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

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Ayaboe K. Edoh – UCLA
Venke Sankaran – AFRL/RQ

2015 AIAA SciTech
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 $> 2^{nd}$-order accuracy
• Thus, multistage methods, like Runge-Kutta (RK) methods, must be used for $3^{rd}$- 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:

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

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

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

• Quasi-linear Form:

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

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

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

• Residual Form:

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

- Central Differences with added artificial dissipation

- Central differences:

\[
\frac{\partial \gamma_j}{\partial x_i} = \frac{\gamma_{j+1} - \gamma_{j-1}}{2 \Delta x_i}
\]

\[
\frac{\partial \gamma_j}{\partial x_i} = \frac{-\gamma_{j+2} + 8\gamma_{j+1} - 8\gamma_{j-1} + \gamma_{j-2}}{12 \Delta x_i}
\]

\[
\frac{\partial \gamma_j}{\partial x_i} = \frac{\gamma_{j+3} - 9\gamma_{j+2} + 45\gamma_{j+1} - 45\gamma_{j-1} + 9\gamma_{j-2} - \gamma_{j-3}}{60 \Delta x_i}
\]

where \( \gamma \) could be \( F_i \) or \( Q \) depending on the form of the equations.

- Scalar artificial dissipation:

\[
R_s = \frac{\partial F_i}{\partial x_i} - \varepsilon_\eta \| \lambda \| \frac{\partial^\eta Q}{\partial x_i^\eta} - \frac{\partial V_i}{\partial x_i} - H
\]

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:**

<table>
<thead>
<tr>
<th>$c_1$</th>
<th>$a_{11}$</th>
<th>$a_{12}$</th>
<th>$a_{13}$</th>
<th>$\ldots$</th>
<th>$a_{1(s-1)}$</th>
<th>$a_{1s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_2$</td>
<td>$a_{21}$</td>
<td>$a_{22}$</td>
<td>$a_{23}$</td>
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<td>$a_{2(s-1)}$</td>
<td>$a_{2s}$</td>
</tr>
<tr>
<td>$c_3$</td>
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<td>$a_{32}$</td>
<td>$a_{33}$</td>
<td>$\ldots$</td>
<td>$a_{3(s-1)}$</td>
<td>$a_{3s}$</td>
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<tr>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
</tr>
<tr>
<td>$c_{s-1}$</td>
<td>$a_{(s-1)1}$</td>
<td>$a_{(s-1)2}$</td>
<td>$a_{(s-1)3}$</td>
<td>$\ldots$</td>
<td>$a_{(s-1)(s-1)}$</td>
<td>$a_{(s-1)s}$</td>
</tr>
<tr>
<td>$c_s$</td>
<td>$a_{s1}$</td>
<td>$a_{s2}$</td>
<td>$a_{s3}$</td>
<td>$\ldots$</td>
<td>$a_{s(s-1)}$</td>
<td>$a_{ss}$</td>
</tr>
</tbody>
</table>
| \hline
| $b_1$ | $b_2$ | $b_3$ | $\ldots$ | $b_{s-1}$ | $b_s$ |
| $\hat{b}_1$ | $\hat{b}_2$ | $\hat{b}_3$ | $\ldots$ | $\hat{b}_{s-1}$ | $\hat{b}_s$ |

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

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

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

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

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<th>(0)</th>
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<td>(0)</td>
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<tr>
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<td>(\vdots)</td>
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<td>(\vdots)</td>
<td>(\vdots)</td>
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<td>(\vdots)</td>
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<tr>
<td>(c_{s-1})</td>
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<td></td>
<td>(b_1)</td>
<td>(\hat{b}_2)</td>
<td>(\hat{b}_3)</td>
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<td>(\hat{b}_{s-1})</td>
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# ESDIRK3 and 4

## Implicit, Third-order ESDIRK3

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## Implicit, Fourth-order ESDIRK4

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<td>8211</td>
</tr>
</tbody>
</table>

