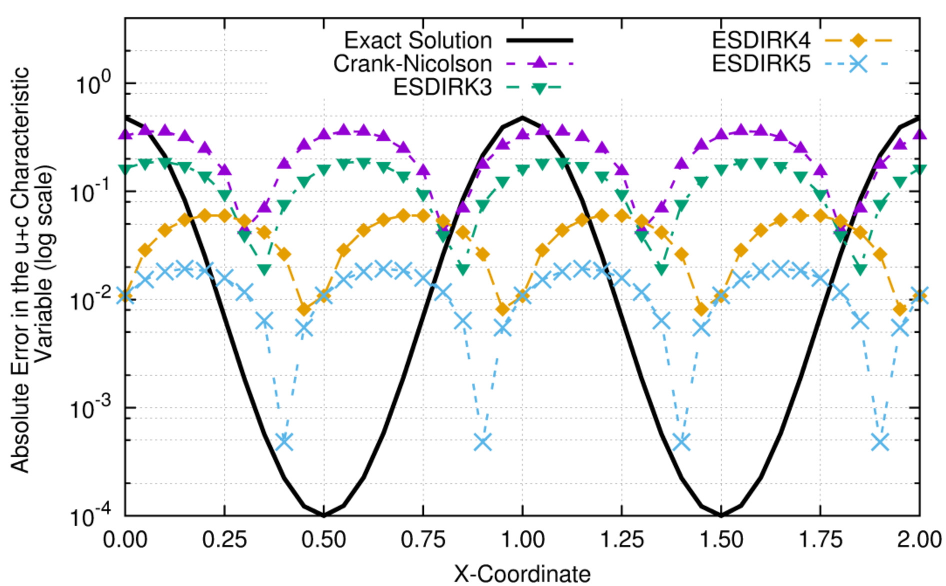




1-D, *CFL = 10.0*, 1 Period

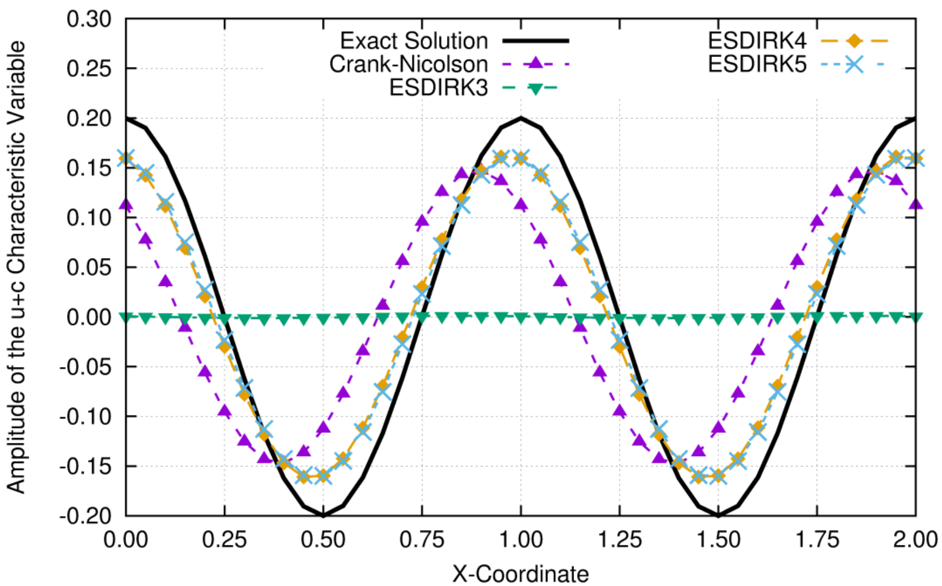
	Dissipation Error		Dispersion Error	
Scheme	VNA	Simulation	VNA	Simulation
Crank-Nicolson	9.02×10^{-5}	2.44×10^{-3}	3.61×10^{-1}	3.61×10^{-1}
ESDIRK3	4.99×10^{-1}	4.90×10^{-1}	1.92×10^{-1}	1.92×10^{-1}
ESDIRK4	7.22×10^{-3}	7.25×10^{-3}	4.90×10^{-2}	4.90×10^{-2}
ESDIRK5	5.10×10^{-2}	5.46×10^{-2}	1.38×10^{-2}	1.39×10^{-2}

