High-Order RD Hyperbolic Advection-Diffusion Schemes: 3rd-, 4th-, and 6th-Order

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June 16, 2014

Overview

Objectives

- Develop a Robust, Accurate, and Efficient Viscous Solver
  a) Residual Distribution (RD)
     - Compact Second-Order
     - Newton Method
       (≤ 10 sub-iterations for implicit time stepping)
  b) Hyperbolic System Formulation
     - Compact Viscous Stencil
     - No Second Derivatives

Basic Formulation

Consider an Advection-Diffusion equation:

$$\partial_t u + a\,\partial_x u = \nu\,\partial_{xx} u + \tilde{S}(x)$$

We hyperbolize the equation by setting $p = u_x$ as:

$$\partial_\tau u + \boxed{a\,\partial_x u} = \boxed{\nu\,\partial_x p} - \boxed{\frac{\alpha}{\Delta t} u + S(x)}$$

$$\partial_\tau p = \boxed{(\partial_x u - p)/T_r}$$

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- Hyperbolic Diffusion
- Source Terms
- Pseudo-Steady-State: i.e., Solution at the next physical time step

Hyperbolic Advection-Diffusion

With the hyperbolic formulation, we can rewrite our advection-diffusion equation as a first-order system:

$$\frac{\partial \mathbf{U}}{\partial \tau} + \mathbf{A}\frac{\partial \mathbf{U}}{\partial x} = \mathbf{S}$$

$$\mathbf{U} = \begin{bmatrix} u \\ p \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} a & -\nu \\ -1/T_r & 0 \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} -\alpha u/\Delta t + S(x) \\ -p/T_r \end{bmatrix}$$

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With two real wave speeds of

$$\lambda_{1,2} = \frac{a}{2}\left[1 \pm \sqrt{1 + \frac{4\nu}{a^2 T_r}}\,\right]$$

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Hyperbolic in Pseudo Time (T_r is a free parameter.)

RD Scheme

RD Scheme: Cell Residuals

We can now evaluate the cell residuals for a general time-dependent hyperbolic advection-diffusion system as

$$\mathbf{\Phi}^C = \int_{x_i}^{x_{i+1}} (-\mathbf{A}\mathbf{U}_x + \mathbf{S})dx$$

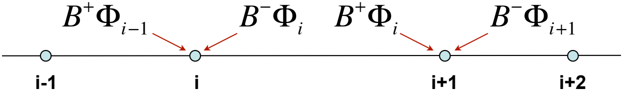
RD Scheme: Cell Residuals

We can now evaluate the cell residuals for a general time-dependent hyperbolic advection-diffusion system as

$$
\begin{aligned}
\mathbf{\Phi}^C &= \int_{x_i}^{x_{i+1}} (-\mathbf{A}\mathbf{U}_x + \mathbf{S})dx \\
&= \left\{ \begin{array}{l} -a(u_{i+1} - u_i)^{k+1} + \nu(p_{i+1} - p_i)^{k+1} \\[2ex] \dfrac{1}{T_r}(u_{i+1} - u_i)^{k+1} \end{array} \right. \\
&+ \left[\int_{x_i}^{x_{i+1}} \mathbf{S}\, dx \right]^{k+1,n-1,n}
\end{aligned}
$$

Details at NASA/TM-2014-218175, 2014.

RD Scheme: Nodal Residuals

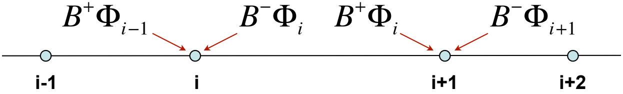


Nodal residuals are evaluated by distributing the cell residuals $\mathbf{\Phi}^C$ to the nodes:

$$\cancel{\frac{d\mathbf{U}_i}{d\tau}} = \frac{1}{h_i}(\mathbf{B}^+\mathbf{\Phi}^L + \mathbf{B}^-\mathbf{\Phi}^R) = \mathbf{Res}_i$$

$$h_i = \frac{h_L + h_R}{2}$$

RD Scheme: Nodal Residuals



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$$h_i = \frac{h_L + h_R}{2}$$

Therefore, we solve $\mathbf{Res}_i = 0$.

