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On Exponential Integrators

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Outline

- Motivation
- History
- Numerical schemes
- Numerical experiments
- Generalized IF methods
- Conclusions
- Future work

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Motivation

A new interest in exponential integrators for semilinear problems

$$u_t = \mathcal{L}u + \mathcal{N}(u, t), \quad u(t_0) = u_0$$

where \mathcal{L} is a higher-order linear term and \mathcal{N} is low-order nonlinear term.

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where \mathcal{L} is a higher-order linear term and \mathcal{N} is low-order nonlinear term.

After discretization in space we obtain a systems of ODEs

$$u_t = \mathbf{L}u + \mathbf{N}(u(t)) = \mathbf{F}(u, t), \quad u(t_0) = u_0$$

History

- Certaine, 1960
 - Implicit ETD3?

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- Hochbruck and Lubich, 1997
 - Exp. Integrators (EXP4) with inexact Jacobian

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 - Exp. Collocation Methods, convergence analyze

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Rosenbrock Methods

$$\begin{aligned} k_i &= h\mathbf{F}\left(u_0 + \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + h\mathbf{J} \sum_{j=1}^{i-1} \gamma_{i,j} k_j + h\mathbf{J}\gamma k_i \\ u_1 &= u_0 + \sum_{j=1}^s \beta_j k_j, \end{aligned}$$

where $J = \frac{\partial F}{\partial u}$

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or

$$\begin{aligned} (I - h\gamma\mathbf{J})k_i &= h\mathbf{F}\left(u_0 + \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + h\mathbf{J} \sum_{j=1}^{i-1} \gamma_{i,j} k_j \\ u_1 &= u_0 + \sum_{j=1}^s \beta_j k_j, \end{aligned}$$

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W - Methods

$$\begin{aligned} k_i &= h\mathbf{L}\left(u_0 + \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + h\mathbf{N}\left(u_0 + \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + h\mathbf{L} \sum_{j=1}^{i-1} \gamma_{i,j} k_j + h\mathbf{L}\gamma k_i \\ u_1 &= u_0 + \sum_{j=1}^s \beta_j k_j, \end{aligned}$$

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or

$$\begin{aligned} (I - h\gamma\mathbf{L})k_i &= h\mathbf{L}\left(u_0 + \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + h\mathbf{N}\left(u_0 + \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + h\mathbf{L} \sum_{j=1}^{i-1} \gamma_{i,j} k_j \\ u_1 &= u_0 + \sum_{j=1}^s \beta_j k_j, \end{aligned}$$

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$$\begin{aligned} U_i &= u_0 + h \mathbf{L} \sum_{j=1}^{i-1} A_{i,j} u_0 + h \sum_{j=1}^{i-1} A_{i,j} N(U_j) \\ u_1 &= u_0 + h \mathbf{L} \sum_{j=1}^s B_j u_0 + h \sum_{j=1}^s B_j N(U_j), \end{aligned}$$

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where

$$A = \alpha(\Gamma - h\tilde{L}\alpha)^{-1}$$

$$B = \beta(\Gamma - h\tilde{L}\alpha)^{-1}$$

$$\tilde{L} = \text{diag}(L, \dots, L)$$

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Denote

$$\begin{aligned} R_i^{[0]}(c_i h\mathbf{L}) &= I + h\mathbf{L} \sum_{j=1}^{i-1} A_{i,j} \\ R_{s+1}^{[0]}(h\mathbf{L}) &= I + h\mathbf{L} \sum_{j=1}^{i-1} B_j \end{aligned}$$

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Then the method is

$$\begin{aligned} U_i &= R_i^{[0]}(c_i h\mathbf{L}) u_0 + h \sum_{j=1}^{i-1} A_{i,j} N(U_j) \\ u_1 &= R_{s+1}^{[0]}(h\mathbf{L}) u_0 + h \sum_{j=1}^s B_j N(U_j), \end{aligned}$$

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and

$$R_i^{[l+1]}(z) = \frac{R_i^{[l]}(z) - R_i^{[l]}(0)}{z}$$

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Exp. Integrators of H&L

They are a modification of Rosenbock Methods

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- Methods with inexact Jacobian suffer from order reductions

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Integrating Factor

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Solve exactly the linear part then make a change of variables

$$\begin{aligned} v(t) &= \exp(-\mathbf{L}t)u(t) \\ \underbrace{\exp(-\mathbf{L}t)(u_t - \mathbf{L}u)}_{v_t} &= \exp(-\mathbf{L}t)\mathbf{N}(u) \\ v_t &= \exp(-\mathbf{L}t)\mathbf{N}(\exp(\mathbf{L}t)v) \end{aligned}$$

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Transform back the approximate solution to the original variable

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Example of IF

In terms of the original variable the computations performed are

$$U_1 = u_0$$

$$U_2 = e^{c_2 h L} (u_0 + a_{21} h N(U_1))$$

$$U_3 = e^{c_3 h L} (u_0 + a_{31} h N(U_1) + a_{32} h e^{-c_2 h L} N(U_2))$$

$$\begin{aligned} U_4 = & e^{c_4 h L} (u_0 + a_{41} h N(U_1) + a_{42} h e^{-c_2 h L} N(U_2) \\ & + a_{43} h e^{-c_3 h L} N(U_3)) \end{aligned}$$

$$\begin{aligned} u_1 = & e^{h L} (u_0 + b_1 h N(U_1) + b_2 h e^{-c_2 h L} N(U_2) \\ & + b_3 h e^{-c_3 h L} N(U_3) + b_4 h e^{-c_4 h L} N(U_4)) \end{aligned}$$

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Example of IF

General form of the order 4 integrating factor method is

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & 1 \\ a_{21}e^{c_2 hL} & 0 & 0 & 0 & e^{c_2 hL} \\ a_{31}e^{c_3 hL} & a_{32}e^{(c_3 - c_2)hL} & 0 & 0 & e^{c_3 hL} \\ a_{41}e^{c_4 hL} & a_{42}e^{(c_3 - c_2)hL} & a_{43}e^{(c_4 - c_3)hL} & 0 & e^{c_4 hL} \\ \hline b_1e^{hL} & b_2e^{(1-c_2)hL} & b_3e^{(1-c_3)hL} & b_4e^{(1-c_4)hL} & e^{hL} \end{array} \right]$$

- Uniformly distributed c vector provides cheapest methods.
- This structure requires only classical order conditions.