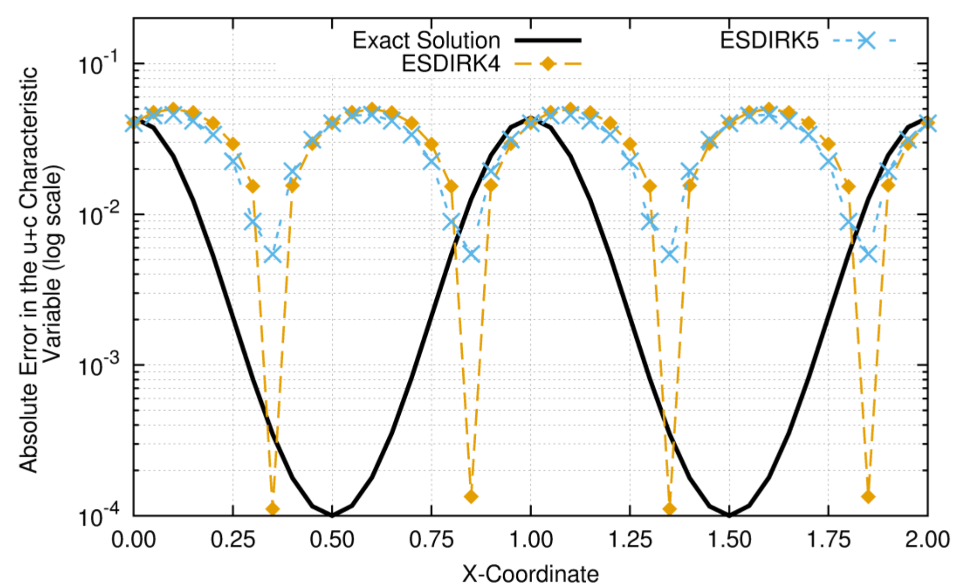




1-D, *CFL = 1.0*, 1000 Periods

	Dissipation Error		Dispersion Error	
Scheme	VNA	Simulation	VNA	Simulation
Crank-Nicolson	2.63×10^{-1}	2.65×10^{-1}	8.11×10^{0}	8.10×10^{0}
ESDIRK3	9.94×10^{-1}	9.94×10^{-1}	1.51×10^{-1}	1.00×10^{-1}
ESDIRK4	2.69×10^{-1}	1.95×10^{-1}	1.50×10^{-2}	3.00×10^{-2}
ESDIRK5	2.70×10^{-1}	2.01×10^{-1}	6.78×10^{-3}	2.50×10^{-2}





3-D Isentropic Vortex

- **Free-stream Mach number of *0.5***

$$\rho_\infty = 1.0\frac{kg}{m^3}, \quad \rho u_\infty = 200.0\frac{kg}{m^2 \cdot s}, \quad \rho v_\infty = 0.0\frac{kg}{m^2 \cdot s}, \quad \rho w_\infty = 0.0\frac{kg}{m^2 \cdot s}, \quad \rho e_{0,\infty} = 305714.3\frac{kg}{m \cdot s^2}$$

$$R_\infty = 287.11\frac{J}{kg \cdot K} \text{ and } \gamma = 1.4$$

- **Perturbation - 11 points across the vortex**

$$\delta u = -\sqrt{R_\infty T_\infty}\frac{\alpha}{2\pi}(y - y_0)\, e^{\phi\left(1-r^2\right)}$$