Implicit Solver

Implicit Solver

Implicit formulation for $\mathbf{U} = (u_1, p_1, u_2, p_2, \ldots, u_N, p_N)$:

$$\mathbf{U}^{k+1} = \mathbf{U}^k + \Delta\mathbf{U}^k$$

The correction, $\Delta\mathbf{U}^k = \mathbf{U}^{k+1} - \mathbf{U}^k$, is determined by:

$$\frac{\partial \mathbf{Res}}{\partial \mathbf{U}} \Delta\mathbf{U}^k = -\mathbf{Res}^k$$

- Jacobian: Exact for 2nd-order scheme
- Gauss-Seidel Relaxation

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- Jacobian: Exact for 2nd-order scheme
- Gauss-Seidel Relaxation

This is Newton's Method for second-order scheme.

Second-Order Discretization

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With simple trapezoidal rule for the source terms,

$$\Phi^C = \begin{bmatrix} -a(u_{i+1}-u_i)+\nu(p_{i+1}-p_i)-h_R\dfrac{\alpha}{\Delta t}(u_{i+1}+u_i)/2 \\ \dfrac{1}{T_r}\left[u_{i+1}-u_i-\dfrac{h_R}{2}(p_{i+1}+p_i)\right] \end{bmatrix}^{k+1}$$

$$+ \begin{bmatrix} \frac{h_R}{2}(\tilde{s}_{i+1}+\tilde{s}_i) \\ 0 \end{bmatrix}^{n-1,n}$$

Second-Order Discretization

With simple trapezoidal rule for the source terms, we get a uniform second-order scheme for all variables:

$$\Phi^C = \begin{bmatrix} -a(u_{i+1}-u_i) + \nu(p_{i+1}-p_i) - h_R \dfrac{\alpha}{\Delta t}(u_{i+1}+u_i)/2 \\ \dfrac{1}{T_r}\left[u_{i+1}-u_i-\dfrac{h_R}{2}(p_{i+1}+p_i)\right] \end{bmatrix}^{k+1}$$

$$+ \begin{bmatrix} \frac{h_R}{2}(\tilde{s}_{i+1}+\tilde{s}_i) \\ 0 \end{bmatrix}^{n-1,n}$$

$$\begin{aligned} T.E.\,(\partial_\tau p) &= \cancelto{0}{(\partial_x u_i - p_i)} + \frac{h}{2}\cancelto{0}{(\partial_{xx} u_i - \partial_x p_i)} \\ &+ \frac{h^2}{6}(\partial_{xxx} u_i - \frac{6}{4}\partial_{xx} p_i) + O(h^3) \end{aligned}$$

Extension to High-Order

$$\mathbf{\Phi}^C = \int_{x_i}^{x_{i+1}} (-\mathbf{A}\mathbf{U}_x + \mathbf{S})dx$$

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Methods

1. Divergence Formulation of Source Terms (RD-D)

Extension to High-Order

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Methods

1. Divergence Formulation of Source Terms (RD-D)

$$\int_{x_i}^{x_{i+1}} \mathbf{S}dx = \int_{x_i}^{x_{i+1}} \mathbf{f}_x^S dx$$

Extension to High-Order

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Methods

1. Divergence Formulation of Source Terms (RD-D)
$$\int_{x_i}^{x_{i+1}} \mathbf{S}dx = \int_{x_i}^{x_{i+1}} \mathbf{f}_x^S dx$$
2. General Trapezoidal Rule (RD-GT)

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Methods

1. Divergence Formulation of Source Terms (RD-D)
$$\int_{x_i}^{x_{i+1}} \mathbf{S}dx = \int_{x_i}^{x_{i+1}} \mathbf{f}_x^S dx$$
2. General Trapezoidal Rule (RD-GT)
$$\int_{x_i}^{x_{i+1}} \mathbf{S}dx = \frac{h_R}{2}(\mathbf{S}_L + \mathbf{S}_R)$$

Third-Order RD-D Scheme

- Third-Order Scheme:

Third-Order RD-D Scheme

- Third-Order Scheme:
  See the paper!