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Exponential Time Differencing

Similar approach to *IF* but we do not make a complete change of variables

$$\frac{d}{dt}(\exp(-\mathbf{L}t)u) = \exp(-\mathbf{L}t)\mathbf{N}(u(t))$$

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Integrate over a single time step of length $c_i h$

$$u(t_n + c_i h) = \exp(c_i h \mathbf{L}) u_n + \exp(c_i h \mathbf{L}) \int_0^{c_i h} \exp(-\mathbf{L}\tau) \mathbf{N}(u(t_n + \tau)) d\tau$$

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ETD methods of multistep type use polynomial approximation to the function $\mathbf{N}(u(t_n + \tau))$

(Nørsett'69,..., Cox and Matthews'02)

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Approximations to $N(u(t))$

- If $N(u(t)) \approx \delta_i e^{Lt}$, where δ_i is a constant such that the approximation matches $N(u(t))$ for $t = c_i h$, then the coefficients of the method will be linear combinations of

$$\phi^{[i]}(\lambda)(hL) = e^{(\lambda - c_i)hL} \quad i = 1, 2, 3, \dots$$

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Approximations to $N(u(t))$

- If $N(u(t)) \approx P_{s-1}(t)$, where $P_{s-1}(t)$ is a Lagrange interpolation polynomial of degree $s - 1$ that matches $N(u(t))$ at the points $t = c_1 h, c_2 h, \dots, c_s h$ then

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$$\phi^{[1]}(\lambda)(hL) = \frac{e^{\lambda hL} - I}{\lambda hL}, \quad \phi^{[2]}(\lambda)(hL) = \frac{e^{\lambda hL} - \lambda hL - I}{(\lambda hL)^2},$$

$$\phi^{[i+1]}(\lambda)(hL) = \frac{\phi^{[i]}(\lambda)(hL) - \phi^{[i]}(0)(hL)}{\lambda hL} \quad i = 1, 2, 3, \dots$$

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$$\phi^{[1]}(\lambda)(hL) = 1I_m + \frac{\lambda}{2!}hL + \frac{\lambda^2}{3!}(hL)^2 + \frac{\lambda^3}{4!}(hL)^3 + \frac{\lambda^4}{5!}(hL)^4 + \dots,$$

$$\phi^{[2]}(\lambda)(hL) = \frac{1}{2!}I_m + \frac{\lambda}{3!}(hL) + \frac{\lambda^2}{4!}(hL)^2 + \frac{\lambda^3}{5!}(hL)^3 + \frac{\lambda^4}{6!}(hL)^4 + \dots,$$

$$\phi^{[3]}(\lambda)(hL) = \frac{1}{3!}I_m + \frac{\lambda}{4!}(hL) + \frac{\lambda^2}{5!}(hL)^2 + \frac{\lambda^3}{6!}(hL)^3 + \frac{\lambda^4}{7!}(hL)^4 + \dots.$$

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- If $N(u(t)) \approx P_{s-1}(t)$, where $P_{s-1}(t)$ is a Lagrange interpolation polynomial of degree $s-1$ that matches $N(u(t))$ at the points $t = c_1 h, c_2 h, \dots, c_s h$ then

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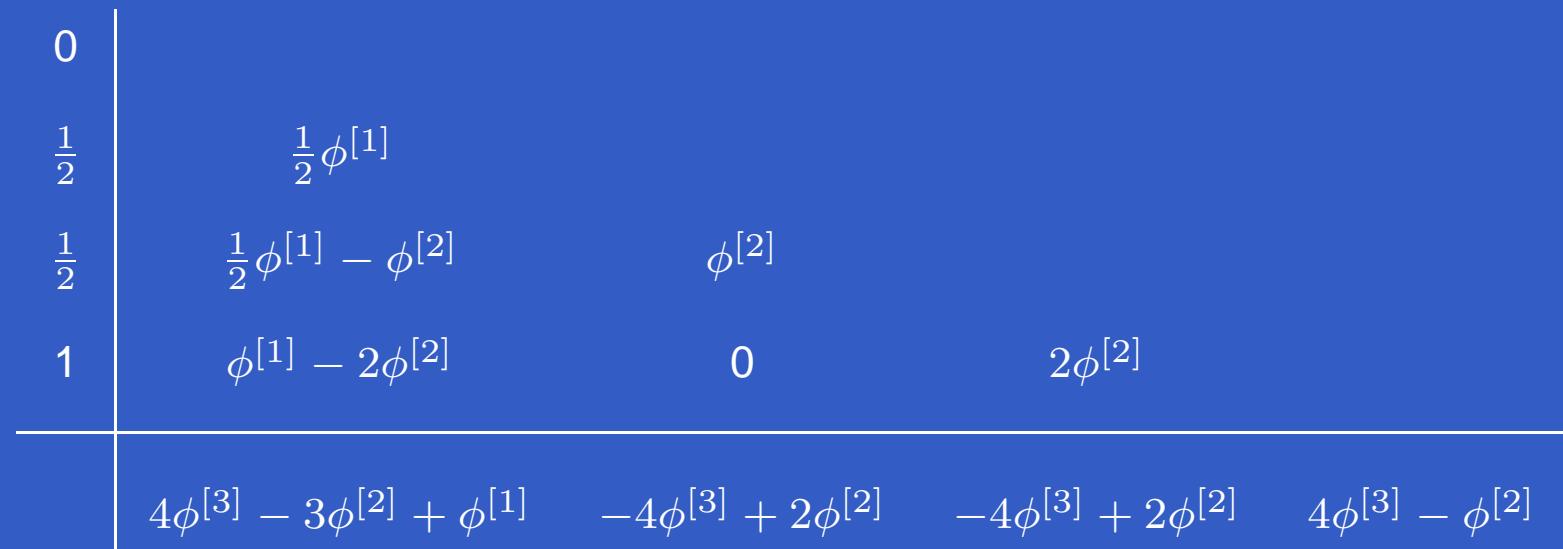
- If $N(u(t)) \approx T_{s-1}(t)$, where $T_{s-1}(t)$ is a trigonometrical polynomial of $\sin(\alpha t)$, then

$$\phi^{[1]}(\lambda)(hL) = \frac{e^{\lambda hL} - I}{\lambda hL}, \quad \phi^{[2]}(\lambda)(hL) = \frac{e^{\lambda hL} - L \sin(\lambda h) - \cos(\lambda h)}{\lambda h(L + I)^2},$$

$$\phi^{[\alpha+1]}(\lambda)(hL) = \frac{\alpha e^{\lambda hL} - L \sin(\alpha \lambda h) - \alpha \cos(\alpha \lambda h)}{\lambda h(L^2 + \alpha^2 I)} \quad \alpha = 1, 2, 3, \dots$$

