Implicit Two-Derivative Runge-Kutta Methods

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(joint work with Shixiao Wang and Robert Chan)

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Outline of Topics

Basic Background

- Two-derivative Runge-Kutta (TDRK) methods belong to the family of multi-derivative Runge-Kutta methods – they are one-step multi-stage methods.
- We consider an autonomous ODE system $y'(t) = f(y)$ with initial condition $y_0 = y(t_0)$ and known second derivative $y''(t) = f'(y)f(y) =: g(y)$.
- Numerical Scheme:

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_j) + h^2 \sum_{j=1}^{s} \widehat{a}_{ij} g(Y_j), \quad i = 1, \ldots, s,$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_i) + h^2 \sum_{i=1}^{s} \widehat{b}_i g(Y_i).$$

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- In a non-autonomous system, the variable t can be treated as a component of the y vector.
- Block Matrix Form:

$$Y = e \otimes y_n + h(A \otimes I_N)F(Y) + h^2(\widehat{A} \otimes I_N)G(Y),$$
$$y_{n+1} = y_n + h(b^T \otimes I_N)F(Y) + h^2(\widehat{b}^T \otimes I_N)G(Y),$$

where $e = [1]_{s\times 1}$, $A = [a_{ij}]_{s\times s}$, $\widehat{A} = [\widehat{a}_{ij}]_{s\times s}$, $b = [b_i]_{s\times 1}$, $\widehat{b} = [\widehat{b}_i]_{s\times 1}$, and

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F(Y) = \begin{bmatrix} f(Y_1) \\ f(Y_2) \\ \vdots \\ f(Y_s) \end{bmatrix}, \quad G(Y) = \begin{bmatrix} g(Y_1) \\ g(Y_2) \\ \vdots \\ g(Y_s) \end{bmatrix}.$$

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- Extended Butcher Tableau:

$$\begin{array}{c|c||c} c & A & \widehat{A} \\ \hline & b^T & \widehat{b}^T \end{array}$$

- Stability Function: For the standard test problem $y'(t) = \lambda y$, $y_{n+1} = R(z) y_n$, where

$$R(z) = 1 + (zb^T + z^2 \widehat{b}^T)(I - zA - z^2 \widehat{A})^{-1} e, \quad \text{with } z = h\lambda.$$

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(t_n, y_n) •

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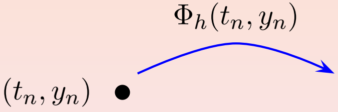

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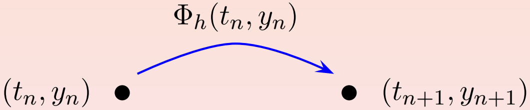

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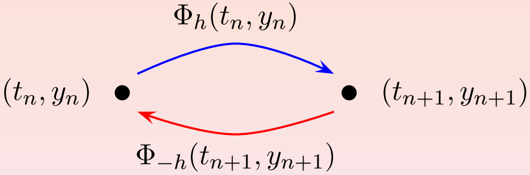

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\begin{aligned}
PAP &= eb^T - A \\
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Pb &= b \\
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  where P is the permutation matrix which reverses the stages.

- Order Conditions: As for RK methods, we compare the Taylor Series expansions of the exact and numerical solutions, $y(t_n + h)$ and y_{n+1} respectively, to derive the order conditions of methods.

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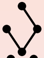
Order Conditions

- Order conditions assuming $C(1)$:

Order	Tree	Order Condition
1		$b^T e = 1$
2		$b^T c + \widehat{b}^T e = \frac{1}{2}$
3		$b^T c^2 + 2\widehat{b}^T c = \frac{1}{3}$
		$b^T A c + b^T \widehat{A} e + \widehat{b}^T c = \frac{1}{6}$
4		$b^T c^3 + 3\widehat{b}^T c^2 = \frac{1}{4}$
		$b^T c A c + b^T c \widehat{A} e + \widehat{b}^T c^2 + \widehat{b}^T A c + \widehat{b}^T \widehat{A} e = \frac{1}{8}$
		$b^T A c^2 + 2 b^T \widehat{A} c + \widehat{b}^T c^2 = \frac{1}{12}$
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		$b^T cAc + b^T c\widehat{A}e + \widehat{b}^T c^2 + \widehat{b}^T Ac + \widehat{b}^T \widehat{A}e = \frac{1}{8}$
		$b^T Ac^2 + 2b^T \widehat{A}c + \widehat{b}^T c^2 = \frac{1}{12}$
		$b^T A^2 c + b^T A\widehat{A}e + b^T \widehat{A}c + \widehat{b}^T Ac + \widehat{b}^T \widehat{A}e = \frac{1}{24}$