Fourth-Order RD-D Scheme

$$\mathbf{\Phi}^C = \int_{x_i}^{x_{i+1}} (-\mathbf{A}\mathbf{U}_x + \mathbf{f}_x^S)dx$$

We introduce a source function, f^S, based on mid-point:

$$\begin{aligned} f^S &= \sum_{n=1}^{m\geq 3} \frac{(-1)^{n-1}}{n!}(x-\bar{x})^n \partial_{x^{n-1}} S \\ &= (x-\bar{x})S - \frac{1}{2}(x-\bar{x})^2 \partial_x S + \frac{1}{6}(x-\bar{x})^3 \partial_{xx} S + \dots \end{aligned}$$

where $\bar{x} = (x_i + x_{i+1})/2$.

Fourth-Order RD-D Scheme

- What happens to our Original equation with the use of divergence formulation?

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  Let's consider $m = 3$; we have:

$$\partial_x f^S = S + \frac{(x-\bar{x})^3}{6}\partial_{xxx} S = S + O(h^3)$$

Fourth-Order RD-D Scheme

- What happens to our Original equation with the use of divergence formulation?

  Let's consider $m = 3$; we have:

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  - That is, we recover the original S up to $O(h^m)$.

Fourth-Order RD-D Scheme

- Examining the order of accuracy of the discretized system with the divergence form of the source term:

$$
\begin{aligned}
T.E.\,(\partial_\tau p) &= \underbrace{(\partial_x u_i - p_i)}_{0} + \frac{h_R}{2}\underbrace{(\partial_{xx} u_i - \partial_x p_i)}_{0} \\
&+ \frac{h_R^2}{6}\underbrace{(\partial_{xxx} u_i - \partial_{xx} p_i)}_{0} \\
&+ \frac{h_R^3}{24}\underbrace{(\partial_{xxxx} u_i - \partial_{xxx} p_i)}_{0} \\
&+ \frac{h_R^4}{120}(\partial_{xxxxx} u_i - \frac{5}{4}\partial_{xxxx} p_i) + O(h^5)
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- How come we got 4th-order instead of 3rd-order?

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- How come we got 4th-order instead of 3rd-order?
  Because we used the mid-point in the divergence formulation!

Overview of Fourth-Order RD-D Scheme

For uniform 4th-order results, we discretize the system as

$$
\begin{aligned}
\mathbf{\Phi}^C &= \int_{x_i}^{x_{i+1}} (-\mathbf{A}\mathbf{U}_x + \mathbf{S})dx \\
&\simeq \int_{x_i}^{x_{i+1}} (-\mathbf{A}\mathbf{U}_x + \mathbf{f}_x^S)dx \\
&\simeq -\mathbf{A}(\mathbf{U}_{i+1} - \mathbf{U}_i) + h_R\, \partial_x \mathbf{S}_i + \frac{h_R^2}{2}\, \partial_{xx} \mathbf{S}_i
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- The cost relative to 2nd-order?

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  - evaluation of the first derivative (2nd-order accurate)

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- The cost relative to 2nd-order?
  - evaluation of the first derivative (2nd-order accurate)
  - evaluation of the second derivative (1st-order accurate)
- We can use quadratic fit to evaluate the above derivatives.

Generalized Trapezoidal Rule

$$\mathbf{\Phi}^C = \int_{x_i}^{x_{i+1}} \left(-\mathbf{A}\mathbf{U}_x + \mathbf{S}\right) dx$$

Introducing a new source term integration:

$$\int \mathbf{S}\, dx \simeq \frac{h_R}{2}(\mathbf{S}_L + \mathbf{S}_R)$$

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$$\int \mathbf{S}\, dx \simeq \frac{h_R}{2}(\mathbf{S}_L + \mathbf{S}_R)$$

where we define the left and right states of S as

$$\begin{aligned} S_L &= S_i + C_1^L \partial_x S_i + C_2^L \partial_{xx} S_i \\ S_R &= S_{i+1} + C_1^R \partial_x S_{i+1} + C_2^R \partial_{xx} S_{i+1} \end{aligned}$$

Third-Order RD-GT Scheme

$$\int \mathbf{S}\, dx \simeq \frac{h_R}{2}[\mathbf{S}_i + \mathbf{S}_{i+1} \\ + (C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1}) \\ + (C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1})]$$

Note: The first two terms are what we had in 2nd-order. The rest are the corrections to get to high-order schemes.