Distribution A – Approved for public release; Distribution Unlimited
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
  \[ Q_o = Q_\infty + M \delta Q_{u,u \pm c} \]
  \[ \delta Q_{u,u \pm c} = \delta \cdot \cos(kx) \]
  where \( \delta = 0.01 \)

- More results in the paper
### Dissipation Error

<table>
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<tr>
<th>Scheme</th>
<th>VNA</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crank-N-colson</td>
<td>$3.05 \times 10^{-3}$</td>
<td>$1.00 \times 10^{-2}$</td>
</tr>
<tr>
<td>ESDIRK3</td>
<td>$5.02 \times 10^{-2}$</td>
<td>$5.02 \times 10^{-2}$</td>
</tr>
<tr>
<td>ESDIRK4</td>
<td>$3.13 \times 10^{-3}$</td>
<td>$3.13 \times 10^{-3}$</td>
</tr>
<tr>
<td>ESDIRK5</td>
<td>$3.14 \times 10^{-3}$</td>
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</tbody>
</table>

### Dispersion Error

<table>
<thead>
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<th>VNA</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
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<td>$8.11 \times 10^{-2}$</td>
<td>$8.11 \times 10^{-2}$</td>
</tr>
<tr>
<td>ESDIRK3</td>
<td>$1.51 \times 10^{-3}$</td>
<td>$1.53 \times 10^{-3}$</td>
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<tr>
<td>ESDIRK4</td>
<td>$1.50 \times 10^{-4}$</td>
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<tr>
<td>ESDIRK5</td>
<td>$6.78 \times 10^{-5}$</td>
<td>$6.90 \times 10^{-5}$</td>
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</table>
1-D, $CFL = 10.0$, 1 Period

<table>
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<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>
</tr>
<tr>
<td>Crank-Nicolson</td>
<td>$9.02 \times 10^{-5}$</td>
<td>$2.44 \times 10^{-3}$</td>
</tr>
<tr>
<td>ESDIRK3</td>
<td>$4.99 \times 10^{-1}$</td>
<td>$4.90 \times 10^{-1}$</td>
</tr>
<tr>
<td>ESDIRK4</td>
<td>$7.22 \times 10^{-3}$</td>
<td>$7.25 \times 10^{-3}$</td>
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<tr>
<td>ESDIRK5</td>
<td>$5.10 \times 10^{-2}$</td>
<td>$5.46 \times 10^{-2}$</td>
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</table>
1-D, $CFL = 1.0$, 1000 Periods

<table>
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<th>Dispersion Error</th>
</tr>
</thead>
<tbody>
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<td>$2.65 \times 10^{-1}$</td>
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<td>$9.94 \times 10^{-1}$</td>
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<td>ESDIRK4</td>
<td>$2.69 \times 10^{-1}$</td>
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<td>$2.70 \times 10^{-1}$</td>
<td>$2.01 \times 10^{-1}$</td>
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</table>

**Diagram:**

- **Left Diagram**: Amplitude of the u-c Characteristic Variable vs X-Coordinate.
- **Right Diagram**: Absolute Error in the u-c Characteristic Variable (log scale) vs X-Coordinate.

Distribution A – Approved for public release; Distribution Unlimited
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**
  \[
  \delta u = -\sqrt{R_\infty T_\infty} \frac{\alpha}{2\pi} (y - y_0) e^{\phi (1 - r^2)}
  \]
  \[
  \delta v = \sqrt{R_\infty T_\infty} \frac{\alpha}{2\pi} (x - x_0) e^{\phi (1 - r^2)}
  \]
  \[
  \delta T = T_\infty \frac{\alpha^2 (\gamma - 1)}{16\phi \gamma \pi^2} e^{2\phi (1 - r^2)}
  \]
  \[\alpha = 4 \text{ and } \phi = 1\]
  \[][\text{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

![Graph showing 3-D CFL = 1.0 with different resolutions.](image)

Distribution A – Approved for public release; Distribution Unlimited
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
Extra Slides
3-D, $CFL = 8.0$
Different Resolutions