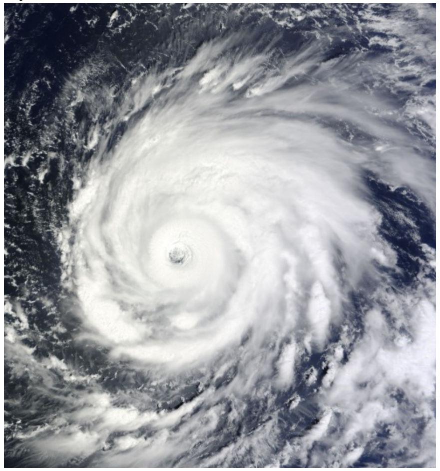
$$\delta v = \sqrt{R_\infty T_\infty}\frac{\alpha}{2\pi}(x - x_0)\, e^{\phi\left(1-r^2\right)}$$

$$\delta T = T_\infty \frac{\alpha^2(\gamma - 1)}{16\phi\gamma\pi^2} e^{2\phi\left(1-r^2\right)}$$

$$\alpha = 4 \text{ and } \phi = 1$$

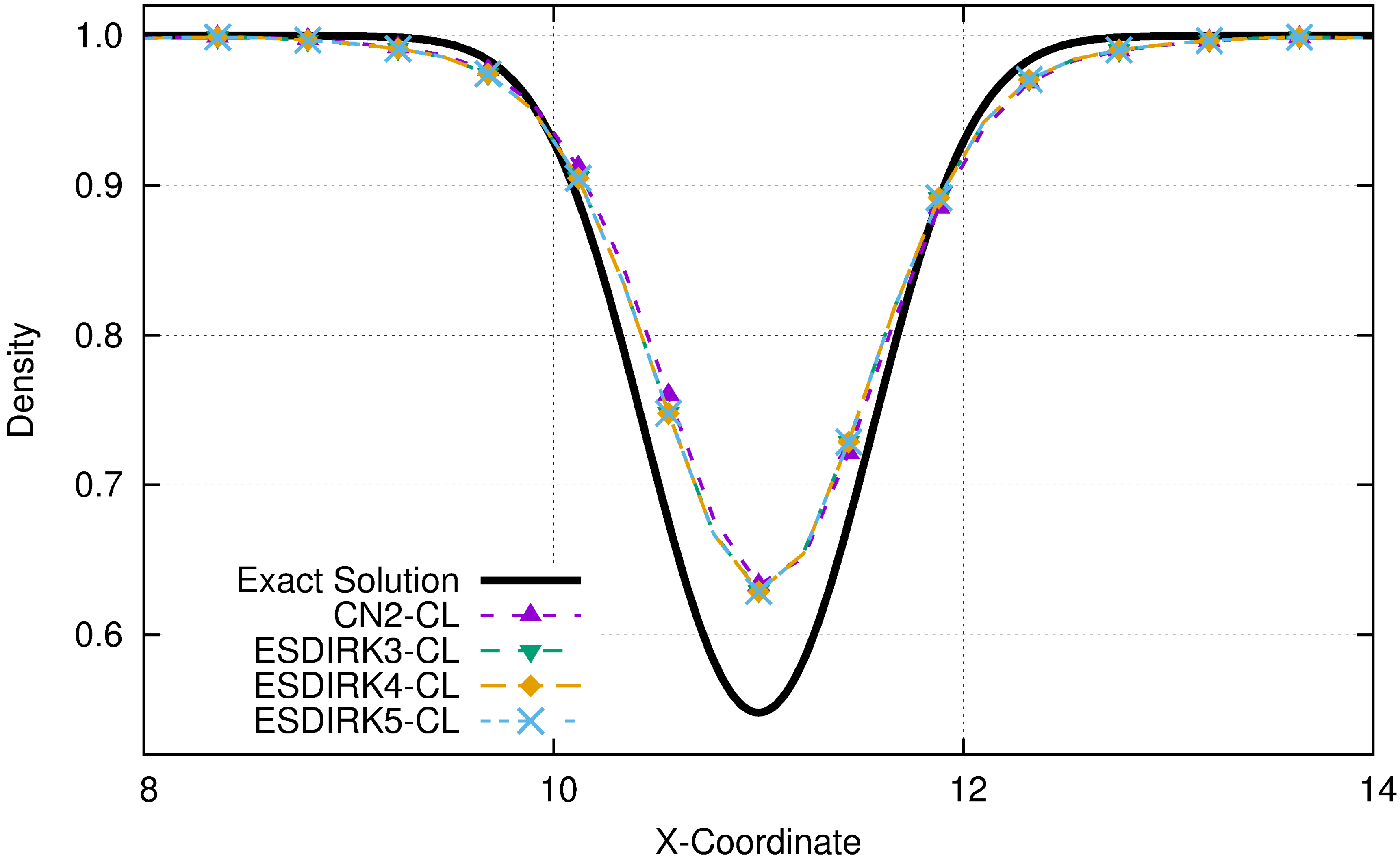
Vortex center: (x_0, y_0)