- Third-Order RD-GT:

Third-Order RD-GT Scheme

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- Third-Order RD-GT:

$$C_1^L + C_1^R = 0, \quad C_1^R h_R + C_2^L + C_2^R = -\frac{h_R^2}{6}, \quad C_1^R h_R + 2C_2^R \neq -\frac{h_R^2}{6}$$

Third-Order RD-GT Scheme

$$\int \mathbf{S}\, dx \simeq \frac{h_R}{2}[\mathbf{S}_i + \mathbf{S}_{i+1} + (C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1}) + (C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1})]$$

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- Many possibilities, for example:

$$C_1^R = -C_1^L = -h_R/6$$
$$C_2^R = -C_2^L = -h_R^2/10$$

Fourth-Order RD-GT Scheme

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- Fourth-Order RD-GT:

$$C_1^L + C_1^R = 0, \quad C_1^R h_R + C_2^L + C_2^R = -\frac{h_R^2}{6}, \quad \frac{C_1^R}{2} h_R + C_2^R = -\frac{h_R^2}{12}$$

Fourth-Order RD-GT Scheme

$$\int \mathbf{S}\,dx \simeq \frac{h_R}{2}[\mathbf{S}_i + \mathbf{S}_{i+1}$$
$$+ (C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1})$$
$$+ (C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1})]$$

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- Again, many possibilities. In particular, we can select the most efficient and attractive coefficients:

Fourth-Order RD-GT Scheme

$$\int \mathbf{S}\,dx \simeq \frac{h_R}{2}[\mathbf{S}_i + \mathbf{S}_{i+1} + (C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1}) + (C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1})]$$

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$$C_1^L + C_1^R = 0, \quad C_1^R h_R + C_2^L + C_2^R = -\frac{h_R^2}{6}, \quad \frac{C_1^R}{2} h_R + C_2^R = -\frac{h_R^2}{12}$$

- Again, many possibilities. In particular, we can select the most efficient and attractive coefficients:

$C_1^R = -C_1^L = -h_R/6, \quad C_2^R = C_2^L = 0,$ no second derivatives!

Fourth-Order RD-GT Scheme

Expanding the cell residual around node i:

$$
\begin{aligned}
T.E.(\partial_\tau u_i) &= \cancelto{0}{(-a\partial_x u_i + \nu\partial_x p_i + S_i)} \\
&+ \cancelto{0}{\frac{h_R}{2}(-a\partial_{xx} u_i + \nu\partial_{xx} p_i + \partial_x S_i)} \\
&+ \cancelto{0}{\frac{h_R^2}{6}(-a\partial_{xxx} u_i + \nu\partial_{xxx} p_i + \partial_{xx} S_i)} \\
&+ \cancelto{0}{\frac{h_R^3}{24}(-a\partial_{xxxx} u_i + \nu\partial_{xxxx} p_i + \partial_{xxx} S_i)} \\
&+ \frac{h_R^4}{120}(-a\partial_{xxxxx} u_i + \nu\partial_{xxxxx} p_i + \frac{5}{6}\partial_{xxxx} S_i) + O(h^5) \\
&= 0 + O(h^4)
\end{aligned}
$$

Sixth-Order RD-GT Schemes

$$\int \mathbf{S}\,dx \simeq \frac{h_R}{2}[\mathbf{S}_i + \mathbf{S}_{i+1} + (C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1}) + (C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1})]$$

- Fifth-Order RD-GT:

Sixth-Order RD-GT Schemes

$$\int \mathbf{S}\, dx \simeq \frac{h_R}{2}[\mathbf{S}_i + \mathbf{S}_{i+1} + (C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1}) + (C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1})]$$

- Fifth-Order RD-GT:

  Fourth-Order Constraints & $\frac{C_1^R}{3} h_R + C_2^R = -\frac{h_R^2}{20}$

Sixth-Order RD-GT Schemes

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- A Unique Solution:

$$C_1^R = -C_1^L = -h_R/5$$
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Sixth-Order RD-GT Schemes

$$\int \mathbf{S}\, dx \simeq \frac{h_R}{2}\Big[\mathbf{S}_i + \mathbf{S}_{i+1} + \left(C_1^L \partial_x S_i + C_1^R \partial_x S_{i+1}\right) + \left(C_2^L \partial_{xx} S_i + C_2^R \partial_{xx} S_{i+1}\right)\Big]$$

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$$C_1^R = -C_1^L = -h_R/5$$
$$C_2^R = C_2^L = h_R^2/60$$

- Why then 6th-order not fifth-order?

