#### **Exp**<sup>3</sup> Integrators for semilinear problems

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Exp<sup>3</sup> = Explaining Explicit Exponential Integrators

#### **Outline**

- Motivation and History
- Formulation of the method
- Connections with Lie group methods
- Numerical schemes
- Numerical experiments
- Generalized IF methods
- Conclusions
- Future work

# **Motivation and History**

A new interest in exponential integrators for semilinear problems

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#### **Brief History**

- Lawson, 1967
  - IF methods, A-stability
- Friedli, 1978
  - Exp. Exp. RK Methods, nonstiff order
- Strehmel and Weiner, 1987
  - Adaptive RK Methods, Order theory, B-stability
- Hochbruck and Lubich, 1997
  - Exp. Integrators (EXP4) with inexact Jacobian

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

- Cox and Matthews, 2002
  - ETDRK Methods of 3<sup>-th</sup> and 4<sup>-th</sup> order
- Kasam and Trefethen, 2002
  - Extensive numerical experiments, overcome the numerical instability
- Celledoni, Marthinsen, Owren, 2003
  - Commutator Free Lie group methods
- Krogstad, 2003
  - Generalized IF Methods, connection with CF
- Hochbruck and Osterman, 2003
  - Exp. Collocation Methods, convergence analyze

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- GIF = Generalized Integrating Factor

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$$v(t) = \exp(-\mathbf{L}t)u(t)$$

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Apply a numerical method to the transformed equation

Transform back the approximate solution to the original variable

#### **Example of IF**

In terms of the original variable the computations performed are

$$U_{1} = u_{0}$$

$$U_{2} = e^{c_{2}hL}(u_{0} + a_{21}hN(U_{1}))$$

$$U_{3} = e^{c_{3}hL}(u_{0} + a_{31}hN(U_{1}) + a_{32}he^{-c_{2}hL}N(U_{2}))$$

$$U_{4} = e^{c_{4}hL}(u_{0} + a_{41}hN(U_{1}) + a_{42}he^{-c_{2}hL}N(U_{2}) + a_{43}he^{-c_{3}hL}N(U_{3}))$$

$$u_{1} = e^{hL}(u_{0} + b_{1}hN(U_{1}) + b_{2}he^{-c_{2}hL}N(U_{2}) + b_{3}he^{-c_{3}hL}N(U_{3}) + b_{4}he^{-c_{4}hL}N(U_{4}))$$

#### **Example of IF**

General form of the order 4 integrating factor method is

Γ	0	0	0	0	1
	$a_{21}e^{c_2hL}$	0	0	0	$e^{c_2 hL}$
	$a_{31}e^{c_3hL}$	$a_{32}e^{(c_3-c_2)hL}$	0	0	$e^{c_3hL}$
	$a_{41}e^{c_4hL}$	$a_{42}e^{(c_3-c_2)hL}$	$a_{43}e^{(c_4-c_3)hL}$	0	$e^{c_4 h L}$
	$b_1 e^{hL}$	$b_2 e^{(1-c_2)hL}$	$b_3 e^{(1-c_3)hL}$	$b_4 e^{(1-c_4)hL}$	$e^{hL}$

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

# **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  $N(u(t_n+\tau))$ 

(Nørsett'69, Cox and Matthews'02)

- If  $N(u(t)) \approx \delta_i e^{Lt}$ , where  $\delta_i$  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

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

- 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  $t=c_1h,c_2h,\ldots,c_sh$  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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$$\phi^{[1]}(\lambda)(hL) = 1I_m + \frac{\lambda}{2!}hL + \frac{\lambda^2}{3!}(hL)^2 + \frac{\lambda^3}{4!}(hL)^3 + \frac{\lambda^4}{5!}(hL)^4 + \cdots,$$

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

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

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  $c_1,\ldots,c_s$
- 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  $p_n(c_ih) = \mathbf{N}(U_{n,i})$

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

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

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

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  $\phi^{[1]}, \ldots, \phi^{[s]}$  (Beylkin, Keiser, Vozovi'98) defined as

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

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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?

# The $\phi$ function

The generality of the  $\phi$  functions is not known. For  $\lambda \in \mathbb{R}$  and  $hL \in \mathbb{R}^{m \times m}$ , let

$$\phi^{[i]}(\lambda)(hL) = \sum_{j=0}^{\infty} \phi_j^{[i]}(\lambda)(hL)^j.$$

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The  $\phi$  functions of the IF and ETD work. Certain their linear combinations also work. Are

there others?

#### The method coefficients

The matrix A is defined as

$$A = \sum_{i=1}^{d} \Phi^{[i]}(c)(hL)(\alpha^{(i)} \otimes I_m),$$

where  $\alpha^{(i)}$  are  $s \times s$  strictly lower triangular matrices with the first i rows equal to zero and m is the dimensionality of the problem.