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- Stage Order Conditions:

$$C(q): \quad Ac^{k-1} + (k-1)\widehat{A}c^{k-2} = \frac{c^k}{k}, \quad k = 1, \ldots, q.$$

- Bushy Tree Conditions:
- Example of Labelling Trees:

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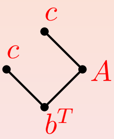

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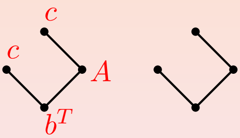

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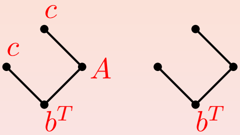

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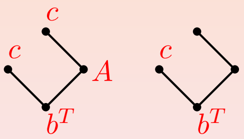

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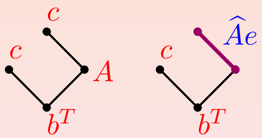

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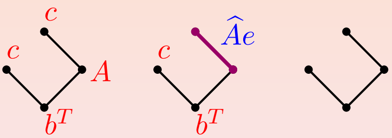

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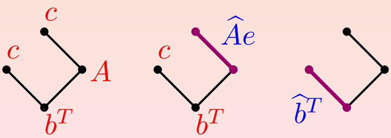

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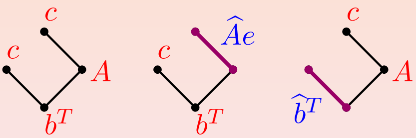

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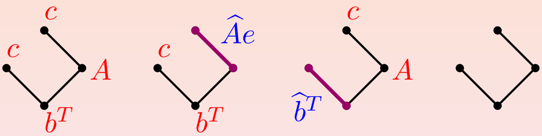

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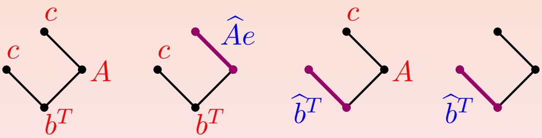

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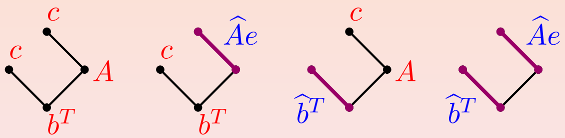

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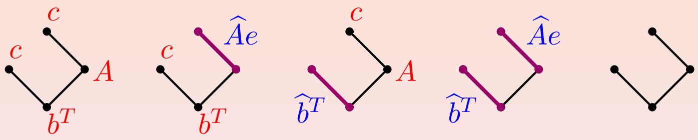

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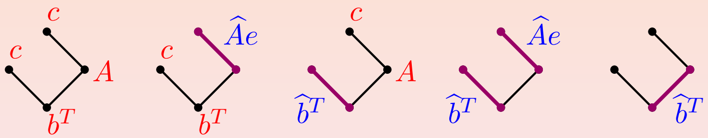

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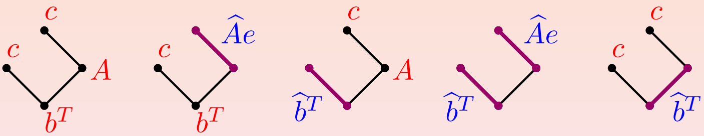

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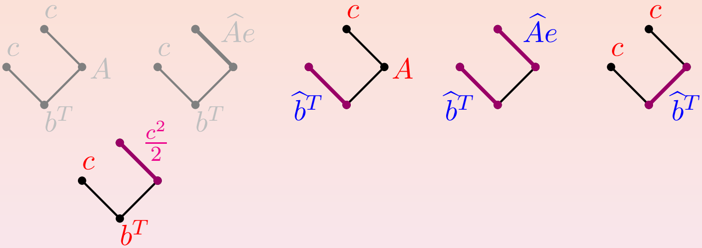