  Because the Sixth-Order Constraint $\frac{C_1^R}{4} h_R + C_2^R = -\frac{h_R^2}{30}$ is also satisfied!

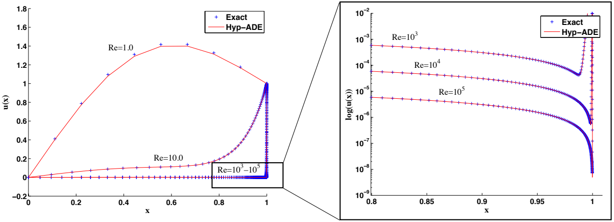
Some Results

Steady state boundary layer problem:

$$\partial_t u + a\partial_x u = \nu\partial_{xx} u + s(x)$$

where

$$s(x) = \frac{\pi}{Re}[a\cos(\pi x) + \pi\nu\sin(\pi x)], \; Re = a/\nu.$$



- GS-Relaxation: 2 orders of magnitude reduction
- Residual tolerance: $\leq 10^{-8}$

$O(N)$ + Newton Convergence

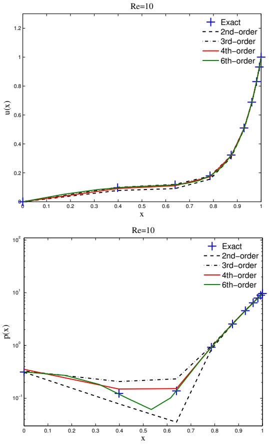
- Fast and Newton + $O(N)$ convergence on irregular grids
- 2nd-order Jacobian acts like exact for 3rd, 4th, and 6th-order schemes

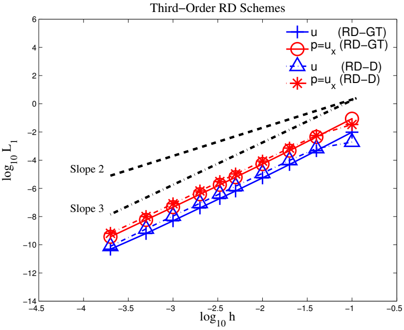
Table: Boundary layer problem (Residuals Criteria : $< 10^{-8}$.)

Nodes	Scheme Order	GS /Newton	Newton iteration
50	3rd	163	8
	4th	163	8
	6th	163	8
100	3rd	324	7
	4th	324	7
	6th	324	7
500	3rd	1647	7
	4th	1647	7
	6th	1647	7

Boundary Layer Problem: 3rd-Order

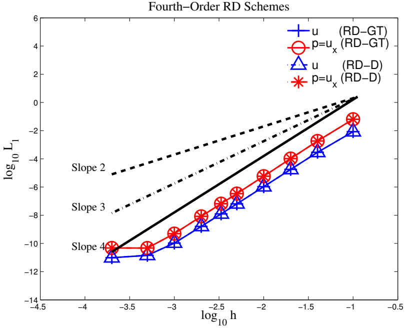
Solutions and Convergence on Irregular Grids



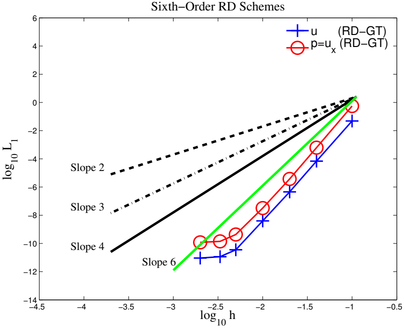


Boundary Layer Problem: 4th- and 6th-Order

Convergence on Irregular Grids



(a) fourth-order ($Re = 1$)



(b) sixth-order ($Re = 10$)