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The matrix  $b^T$  is defined as

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The matrix  $\Phi^{[i]}$  is

$$\Phi^{[i]}(c)(hL) = \operatorname{diag}(\phi^{[i]}(c_1)(hL), \dots, \phi^{[i]}(c_s)(hL))$$

$$U^{[n]} = AhN(U^{[n]}) + e^{chL}u_{n-1},$$
  

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The computations performed in step number n, are

$$\begin{bmatrix} U^{[n]} \\ \hline u_n \end{bmatrix} = \begin{bmatrix} A & e^{chL} \\ \hline b^T & e^{hL} \end{bmatrix} \begin{bmatrix} hN(U^{[n]}) \\ \hline u_{n-1} \end{bmatrix}$$

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where the corresponding vectors are

$$U^{[n]} = \begin{bmatrix} U_1^{[n]} \\ U_2^{[n]} \\ \vdots \\ U_s^{[n]} \end{bmatrix} \qquad N(U^{[n]}) = \begin{bmatrix} N(U_1^{[n]}) \\ N(U_2^{[n]}) \\ \vdots \\ N(U_s^{[n]}) \end{bmatrix} \qquad e^{chL} = \begin{bmatrix} e^{c_1hL} \\ e^{c_2hL} \\ \vdots \\ e^{c_shL} \end{bmatrix}$$

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alternative representation of the method in a more Runge-Kutta tabelau formulation is

### General formulation

A 3 stage example of the general formulation is

$$\begin{bmatrix} 0 & 0 & 0 & e^{c_1hL} \\ a_{21}^1\phi^1 & 0 & 0 & e^{c_2hL} \\ a_{31}^1\phi^1 + a_{31}^2\phi^2 & a_{32}^1\phi^1 + a_{32}^2\phi^2 & 0 & e^{c_3hL} \\ \hline b_1^1\phi^1 + b_1^2\phi^2 + b_1^3\phi^3 & b_2^1\phi^1 + b_2^2\phi^2 + b_3^3\phi^3 & b_3^1\phi^1 + b_3^1\phi^2 + b_3^3\phi^3 & e^{hL} \end{bmatrix}$$

## General formulation

#### ETD4-Kr of Krogstad

	$4\phi^{[3]} - 3\phi^{[2]} + \phi^{[1]}$	$-4\phi^{[3]} + 2\phi^{[2]}$	$-4\phi^{[3]} + 2\phi^{[2]}$	$4\phi^{[3]} - \phi^{[2]}$
1	$\phi^{[1]} - 2\phi^{[2]}$	0	$2\phi^{[2]}$	
$\frac{1}{2}$	$rac{1}{2}\phi^{[1]}-\phi^{[2]}$	$\phi^{[2]}$		
$\frac{1}{2}$	$rac{1}{2}\phi^{[1]}$			
0				

## General formulation

ETDRK4SW of Strehmel and Weiner

	$4\phi^{[3]} - 3\phi^{[2]} + \phi^{[1]}$	0	$-8\phi^{[3]} + 4\phi^{[2]}$	$4\phi^{[3]} - \phi^{[2]}$
1	$\phi^{[1]} - 2\phi^{[2]}$	$-2\phi^{[2]}$	$4\phi^{[2]}$	
$\frac{1}{2}$	$rac{1}{2}\phi^{[1]} - rac{1}{2}\phi^{[2]}$	$\frac{1}{2}\phi^{[2]}$		
$\frac{1}{2}$	$rac{1}{2}\phi^{[1]}$			
0				

## Order theory

- Associate a white node with L and black node with N
- Elementary differentials can be represented by bi-coloured rooted trees where any white node has only one child.

## Order theory

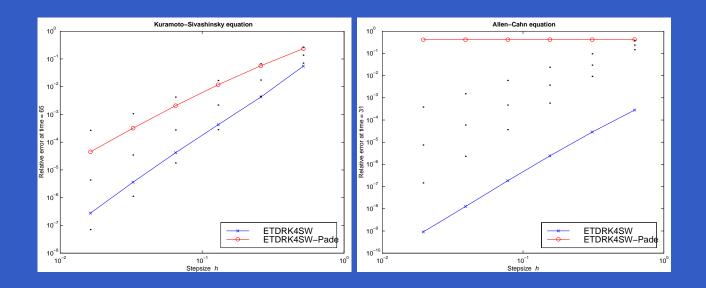
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#### The number of rooted trees

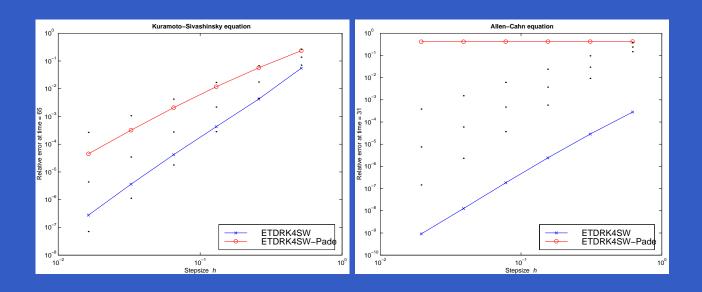
n	1	2	3	4	5	6	7	8
$\overline{ heta_n}$	2	4	11	34	117	421	1589	6162
$\Theta = \sum_{i}^{n} \theta_n$	2	6	17	51	168	589	2178	8340