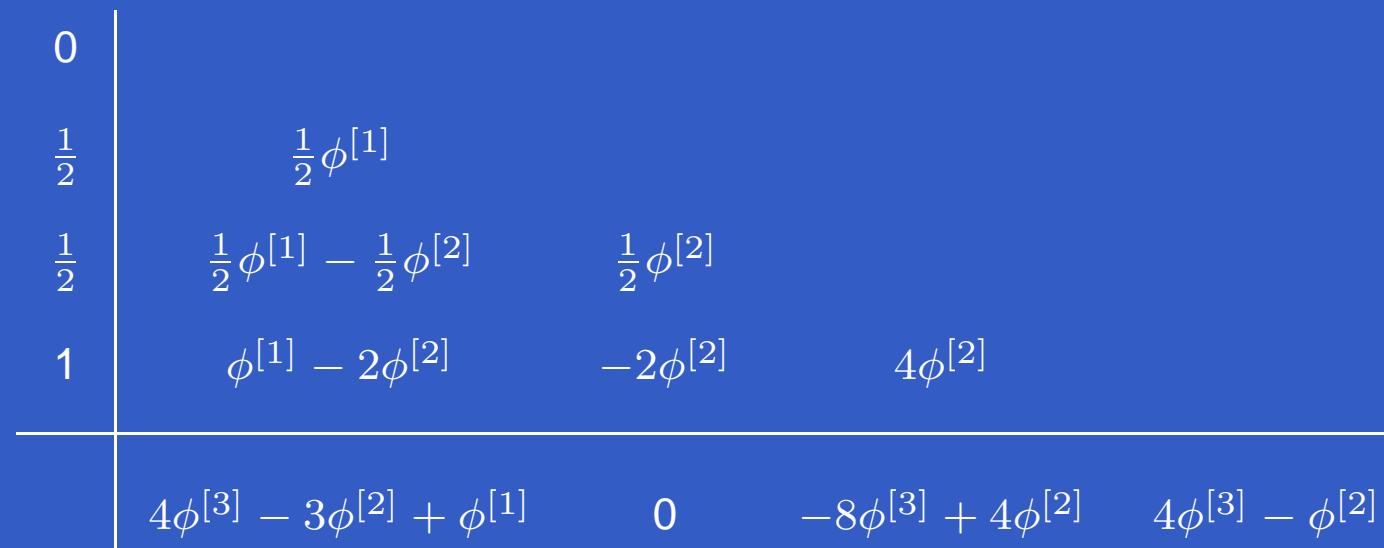
ETD4 Methods

ETD4-Kr of Krogstad



ETD4 Methods

ETDRK4SW of Strehmel and Weiner



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ETD5 Method

$$\begin{aligned}\alpha_{21}^{(1)} &= \frac{1}{4}, & \alpha_{31}^{(1)} &= \frac{1}{4}, & \alpha_{41}^{(1)} &= \frac{1}{2}, & \alpha_{51}^{(1)} &= \frac{3}{4}, & \alpha_{61}^{(1)} &= 1, \\ \alpha_{31}^{(2)} &= -\frac{1}{4}, & \alpha_{32}^{(2)} &= \frac{1}{4}, & \alpha_{41}^{(2)} &= -1, & \alpha_{43}^{(2)} &= 1, & \alpha_{51}^{(2)} &= -\frac{29}{8}, \\ \alpha_{52}^{(2)} &= \frac{5}{4}, & \alpha_{53}^{(2)} &= \frac{15}{4}, & \alpha_{54}^{(2)} &= -\frac{11}{8}, & \alpha_{61}^{(2)} &= -\frac{40}{21}, & \alpha_{62}^{(2)} &= -\frac{32}{7}, \\ \alpha_{63}^{(2)} &= \frac{4}{7}, & \alpha_{64}^{(2)} &= \frac{68}{7}, & \alpha_{65}^{(2)} &= -\frac{80}{21}, & \alpha_{51}^{(3)} &= \frac{15}{2}, & \alpha_{52}^{(3)} &= -6, \\ \alpha_{53}^{(3)} &= -9, & \alpha_{54}^{(3)} &= \frac{15}{2}, & \alpha_{61}^{(3)} &= -\frac{20}{7}, & \alpha_{62}^{(3)} &= \frac{144}{7}, & \alpha_{63}^{(3)} &= \frac{24}{7}, \\ \alpha_{64}^{(3)} &= -\frac{276}{7}, & \alpha_{65}^{(3)} &= \frac{128}{7}, & \beta_1^{(1)} &= 1, & \beta_1^{(2)} &= -\frac{89}{15}, & \beta_3^{(2)} &= \frac{32}{5}, \\ \beta_4^{(2)} &= \frac{12}{5}, & \beta_5^{(2)} &= -\frac{64}{15}, & \beta_6^{(2)} &= \frac{7}{5}, & \beta_1^{(3)} &= \frac{284}{15}, & \beta_3^{(3)} &= -\frac{416}{15}, \\ \beta_4^{(3)} &= -\frac{72}{5}, & \beta_5^{(3)} &= \frac{544}{15}, & \beta_6^{(3)} &= -\frac{196}{15}, & \beta_1^{(4)} &= -\frac{80}{3}, & \beta_3^{(4)} &= \frac{128}{3}, \\ \beta_4^{(4)} &= 32, & \beta_5^{(4)} &= -\frac{256}{3}, & \beta_6^{(4)} &= \bullet \frac{112}{3}, \bullet & \bullet & \bullet & \bullet \end{aligned}$$