Unsteady Non-Linear Problem

Problem Statement:

$$\partial_t u + \partial_x f = \partial_x \left(\nu \, u_x\right) + S(x,t), \quad x \in (0,1)$$

where $f = u^2/2$, $\nu = u$, and

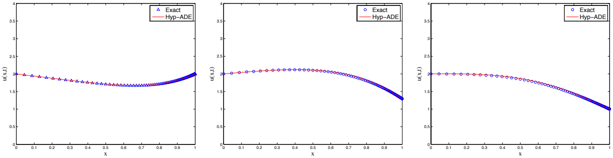
$$S(x,t) = u^e_t + \frac{1}{2}((u^e)^2)_x - (u^e_x)^2 - u^e u^e_{xx}$$

Exact Solution:

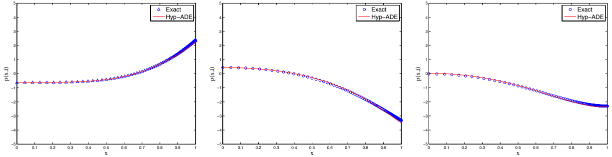
$$u^e(x,t) = Real\left(\frac{\sinh(x\sqrt{i\omega/\nu})}{\sinh(\sqrt{i\omega/\nu})} U e^{i\omega t}\right) + C, \; C > 1$$

Unsteady Non-Linear Problem

Solution: time



Solution gradient:



- GS-Relaxation: 2 orders of magnitude reduction
- Residual tolerance: $\leq 10^{-8}$

Unsteady Non-Linear Problem

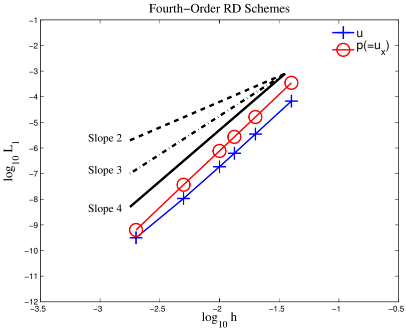
$O(N)$ Convergence and Newton!

Table: Average data over 1000 time steps are shown (Irregular Grids.)

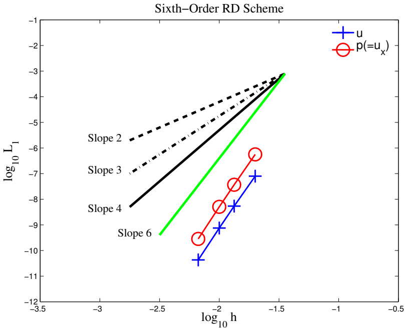
Nodes	RD-GT Scheme Order	GS/Newton	Newton
50	3rd	435	10
	4th	430	10
	6th	431	10
100	3rd	879	10
	4th	868	10
	6th	864	10
200	3rd	1772	10
	4th	1749	10
	6th	1737	10

Unsteady Non-Linear Problem: 4th- and 6th-Order

Convergence on Irregular Grids



(c) fourth-order + BDF4



(d) sixth-order + BDF6

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- Proposed two new source integration techniques:
  1) a new divergence formulation
  2) corrections to the trapezoidal rule
- Proposed a fourth-order scheme that compared to the second-order scheme only costs evaluation of first-derivative of the source term
- Shown $O(N)$ convergence rate for the linear system + Newton for all the proposed high-order schemes

Works Underway:

- Extension to multi-dimensions (snapshot in the next slide)

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- Effects of separating advection and diffusion eigen structures

Works Underway: Extensions to Multi-Dimensions

Problem: Steady 2D Advection-Diffusion

$$\partial_t u + a\,\partial_x u + b\,\partial_y u = \nu\,(\partial_{xx} u + \partial_{yy} u)$$

Exact Solution:

$$u(x,y) = C\cos(A\pi\eta)\exp\left(\frac{-2A^2\pi^2\nu}{1+\sqrt{1+4A^2\pi^2\nu^2}}\xi\right),$$

where $\xi = ax + by$, $\eta = bx - ay$.

- Problem Setup: u is specified on the boundaries.
  Solve for u, $\partial_x u$ and $\partial_y u$.
- GS-Relaxation: 1000 or 5 orders of magnitude reduction
- Residual tolerance: $\leq 10^{-11}$

Works Underway: Extensions to Multi-Dimensions

Newton: 3; GS/Newton : ≤ 300; $a = 2, b = 1, \nu = 0.01$