$$r = \sqrt{(x - x_0)^2 + (y - y_0)^2}$$

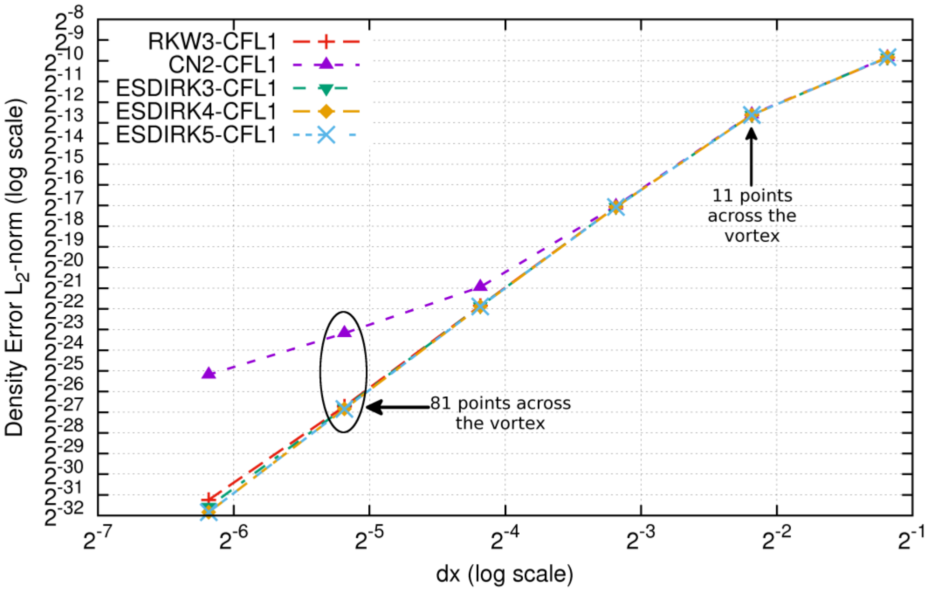


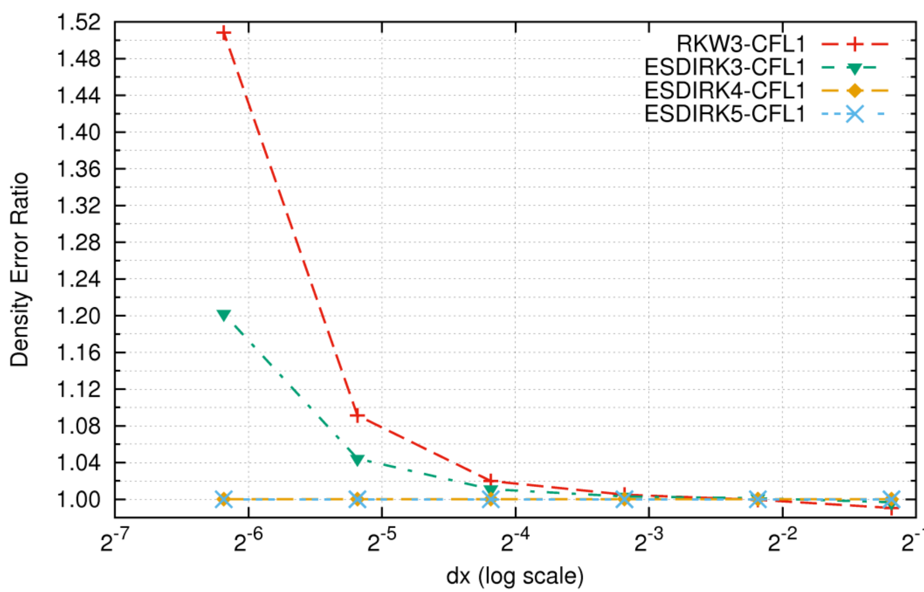