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Exponential Collocation Methods (1/2)

Recall vcf

$$u_{n+1} = \exp(\mathbf{L}h)u_n + \exp(\mathbf{L}h) \int_0^h \exp(-\mathbf{L}\tau)\mathbf{N}(u(t_n + \tau))d\tau$$

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- choose collocation nodes c_1, \dots, c_s
- let $u_n \approx u(t_n)$, $U_{n,i} \approx u(t_n + c_i h)$
- p_n collocational polynomial of degree $s - 1$ $p_n(c_i h) = \mathbf{N}(U_{n,i})$

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- explicit methods: $p_{n,i}$ polynomial of degree $i - 1$ using $\mathbf{N}(U_{n,j})$, $j \leq i - 1$

$$U_{n,i} = e^{\mathbf{L}h} u_n + \int_0^{c_i h} e^{(c_i h - \tau)\mathbf{L}} p_{n,i}(\tau) d\tau$$

$$u_{n,i} = e^{\mathbf{L}h} u_n + \int_0^h e^{(h - \tau)\mathbf{L}} p_n(\tau) d\tau$$

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Exponential Collocation Methods (2/2)

key point: integrals can be calculated exactly

$$\int_0^{c_i h} e^{(c_i h - \tau) \mathbf{L}} p_{n,i}(\tau) d\tau = h \sum_{j=1}^s a_{ij}(c_i h \mathbf{L}) \mathbf{N}(U_{n,j})$$

$$\int_0^h e^{(h - \tau) \mathbf{L}} p_n(\tau) d\tau = h \sum_{i=1}^s b_i(h \mathbf{L}) \mathbf{N}(U_{n,i})$$

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coefficients b_i , a_{ij} are linear combination of $\phi^{[1]}, \dots, \phi^{[s]}$ (Beylkin, Keiser, Vozov'i'98)
defined as

$$\phi^{[i]}(-t \mathbf{L}) = \frac{1}{(i-1)! t^i} \int_0^t (t-\tau)^{i-1} e^{-\tau \mathbf{L}} d\tau, \quad i \geq 1$$

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- No need of new order theory
- Easy to solve all order conditions

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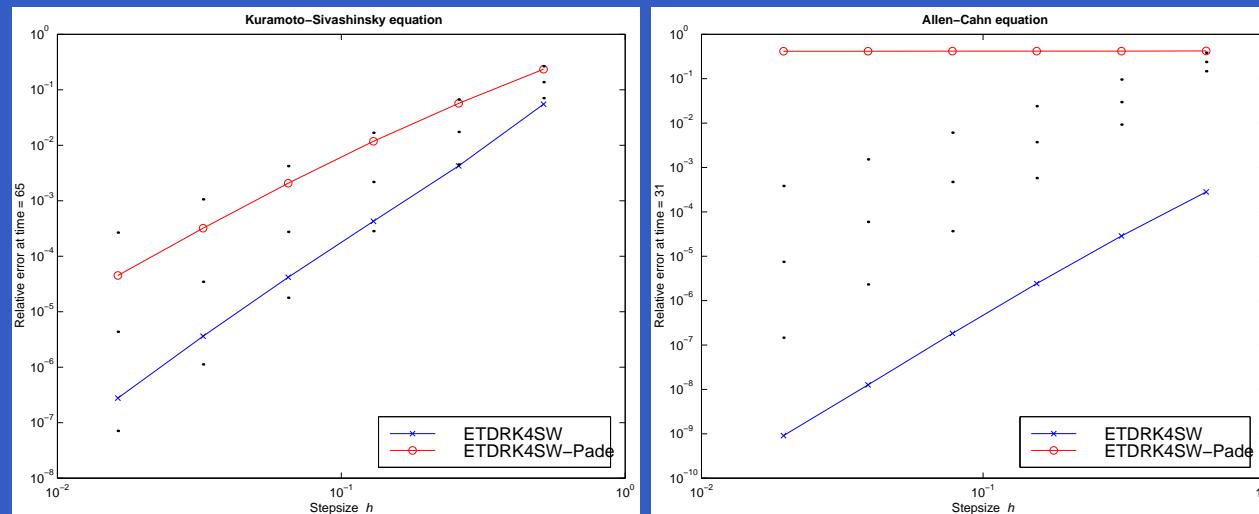
- Are they too restrictive in the choice of the quadrature formula?
- What if $c_i = c_j$?
- How to analyze the methods of Cox and Matthews and Krogstad?

Why exactly?

- ARK use rational approximations to the \exp and $\phi^{[i]}$

Why exactly?

- ARK use rational approximations to the \exp and $\phi^{[i]}$
- The choice of the $\phi^{[i]}$ functions in ARK is restricted to the ETD set.



Connections with CF

We can rewrite the equation (1) in the form

$$u' = (\mathbf{L}, \mathbf{N}(u, t)).u = F_{u,t}(u), \quad u(0) = u_0$$

where . represents the *Lie algebra action*

$$(\mathbf{A}, a).u = \mathbf{A}u + a$$

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Let $\hat{F}_{\hat{u}, \hat{t}}(u)$ be the *Frozen Vector Field* at the point (\hat{u}, \hat{t})

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The flow of such vector field is the solution of $u' = \hat{F}_{\hat{u}, \hat{t}}(u), \quad u(0) = u_0$

$$\phi_{t, \hat{F}}(u_0) = \text{Exp}(t\hat{F}_{\hat{u}, \hat{t}}).u_0 = \exp(t\mathbf{L})u_0 + t\phi^{[1]}(t\mathbf{L})\mathbf{N}(\hat{u}, \hat{t})$$

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CF Method

Algorithm (CF)

for $r = 1 : s$ **do**

$$Y_r = \text{Exp}(\sum_k \alpha_{r,J}^k F_k) \cdots \text{Exp}(\sum_k \alpha_{r,1}^k F_k)(p)$$

$$F_r = hF_{Y_r} = h \sum_i f_i(Y_r)E_i$$

end

$$y_1 = \text{Exp}(\sum_k \beta_J^k F_k) \cdots \text{Exp}(\sum_k \beta_1^k F_k)p$$

