**Report Date (DD-MM-YYYY)**

22 June 2015

**Report Type**

Briefing Charts

**Dates Covered (From - To)**

19 June 2015 – 22 June 2015

**Title and Subtitle**

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

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**Performing Organization Report No.**

AFRL-RQ-ED-VG-2015-268

**Distribution / Availability Statement**

Approved for public release; distribution unlimited

**Supplementary Notes**

For presentation at 22nd AIAA Computational Fluid Dynamics Conference; Dallas, TX; 22 June 2015

PA Case Number: #15352; Clearance Date: 6/29/2015

**Abstract**

Viewgraphs/Briefing Charts

**Subject Terms**

N/A

**Security Classification of:**

a. Report

Unclassified

b. Abstract

Unclassified
c. This Page

Unclassified

17. Limitation of Abstract

SAR

18. Number of Pages

29

19a. Name of Responsible Person

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19b. Telephone No (Include Area Code)

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

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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:**

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

\[Q = \begin{bmatrix} \rho & \rho u_i & \rho e_0 \end{bmatrix}^T\]

\[F_i = \begin{bmatrix} \rho u_i & \rho u_i u_j + p \delta_{ij} & u_i \rho h_0 \end{bmatrix}^T \text{ where } h_0 = e_0 + \frac{\nu}{\rho}\]

- **Quasi-linear Form:**

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

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

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

- **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 \( F_i \) or \( Q \) depending on the form of the equations

• Scalar artificial dissipation:

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

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

\[
\parallel \lambda \parallel = |u_i| + c
\]

\[
\varepsilon_{II} = \frac{\Delta x_i}{2}, \quad \varepsilon_{IV} = -\frac{\Delta x_i^3}{12}, \quad \varepsilon_{VI} = \frac{\Delta x_i^5}{60}.
\]
# 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>
<td>$\ldots$</td>
<td>$a_{2(s-1)}$</td>
<td>$a_{2s}$</td>
</tr>
<tr>
<td>$c_3$</td>
<td>$a_{31}$</td>
<td>$a_{32}$</td>
<td>$a_{33}$</td>
<td>$\ldots$</td>
<td>$a_{3(s-1)}$</td>
<td>$a_{3s}$</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\ddots$</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>

$$t^k = t^n + c_k \Delta t$$

$$Q^k = Q^n - \Delta t \sum_{j=1}^{s} a_{kj} R_j^s(Q^j) \quad k = 1, 2, \ldots, s$$

$$Q^{n+1} = Q^n - \Delta t \sum_{j=1}^{s} b_j R_j^s(Q^j)$$

$$\hat{Q}^{n+1} = Q^n - \Delta t \sum_{j=1}^{s} \hat{b}_j R_j^s(Q^j)$$

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

- **Explicit first stage** **Singly-Diagonally Implicit Runge-Kutta**

  - Stiffly accurate
  - Second-order stage accuracy
  - FSAL – **First is the Same As Last**

| \(c_1 = 0\) | 0 | 0 | 0 | ... | 0 | 0 |
| \(c_2\) | \(a_{21}\) | \(\lambda\) | 0 | ... | 0 | 0 |
| \(c_3\) | \(a_{31}\) | \(a_{32}\) | \(\lambda\) | ... | 0 | 0 |
| \(\vdots\) | \(\vdots\) | \(\vdots\) | \(\vdots\) | ... | \(\vdots\) | \(\vdots\) |
| \(c_{s-1}\) | \(a_{(s-1)1}\) | \(a_{(s-1)2}\) | \(a_{(s-1)3}\) | ... | \(\lambda\) | 0 |
| \(c_s = 1\) | \(b_1\) | \(b_2\) | \(b_3\) | ... | \(b_{s-1}\) | \(\lambda\) |
| \(\hat{c}_1\) | \(\hat{b}_1\) | \(\hat{b}_2\) | \(\hat{b}_3\) | ... | \(\hat{b}_{s-1}\) | \(\hat{b}_s\) |
### Implicit, Third-order ESDIRK3

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### Implicit, Fourth-order ESDIRK4

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</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
Dispersion, $CFL = 1.0$
Dissipation, \( CFL = 10.0 \)
Dispersion, \(\text{CFL} = 10.0\)
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**

\[
Q_o = Q_\infty + M \delta \hat{Q}_{u,u \pm c}
\]
\[
\delta \hat{Q}_{u,u \pm c} = \delta \cdot \cos (kx)
\]

where \(\hat{\delta} = 0.01\)

- **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>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>VNA</td>
<td>Simulation</td>
</tr>
<tr>
<td>Crank-Nicolson</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>
<td>( 3.14 \times 10^{-3} )</td>
</tr>
</tbody>
</table>

Diagram 1: Graph showing the amplitude of the u-c characteristic variable at different x-coordinates for various schemes.

Diagram 2: Graph showing the absolute error in the u-c characteristic variable (log scale) at different x-coordinates for various schemes.
1-D, \( \text{CFL} = 10.0 \), 1 Period

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Dissipation Error</th>
<th>Dispersion Error</th>
</tr>
</thead>
<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>
</tr>
<tr>
<td>ESDIRK5</td>
<td>( 5.10 \times 10^{-2} )</td>
<td>( 5.46 \times 10^{-2} )</td>
</tr>
</tbody>
</table>
1-D, $CFL = 1.0$, 1000 Periods

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Dissipation Error</th>
<th></th>
<th>Dispersion Error</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>VNA</td>
<td>Simulation</td>
<td>VNA</td>
<td>Simulation</td>
</tr>
<tr>
<td>Crank-Nicolson</td>
<td>$2.63 \times 10^{-1}$</td>
<td>$2.65 \times 10^{-1}$</td>
<td>$8.11 \times 10^{-1}$</td>
<td>$8.10 \times 10^{-1}$</td>
</tr>
<tr>
<td>ESDIRK3</td>
<td>$9.94 \times 10^{-1}$</td>
<td>$9.94 \times 10^{-1}$</td>
<td>$1.51 \times 10^{-1}$</td>
<td>$1.00 \times 10^{-1}$</td>
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<tr>
<td>ESDIRK4</td>
<td>$2.69 \times 10^{-1}$</td>
<td>$1.95 \times 10^{-1}$</td>
<td>$1.50 \times 10^{-2}$</td>
<td>$3.00 \times 10^{-2}$</td>
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<tr>
<td>ESDIRK5</td>
<td>$2.70 \times 10^{-1}$</td>
<td>$2.01 \times 10^{-1}$</td>
<td>$6.78 \times 10^{-3}$</td>
<td>$2.50 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

![Graphs showing dissipation and dispersion errors for different schemes](image-url)
3-D Isentropic Vortex

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

\[
\rho_\infty = 1.0 \frac{kg}{m^3}, \quad \rho u_\infty = 200.0 \frac{kg}{m^2.s}, \quad \rho v_\infty = 0.0 \frac{kg}{m^2.s}, \quad \rho w_\infty = 0.0 \frac{kg}{m^2.s}, \quad \rho \epsilon_0,\infty = 305714.3 \frac{kg}{m^2.s^2}
\]

\[
R_\infty = 287.11 \frac{J}{kg.K} \text{ and } \gamma = 1.4
\]

- **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

![Graph showing density vs. x-coordinate with markers and lines labeled as Exact Solution, CN2-CL, CN2-MAX, ESDIRK3-CL, ESDIRK4-CL, ESDIRK5-CL with an annotation indicating 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