- **More results in the paper**

3-D, *CFL = 1.0*, 40 Lengths, 11 Points Across the Vortex

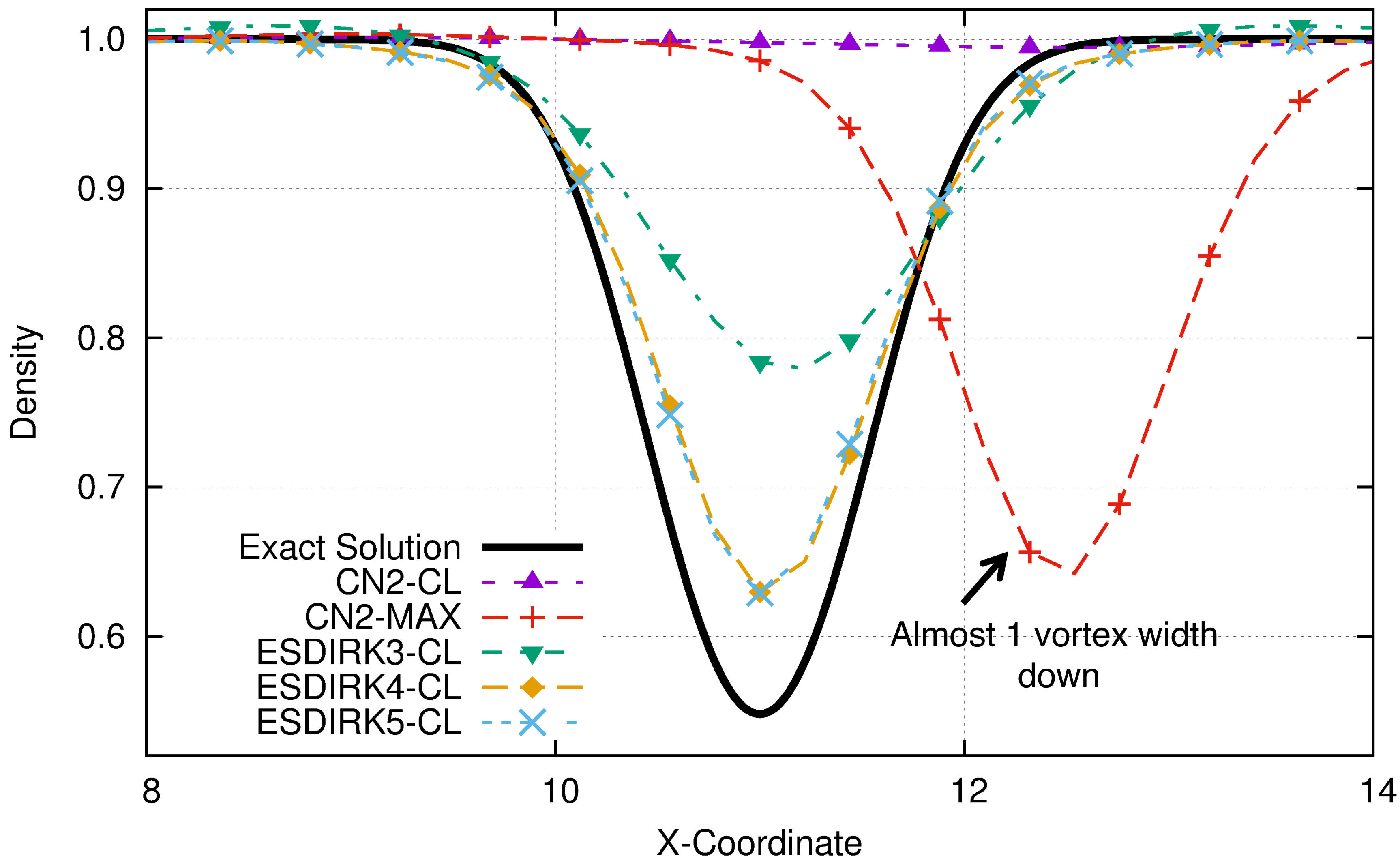


3-D, *CFL = 1.0* Different Resolutions



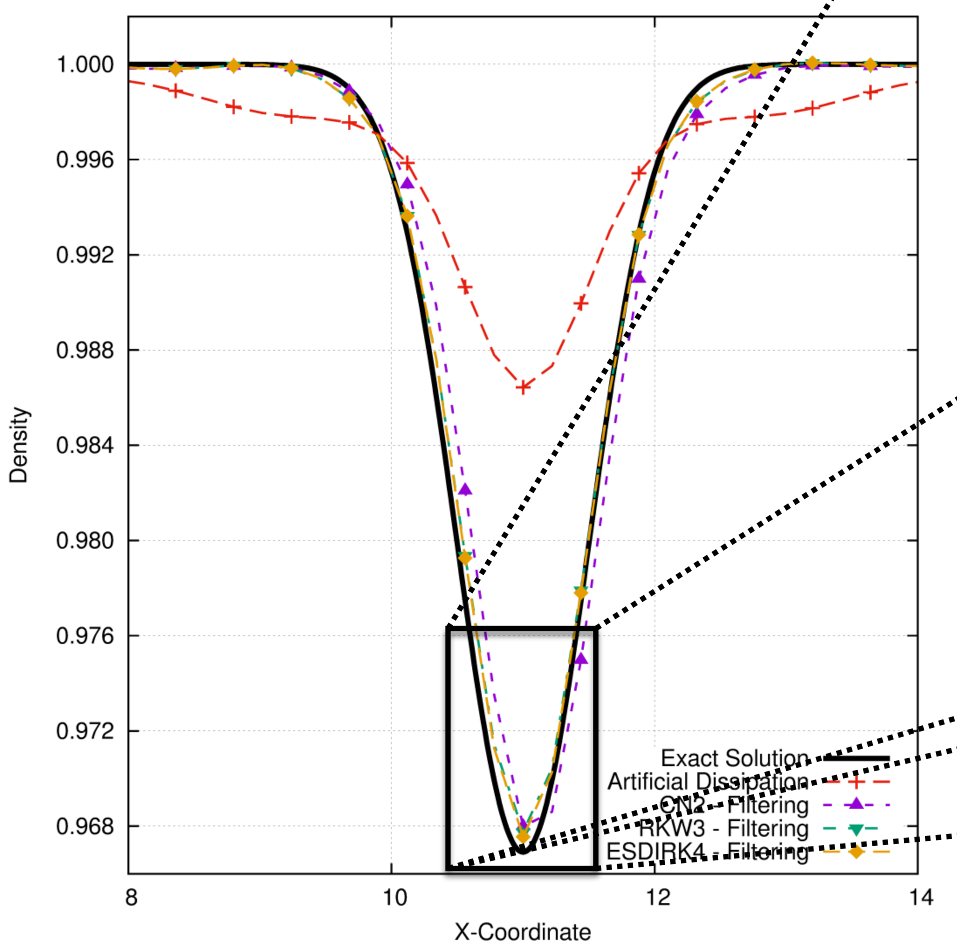