Numerical schemes

ETDCF4 of Celledoni, Marthinse and Owren

0								
$\frac{1}{2}$	$\frac{1}{2}\phi^{[1]}$							
$\frac{1}{2}$	0	$\frac{1}{2}\phi^{[1]}$						
$\frac{1}{2}$	$\frac{1}{2}\phi^{[1]}$	0	0					
$\frac{1}{2}$	$-\frac{1}{2}\phi^{[1]}$	0	$\phi^{[1]}$					
	$\frac{1}{4}\phi^{[1]}$	$\frac{1}{6}\phi^{[1]}$	$\frac{1}{6}\phi^{[1]}$	$-\frac{1}{12}\phi^{[1]}$				
	$-\frac{1}{12}\phi^{[1]}$	$\frac{1}{6}\phi^{[1]}$	$\frac{1}{6}\phi^{[1]}$	$\frac{1}{4}\phi^{[1]}$				

Numerical schemes

ETDRK4 of Cox and Matthews

Numerical experiments

Example 1: Kuramoto-Sivashinsky equation

$$u_t = -uu_x - u_{xx} - u_{xxxx}, \quad x \in [0, 32\pi]$$

with periodic boundary conditions and with the initial condition

$$u(x, 0) = \cos\left(\frac{x}{16}\right)(1 + \sin\left(\frac{x}{16}\right)).$$

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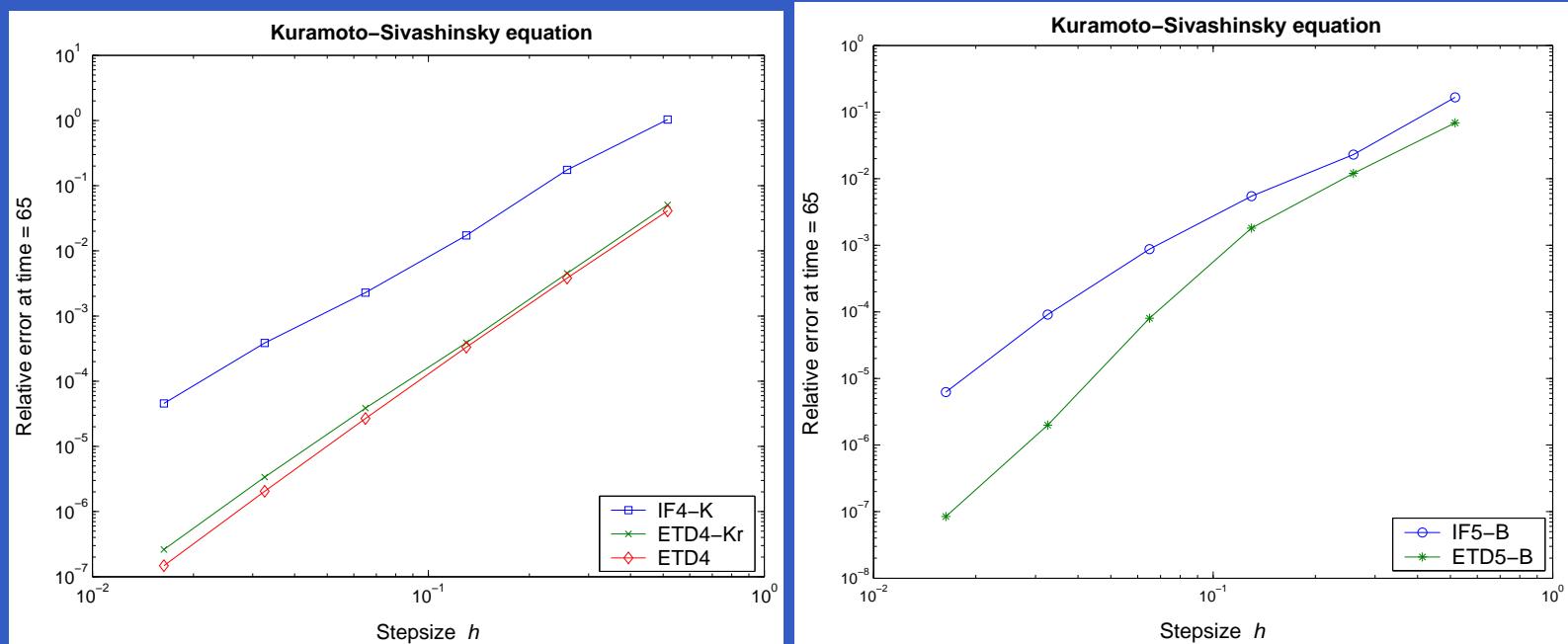
$$u(x, 0) = \cos\left(\frac{x}{16}\right)(1 + \sin\left(\frac{x}{16}\right)).$$

We discretise the spatial part using Fourier spectral method. The transformed equation in the Fourier space is

$$\hat{u}_t = -\frac{ik}{2}\hat{u}^2 + (k^2 - k^4)\hat{u},$$

$$(\mathbf{L}\hat{u})(k) = (k^2 - k^4)\hat{u}(k) \text{ and } \mathbf{N}(\hat{u}, t) = -\frac{ik}{2}(F((F^{-1}(\hat{u}))^2))$$