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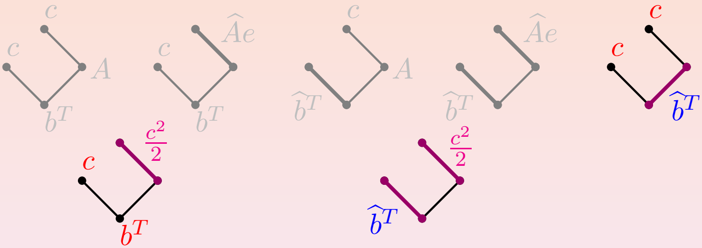

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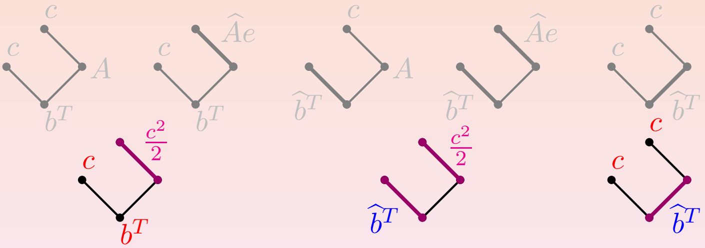

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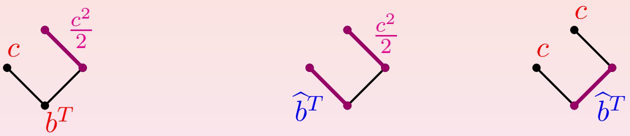

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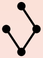
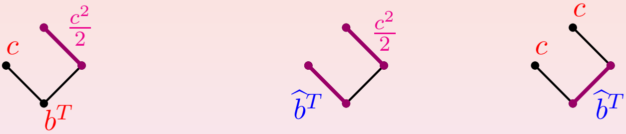
$$\tfrac{1}{2}b^T c^3 + \tfrac{3}{2}\widehat{b}^T c^2 = \tfrac{1}{8}$$ 



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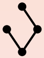
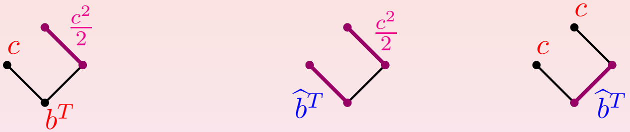
$$\tfrac{1}{2} b^T c^3 + \tfrac{3}{2}\widehat{b}^T c^2 = \tfrac{1}{8}$$ 

$$b^T c^3 + 3\widehat{b}^T c^2 = \tfrac{1}{4}$$ 



Constructing Explicit TDRK Methods

- In our study, we include two special groups of explicit TDRK methods:

GROUP A:

$$\begin{array}{c|c||c} c & Ae_1 & \widehat{A} \\ \hline & b_1 & \widehat{b}^T \end{array} \Rightarrow \begin{array}{c||c} c & \widehat{A} \\ \hline & \widehat{b}^T \end{array}$$

GROUP B:

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- TDRK45b/TDRK5b: $p = 5, q = 2$

0	0	0	0	0	
$\frac{1}{3}$	$\frac{1}{18}$	0	0	0	
$\frac{1}{2}$	$\frac{1}{8}$	0	0	0	
$\frac{4}{5}$	$-\frac{2}{125}$	$\frac{42}{125}$	0	0	
1	$\frac{5}{48}$	$\frac{9}{28}$	0	$\frac{25}{336}$	order 5
1	$\frac{1}{6}$	0	$\frac{1}{3}$	0	order 4

- TDRK5b requires $1f + 3g$ function evaluations per step, and $R(z) = 1 + z + \frac{z^2}{2} + \frac{z^3}{6} + \frac{z^4}{24} + \frac{z^5}{120} + \frac{z^6}{720}$.
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- The implicit TDRK methods we constructed range from order 3 to 6, the order-3 and 5 methods are L-stable and the order-4 and 6 methods are A-stable.