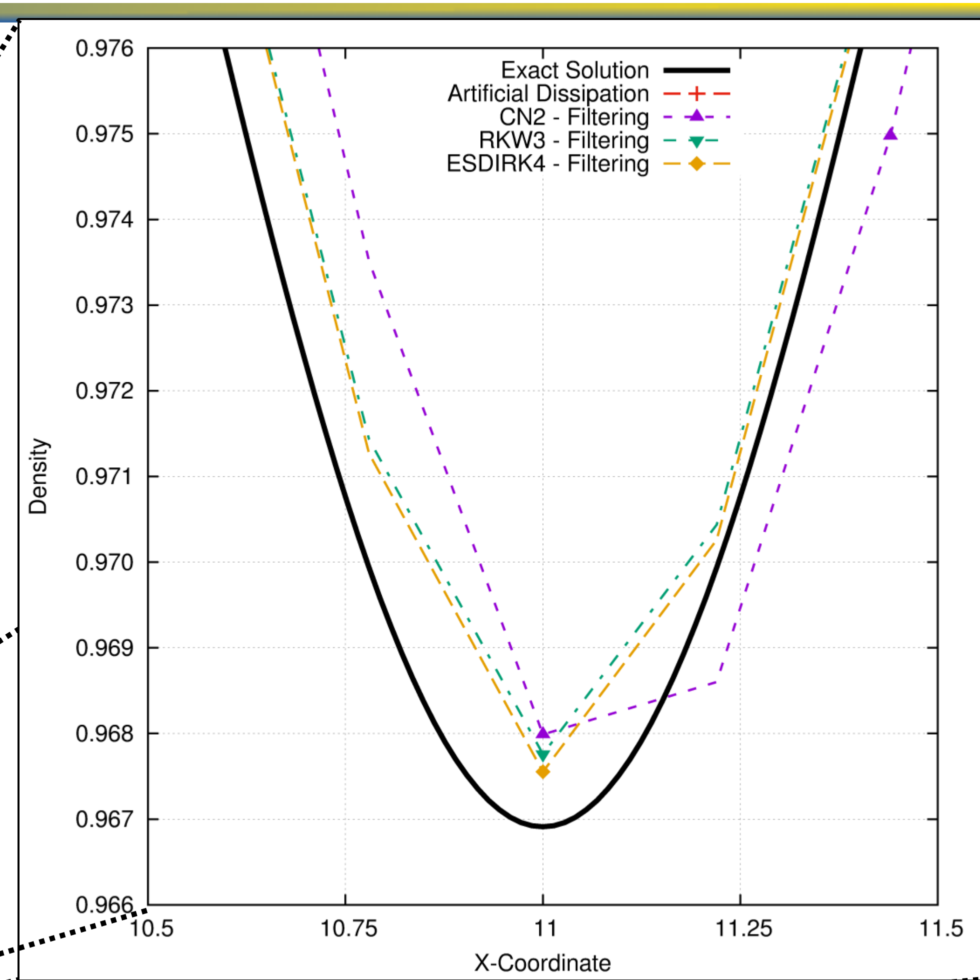
3-D, *CFL* = *8.0*, 40 Lengths, 11 Points Across the Vortex