Kuramoto-Sivashinsky equation



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Numerical experiments

Example 2: Allen-Cahn equation

$$u_t = \varepsilon u_{xx} + u - u^3, \quad x \in [-1, 1]$$

with $\varepsilon = 0.01$ and with boundary and initial conditions

$$u(-1, t) = -1, \quad u(1, t) = 1, \quad u(x, 0) = .53x + .47 \sin(-1.5\pi x)$$

Numerical experiments

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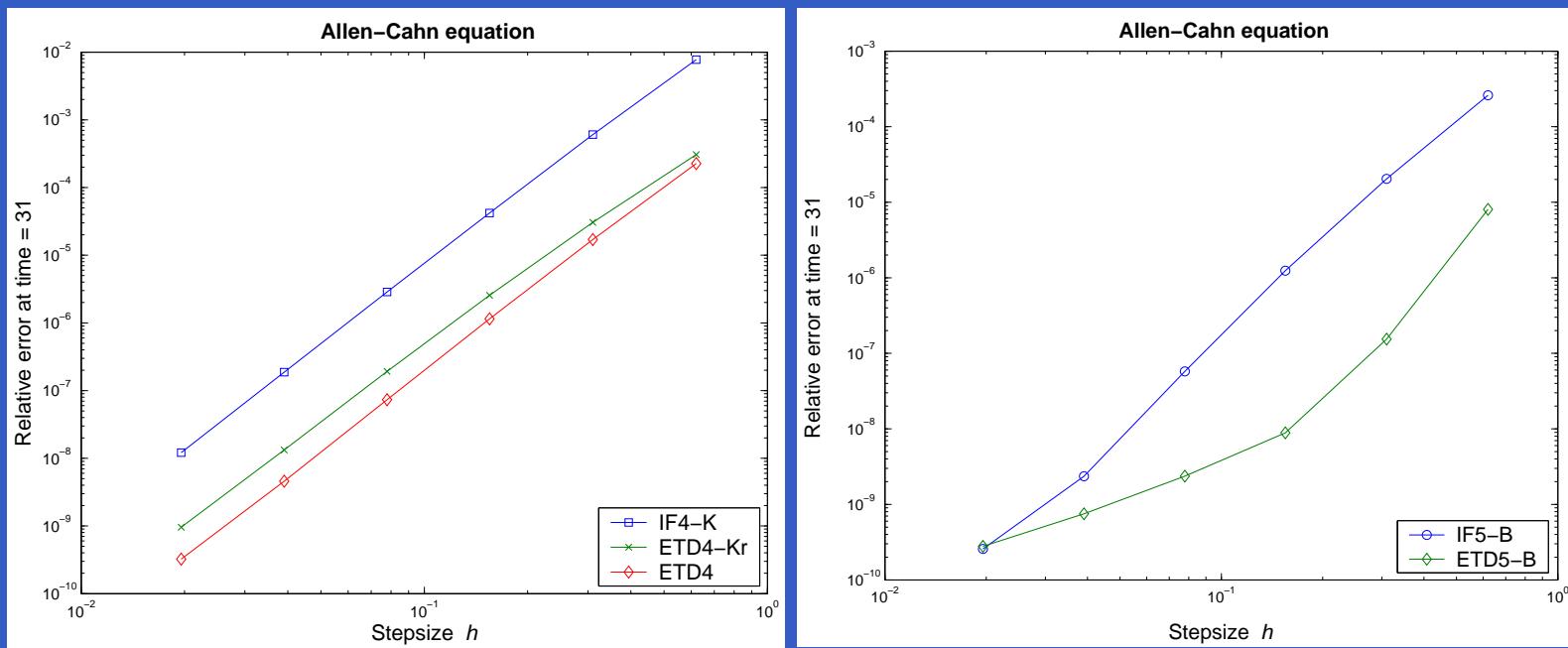
$$u(-1, t) = -1, \quad u(1, t) = 1, \quad u(x, 0) = .53x + .47 \sin(-1.5\pi x)$$

After discretisation in space.

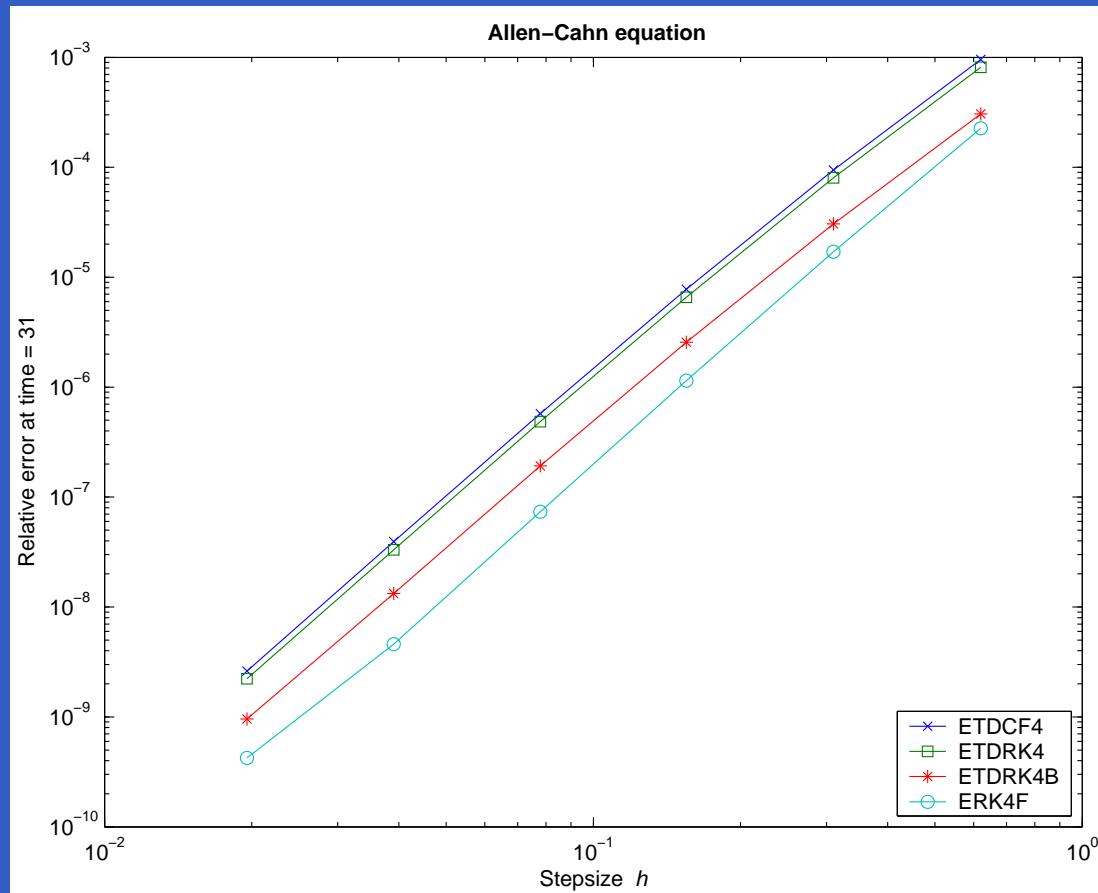
$$u_t = \mathbf{L}u + \mathbf{N}(u(t))$$

where $\mathbf{L} = \varepsilon D^2$, $\mathbf{N}(u(t)) = u - u^3$ and D is the Chebyshev differentiation matrix