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$$y'(t) = \lambda(y(t) - \phi(t)) + \phi'(t),$$

we show the results for $\phi(t) = \sin(t)$ and two cases for the implicit methods,

  - PR1b: $y_0 = \phi_0$ and $\lambda = -10^4$. Exact solution is $y(t) = \phi(t)$.
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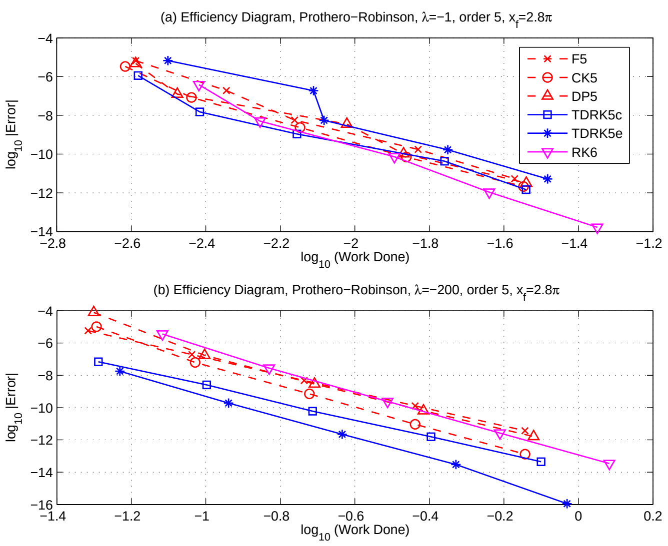
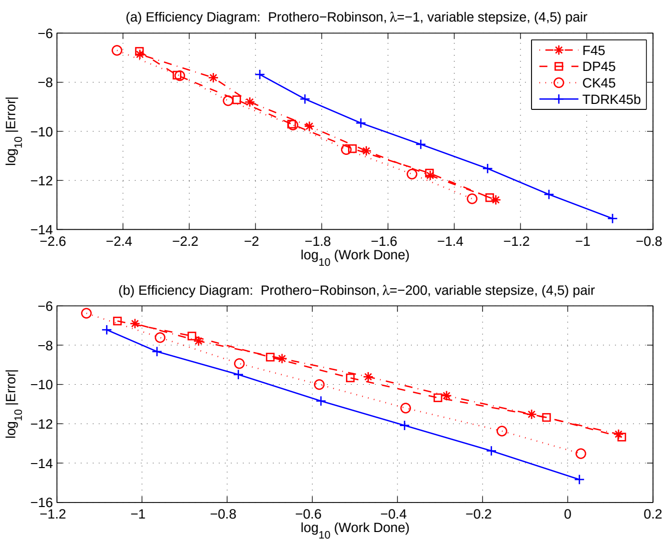
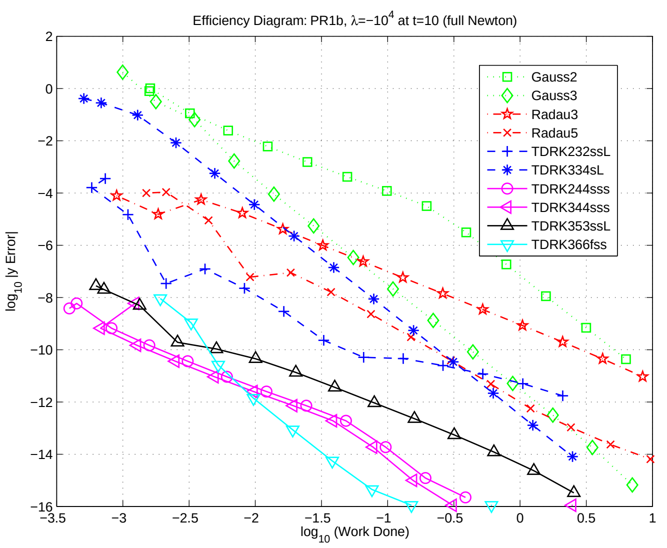


Embedded Explicit Methods for PR Problem



Implicit Methods for PR Problem



Implicit Methods for PR Problem

- Order Behaviour – Error for PR problem when $h \to 0$ and $z = \lambda h \to \infty$:

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p	Method	Local Error	Global Error