Sneak Peak: Filtering

11 points across the vortex
$CFL = 1.0$
80 vortex widths convection





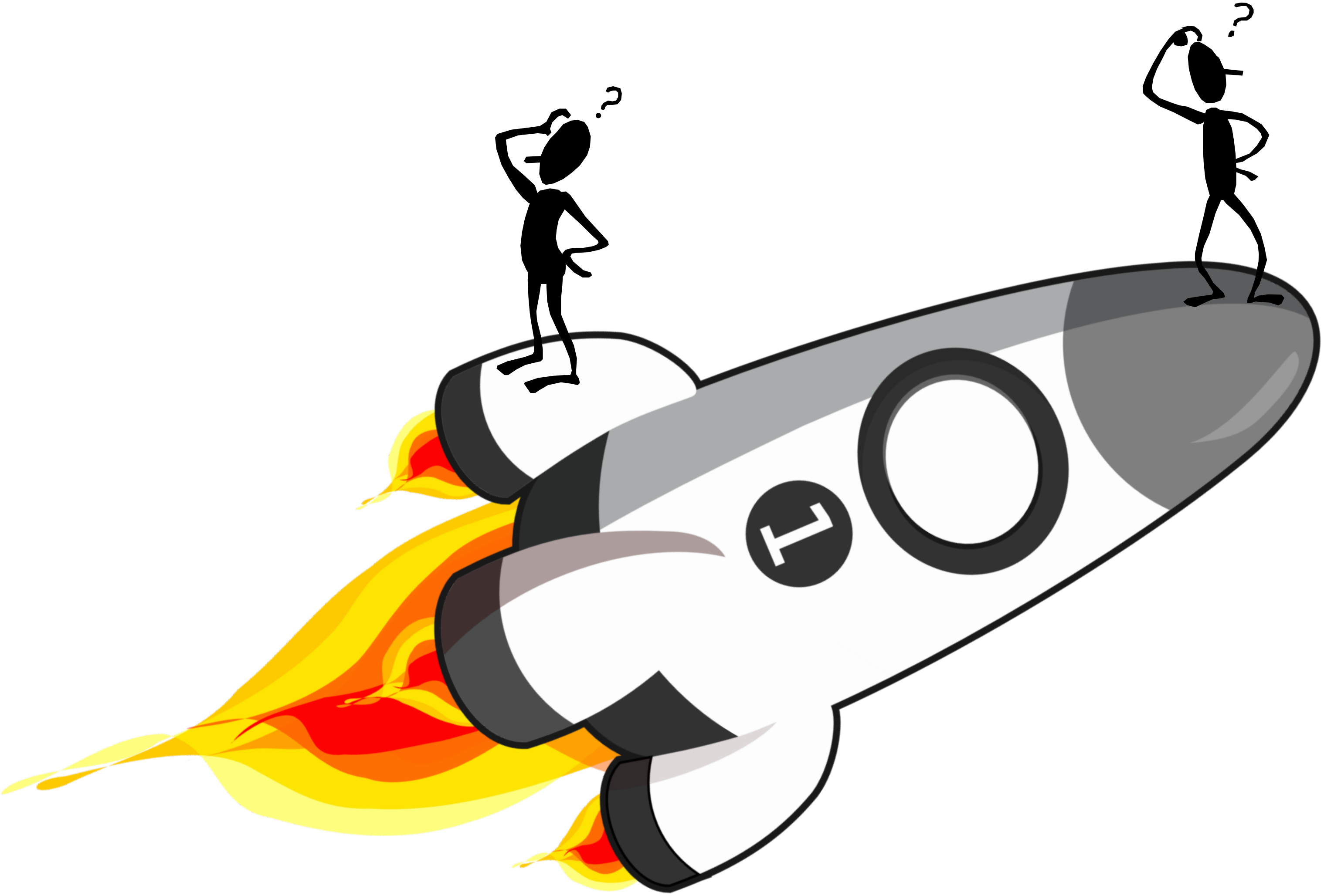
Conclusions

- ***2nd- and 3rd*-order time integrators for *5th*-order spatial schemes are inadequate**
  - The same order of spatial and temporal discretizations is preferable
  - However, ESDIRK5 is not much better than ESDIRK4
    - 7 implicit stages vs. 5 implicit stages
- **Higher-order time integrators:**
  - Do not show significant improvement on coarse grids at *CFL* of one
  - Are better at high *CFL* number
  - Are better on highly refined grids
- **Spatial error usually dominates for typical *CFL* numbers and grid resolutions**
  - Central difference plus artificial dissipation schemes are inadequate

Future Work

- **Implement more accurate spatial schemes of the same orders of accuracy**
  - Compact-difference schemes
  - Filtering schemes
- **Derive better ESDIRK schemes tailored to the desired dissipation and dispersion properties**
- **Add preconditioning to take maximum advantage of the ESDIRK time integrators for stiff problems**
  - Improved convergence efficiency
  - Improved solution accuracy

Questions???



Extra Slides

3-D, *CFL = 8.0*
Different Resolutions