Allen-Cahn equation



Allen-Cahn equation



Numerical experiments

Example 3: Korteweg de Vries equation

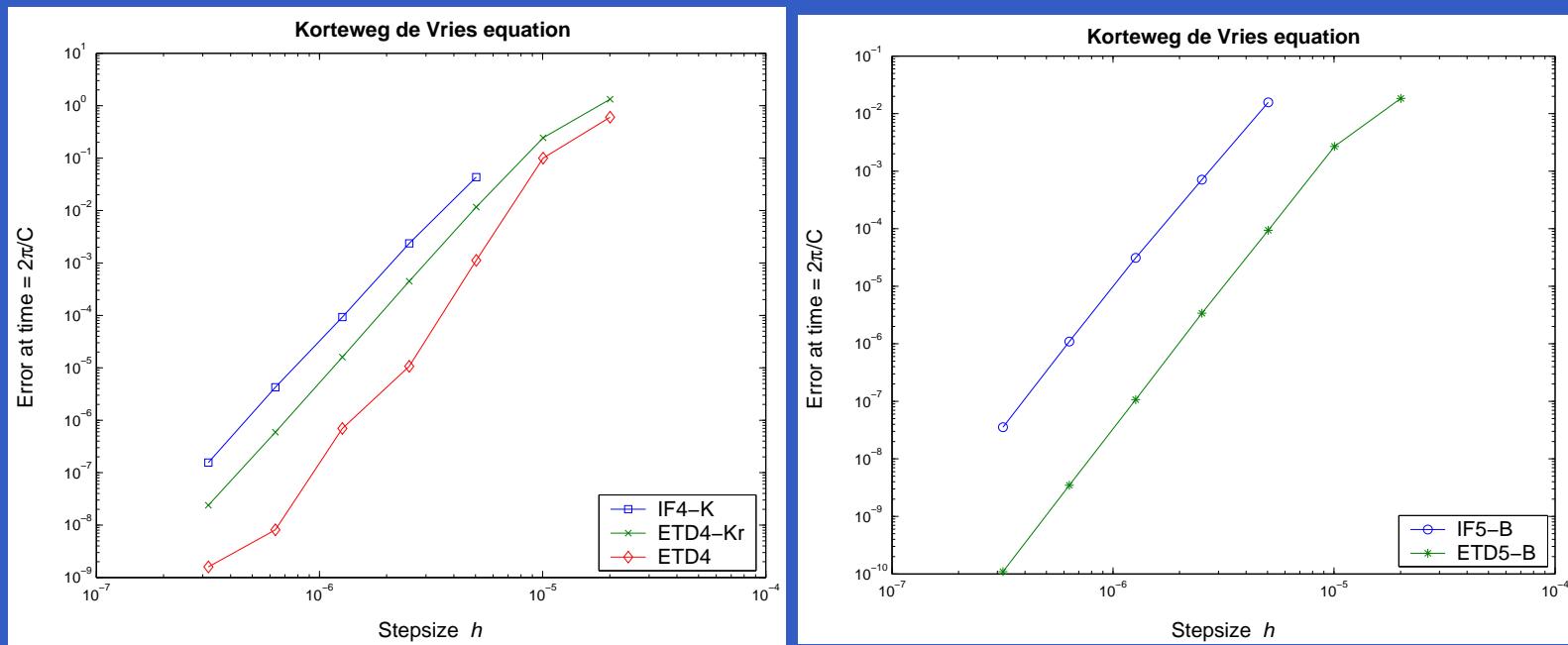
$$u_t = -u_{xxx} - uu_x, \quad x \in [-\pi, \pi],$$