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4	TDRK244sss	$O(h^5/z^2) = O(h^3/\lambda^2)$	$O(h^2/\lambda^2)$
4	TDRK344sss	$O(h^5/z^2) = O(h^3/\lambda^2)$	$O(h^2/\lambda^2)$

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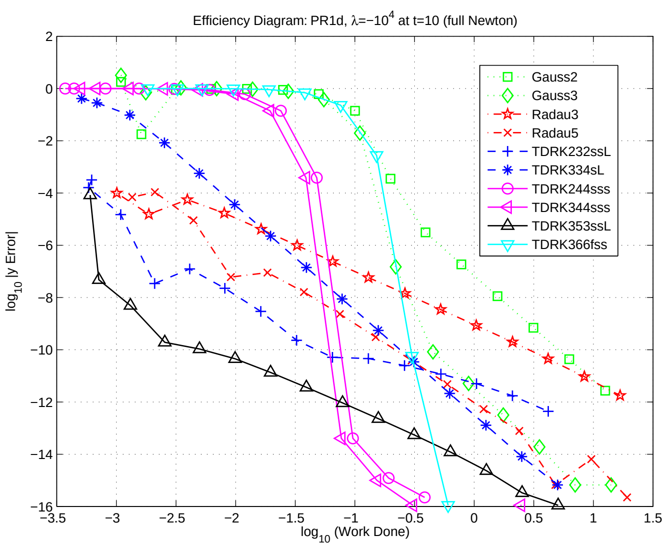
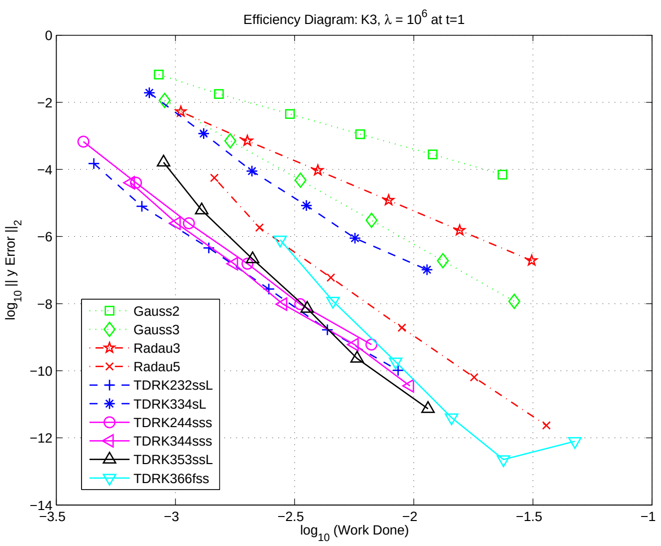
6	TDRK366fss	$O(h^7/z^2) = O(h^5/\lambda^2)$	$O(h^4/\lambda^2)$

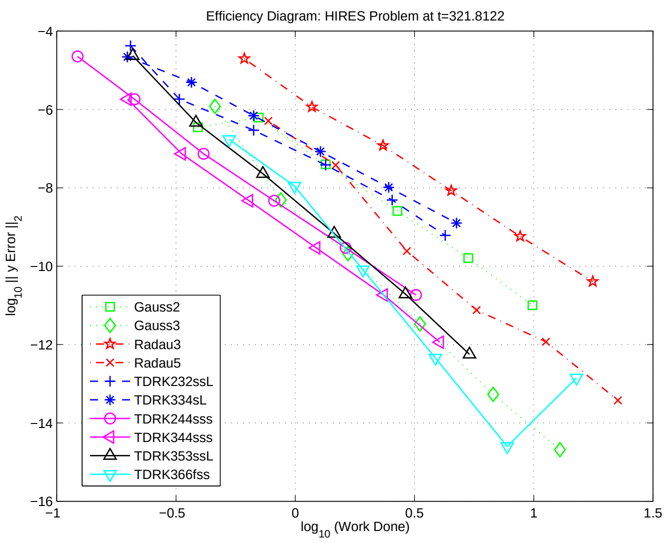
Implicit Methods for PR Problem



Implicit Methods for Kaps Problem



Implicit Methods for HIRES Problem



Classical PDE Methods

- Semi-discretization (or Method of Lines) is used to approximate PDEs by
  - firstly, discretize the spatial variables of PDEs to get a set of ODEs,
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- However, many popular classical PDE methods are not MOL. Why?
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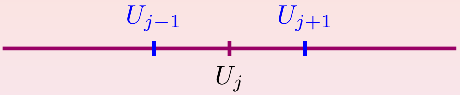

