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

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Viewgraphs/Briefing Charts
Optimal Runge-Kutta Schemes for High-order Spatial and Temporal Discretizations

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Outline

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- Governing Equations
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- Von Neumann Analysis (VNA)
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- 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:**

\[
\frac{\partial Q}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H
\]

\[Q = [\rho \quad \rho u_i \quad \rho e_0]^T\]

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

- **Quasi-linear Form:**

\[
\frac{\partial Q}{\partial \tau} + \frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H
\]

\[A = \frac{\partial F_i}{\partial Q} = MAM^{-1}\]

\[\Lambda = \text{diag} \{u_i + c, u_i, u_i - c\}\]

- **Residual Form:**

\[
\frac{\partial Q}{\partial \tau} + \frac{\partial Q}{\partial t} + R_s(Q) = 0 \quad \text{where} \quad R_s = \frac{\partial F_i}{\partial x_i} - \frac{\partial V_i}{\partial x_i} - H
\]
Spatial Discretizations

- Central Differences with added artificial dissipation

- Central differences:
  \[
  \frac{\partial \gamma_j}{\partial x_i} \bigg|_{II} = \frac{\gamma_{j+1} - \gamma_{j-1}}{2\Delta x_i},
  \]
  \[
  \frac{\partial \gamma_j}{\partial x_i} \bigg|_{IV} = \frac{-\gamma_{j+2} + 8\gamma_{j+1} - 8\gamma_{j-1} + \gamma_{j-2}}{12\Delta x_i},
  \]
  \[
  \frac{\partial \gamma_j}{\partial x_i} \bigg|_{VI} = \frac{\gamma_{j+3} - 9\gamma_{j+2} + 45\gamma_{j+1} - 45\gamma_{j-1} + 9\gamma_{j-2} - \gamma_{j-3}}{60\Delta x_i},
  \]

  where \( \gamma \) could be \( \mathbf{F}_i \) or \( \mathbf{Q} \) depending on the form of the equations

- Scalar artificial dissipation:

\[
R_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \varepsilon_\eta \| \lambda \| \frac{\partial \mathbf{Q}}{\partial x_i} - \varepsilon_{VI} \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}
\]

  where \( \eta \) is even and one more than the order of accuracy

\[
\| \lambda \| = |u_i| + c, \quad \varepsilon_{II} = \frac{\Delta x_i}{2}, \quad \varepsilon_{IV} = -\frac{\Delta x_i^3}{12}, \quad \varepsilon_{VI} = \frac{\Delta x_i^5}{60}.
\]
Temporal Discretizations

- Runge-Kutta Methods:

\[
\begin{array}{c|cccccccc}
\text{c}_1 & a_{11} & a_{12} & a_{13} & \ldots & a_{1(s-1)} & a_{1s} \\
\text{c}_2 & a_{21} & a_{22} & a_{23} & \ldots & a_{2(s-1)} & a_{2s} \\
\text{c}_3 & a_{31} & a_{32} & a_{33} & \ldots & a_{3(s-1)} & a_{3s} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\text{c}_{s-1} & a_{(s-1)1} & a_{(s-1)2} & a_{(s-1)3} & \ldots & a_{(s-1)(s-1)} & a_{(s-1)s} \\
\text{c}_s & a_{s1} & a_{s2} & a_{s3} & \ldots & a_{s(s-1)} & a_{ss} \\
\hline
\text{b}_1 & b_2 & b_3 & \ldots & b_{s-1} & b_s \\
\text{\hat{b}}_1 & \text{\hat{b}}_2 & \text{\hat{b}}_3 & \ldots & \text{\hat{b}}_{s-1} & \text{\hat{b}}_s
\end{array}
\]

\[
t^k = t^n + c_k \Delta t \\
Q^k = Q^n - \Delta t \sum_{j=1}^{s} a_{kj} R_s^j(Q^n_j) \quad k = 1, 2, \ldots, s
\]

\[
Q^{n+1} = Q^n - \Delta t \sum_{j=1}^{s} b_j R_s^j(Q^n_j) \\
\hat{Q}^{n+1} = Q^n - \Delta t \sum_{j=1}^{s} \text{\hat{b}}_j R_s^j(Q^n_j)
\]