with periodic boundary conditions and with initial condition

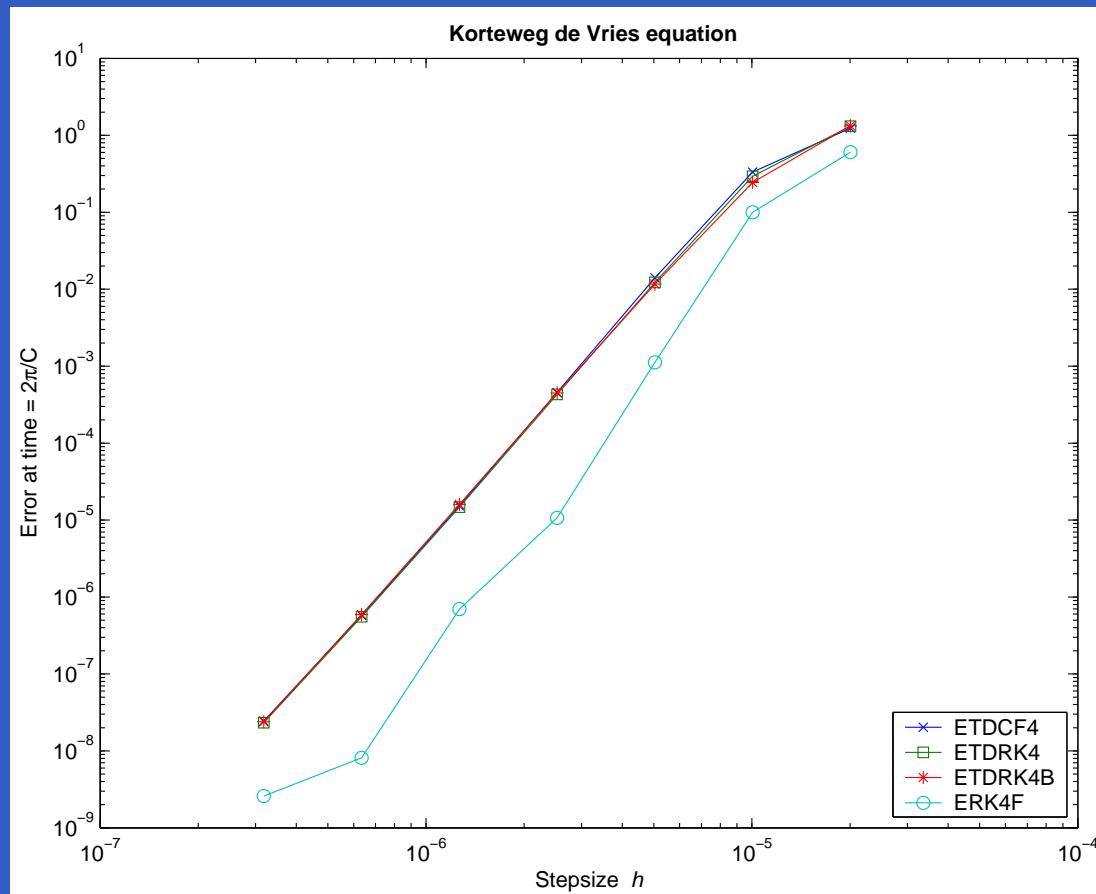
$$u(x, 0) = 3C/\cosh^2(\sqrt{C}x/2),$$

where $C = 625$. The exact solution is $2\pi/C$ periodic and is given by $u(x, t) = u(x - Ct, 0)$. We use a 256-point Fourier spectral discretization in space. In this case the matrix L is again diagonal. The integration in time is done for one period.

KdV equation



KdV equation



Generalized IF Methods

Consider the semi discretised problem (1)

$$u' = \mathbf{L}u + \mathbf{N}(u(t)), \quad u(t_0) = u_0$$

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$$u' = \mathbf{L}u + \mathbf{N}(u(t)), \quad u(t_0) = u_0$$

Change of variables

$$u(t) = \exp(tL)v(t) = \phi_{t,\hat{F}}(v(t)),$$

where $\hat{F}(\hat{u}, t) = L\hat{u}$ approximates F around u_0 .

The transformed equation is

$$v'(t) = \exp(-tL)N(\exp(tL)v(t))$$

Generalized IF Methods

Consider the semi discretised problem (1)

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In general (Krogstad; Mayday, Patera and Rønquist) substitute

$$u(t) = \phi_{t,\hat{F}}(v(t))$$

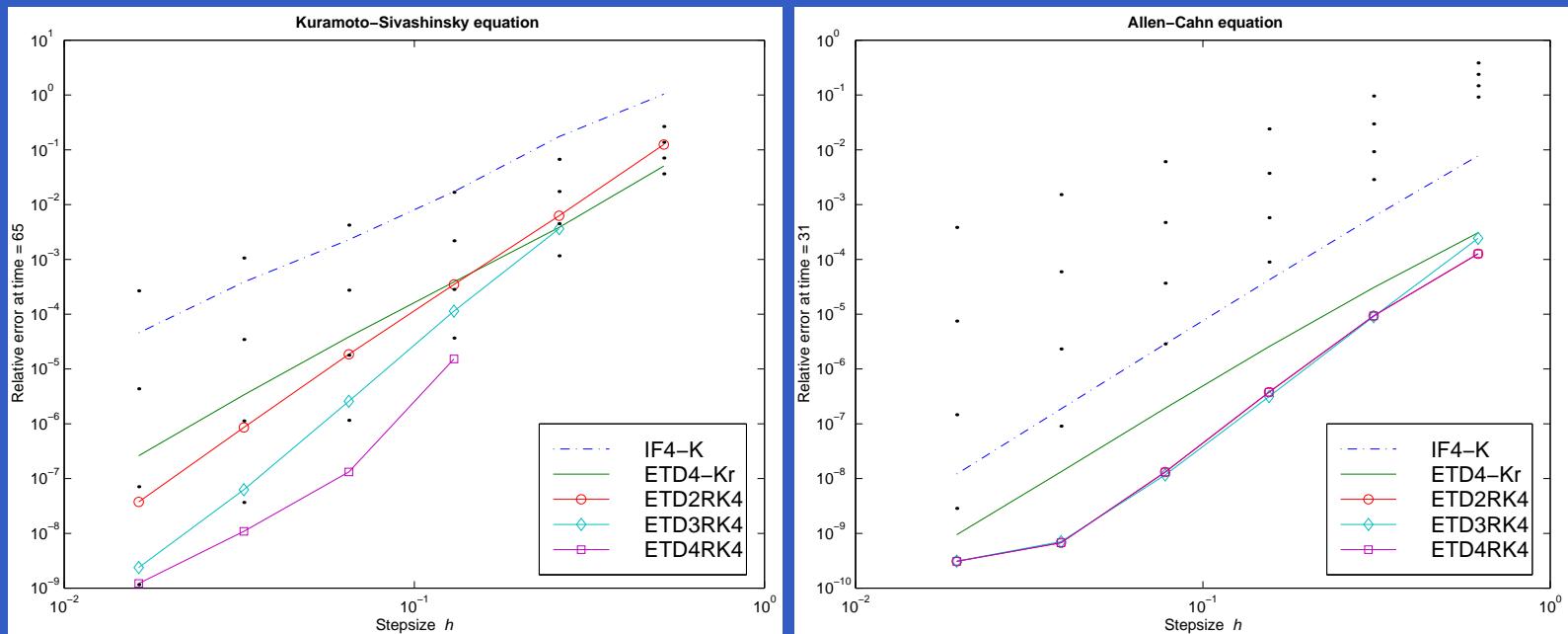
where $\hat{F}(\hat{u}, t) = L\hat{u} + \mathbf{N}(t)$ approximates F around u_0 .

The transformed equation is

$$v'(t) = \exp(-tL) [N(\exp(tL)v(t)) - \mathbf{N}(t)]$$

Now apply a numerical method to the transformed equation.

More Experiments



Conclusion

- The exponential integrators have a long history.

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- The exponential integrators have a long history.
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- Best methods likely to be based on general linear methods.

Work in progress

- Other $\phi^{[i]}$ functions

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