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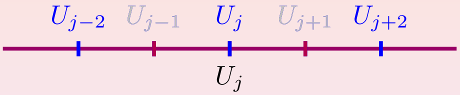

Classical PDE Methods

- Consider the advection/wave equation,

  $$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \quad \text{on the interval } (0,1) \text{ with } u(0,t) = u(1,t).$$

- By using central differences, we semi-discretize the PDE to an ODE system $d\mathbf{u}(t)/dt = A_h\mathbf{u}(t)$ with spatial stepsize $h = 1/N$, and then integrate the system by an explicit RK method with temporal stepsize δ. It follows that z^* must stay inside the stability region of the RK method to ensure the time integration is stable, where $z^* = \delta\lambda_k$, for $k = 1, \ldots, N$ and λ_k are the eigenvalues of A_h.

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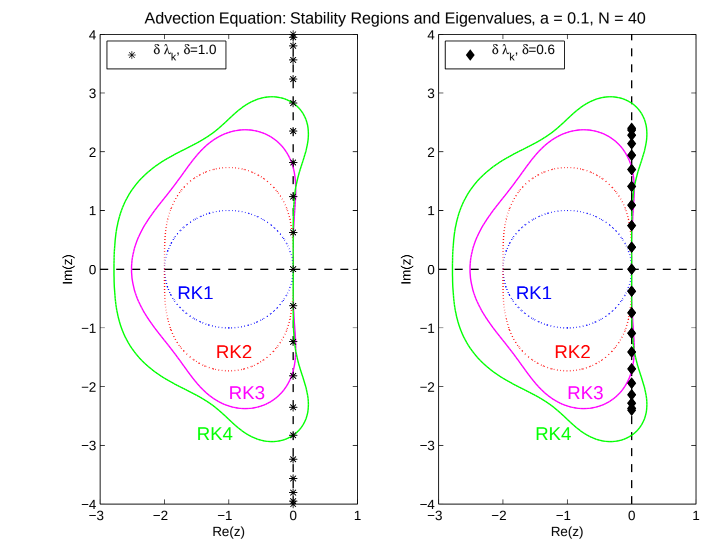
Classical PDE Methods – Method of Lines



A Novel Semi-Discretization Method

- We want to develop new discretization methods which overcome the disadvantages of MOL and unify MOL and other classical PDE methods under the same RK/TDRK structure.
- The idea is simple: we discretize the temporal variable t first. This means that the spatial discretization can then be chosen in a more flexible way to meet stability and/or computational requirements.
- Let $f(\eta)$ be a smooth function of η and we examine

$$\frac{\partial u}{\partial t} = f(\mathcal{P}(u)), \tag{1}$$

where $\mathcal{P}(u)$ be a linear partial differential operator with constant coefficients. For examples: $\mathcal{P}(u) = \frac{\partial}{\partial x} u$ and $\mathcal{P}(u) = \frac{\partial^2}{\partial x^2} u$.

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- Differentiate (1) with respect to t, we get

$$\frac{\partial^2 u}{\partial t^2} = f_\eta(\mathcal{P}(u))\mathcal{P}(f(\mathcal{P}(u))) = f_\eta \mathcal{P}(f).$$

- Compare with $\frac{d^2 y}{dt^2} = f_y f$ for $y'(t) = f(y)$.
- Similarly, we can derive all the higher derivatives and apply the tree theory for ODEs on PDEs.
- This enables us to apply ODE methods directly to PDEs.
- If we apply the explicit trapezoidal rule to the wave equation with appropriate compact schemes to approximate the spatial derivatives, we have a method which has order-2 behaviour in both time and space. In fact, this is the well-known Lax-Wendroff scheme.