\[
\epsilon^{n+1} = Q^{n+1} - \hat{Q}^{n+1}
\]
**ESDIRK Methods**

- **Explicit** first stage **Singly-Diagonally Implicit** **Runge-Kutta**
  - Stiffly accurate
  - Second-order stage accuracy
  - FSAL – **First is the Same As Last**

\[
\begin{array}{cccccc}
\{ & 0 & 0 & 0 & \ldots & 0 & 0 \\
\{ & a_{21} & \lambda & 0 & \ldots & 0 & 0 \\
\{ & a_{31} & a_{32} & \lambda & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\{ & a_{(s-1)1} & a_{(s-1)2} & a_{(s-1)3} & \ldots & \lambda & 0 \\
c_s = 1 & b_1 & b_2 & b_3 & \ldots & b_{s-1} & \lambda \\
\end{array}
\]
ESDIRK3 and 4

Implicit, Third-order ESDIRK3

Implicit, Fourth-order ESDIRK4
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

\[
\begin{align*}
\rho_\infty &= 8.7077 \times 10^{-1} \frac{kg}{m^3} \\
\rho u_\infty &= 1.7458 \times 10^2 \frac{kg}{m^2 \cdot s} \\
T_\infty &= 400K \\
R_\infty &= 2.871 \times 10^2 \frac{J}{kg \cdot K} \\
\gamma &= 1.4
\end{align*}
\]

- Perturbation wave - 20 points per wave resolution

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

- More results in the paper
1-D, $CFL = 1.0$, 10 Periods

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Dissipation Error</th>
<th>Dispersion Error</th>
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<tbody>
<tr>
<td></td>
<td>VNA</td>
<td>Simulation</td>
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<tr>
<td>Crank-Nicolson</td>
<td>$3.05 \times 10^{-3}$</td>
<td>$1.00 \times 10^{-2}$</td>
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<tr>
<td>ESDIRK3</td>
<td>$5.02 \times 10^{-2}$</td>
<td>$5.02 \times 10^{-2}$</td>
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<td>ESDIRK4</td>
<td>$3.13 \times 10^{-3}$</td>
<td>$3.13 \times 10^{-3}$</td>
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<tr>
<td>ESDIRK5</td>
<td>$3.14 \times 10^{-3}$</td>
<td>$3.14 \times 10^{-3}$</td>
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</table>
1-D, CFL = 10.0, 1 Period

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<tr>
<td></td>
<td>VNA</td>
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<tr>
<td>Crank-Nicolson</td>
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<td>$7.22 \times 10^{-3}$</td>
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<td>ESDIRK5</td>
<td>$5.10 \times 10^{-2}$</td>
<td>$5.46 \times 10^{-2}$</td>
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1-D, **CFL = 1.0, 1000 Periods**

<table>
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<tbody>
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<td>VNA</td>
<td>Simulation</td>
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<td>Crank-Nicolson</td>
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<td>ESDIRK5</td>
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</table>

![Graphs showing comparison of Crank-Nicolson, ESDIRK3, ESDIRK4, and ESDIRK5 schemes.](image-url)
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
  \[ \delta u = -\sqrt{R_\infty T_\infty} \frac{\alpha}{2\pi} (y - y_0) e^{\phi(1-r^2)} \]
  \[ \delta v = \sqrt{R_\infty T_\infty} \frac{\alpha}{2\pi} (x - x_0) e^{\phi(1-r^2)} \]
  \[ \delta T = T_\infty \frac{\alpha^2 (\gamma - 1)}{16\phi \gamma \pi^2} e^{2\phi(1-r^2)} \]
  \[ \alpha = 4 \text{ and } \phi = 1 \]
  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

Almost 1 vortex width down
Sneak Peak: Filtering

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

- 2\textsuperscript{nd}- and 3\textsuperscript{rd}-order time integrators for 5\textsuperscript{th}-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
3-D, CFL = 8.0
Different Resolutions

![Graphs showing different resolutions and density error ratios](image)