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An Application to PDE

- One popular method for solving PDE problems, such as the heat equation, is Crank-Nicolson method, which is an order-2 method.
- Heat Equation:

$$U_t = U_{xx},$$

  with I.C. $U(x, 0) = \sin(\pi x)$ and B.C. $U(0, t) = U(1, t) = 0$.
- Crank-Nicolson method: use 3-point second order approximation to U_{xx} and implicit midpoint or trapezoidal rule to solve the resulting tridiagonal system of ODEs.

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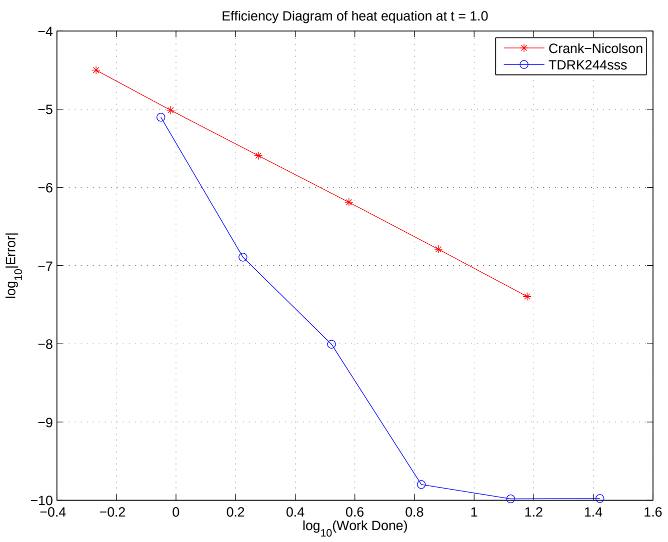

Heat Equation and Order Reduction

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- Analyze the diffusion equation with non-homogeneous boundary values

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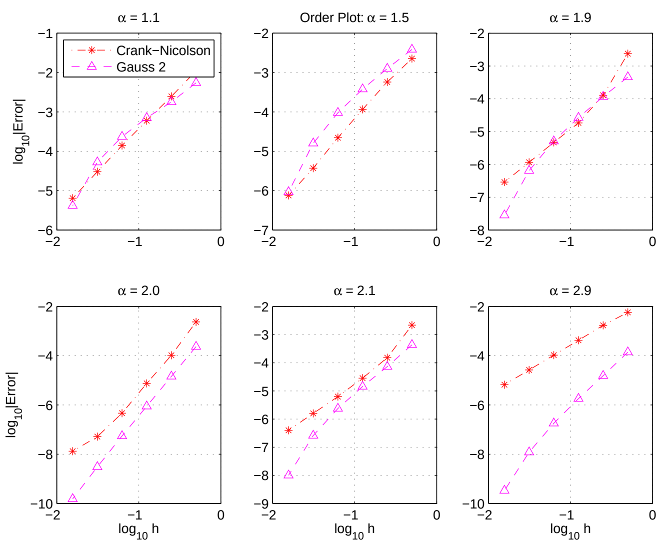

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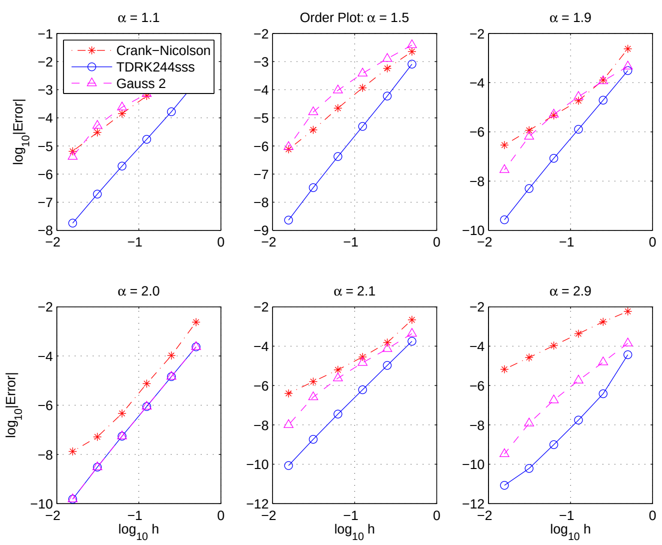

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