The order theory is the same

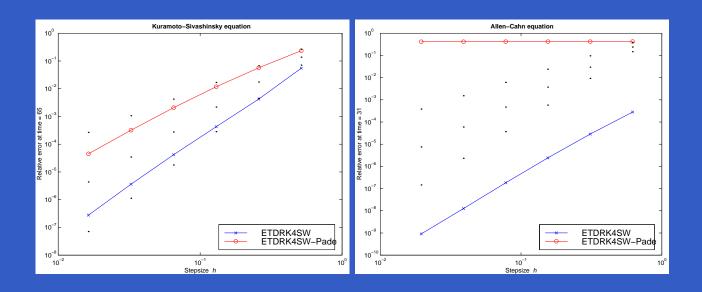
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- The choice of the  $\phi^{[i]}$  functions in ARK is restricted to the ETD set.



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- lacktriangle 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.
- Exp. RK methods include IF, ECM and ETDRK methods of Krogstad and Cox and Matthews as special cases.



### **Connections with CF**

We can rewrite the equation (1) in the form

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

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  $(\hat{u},\hat{t})$ 

$$\hat{F}_{\hat{u},\hat{t}}(u) = (\mathbf{L}, \mathbf{N}(\hat{u},\hat{t})).u = \mathbf{L}u + \mathbf{N}(\hat{u},\hat{t})$$

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$$\hat{F}_{\hat{u},\hat{t}}(u) = (\mathbf{L}, \mathbf{N}(\hat{u},\hat{t})).u = \mathbf{L}u + \mathbf{N}(\hat{u},\hat{t})$$

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

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

### **CF Method**

#### Algorithm (CF)

for 
$$r=1:s$$
 do

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

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

end

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

### Numerical schemes

ETDCF4 of Celledoni, Marthinse and Owren

## Numerical schemes

#### ETDRK4 of Cox and Matthews

0				
$\frac{1}{2}$	$rac{1}{2}\phi^{[1]}$			
$\frac{1}{2}$	0	$rac{1}{2}\phi^{[1]}$		
$\frac{1}{2}$	$rac{1}{2}\phi^{[1]}$	0	0	
$\frac{1}{2}$	$-rac{1}{2}\phi^{[1]}$	0	$\phi^{[1]}$	
	$4\phi^{[3]} - 3\phi^{[2]} + \phi^{[1]}$	$-4\phi^{[3]} + 2\phi^{[2]}$	$-4\phi^{[3]} + 2\phi^{[2]}$	$4\phi^{[3]} - \phi^{[2]}$

## 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

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

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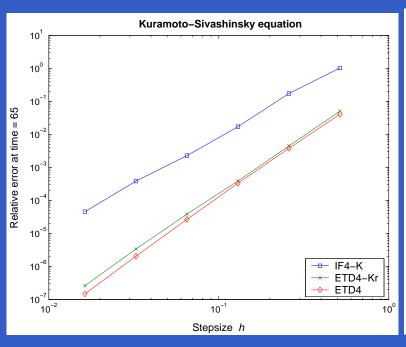
We discretise the spatial part using Fourier spectral method. The transformed equation

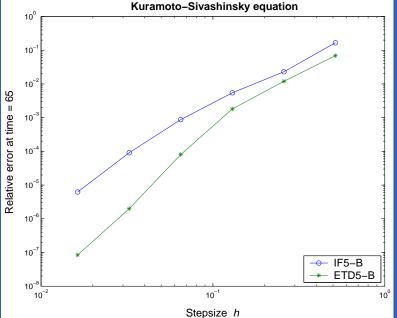
in the Fourier space is

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

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

# Kuramoto-Sivashinsky equation





## 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

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

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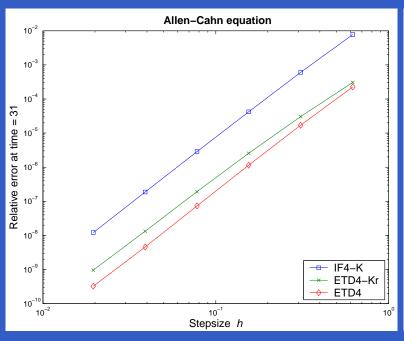
$$u(-1,t) = -1, \quad u(1,t) = 1, \quad u(x,0) = .53x + .47\sin(-1.5\pi x)$$

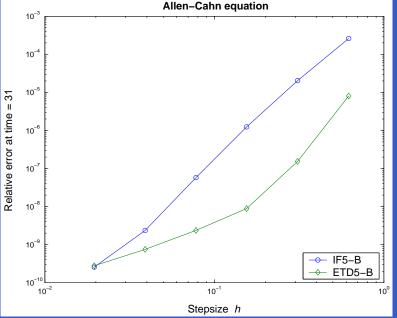
After discretisation in space.

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

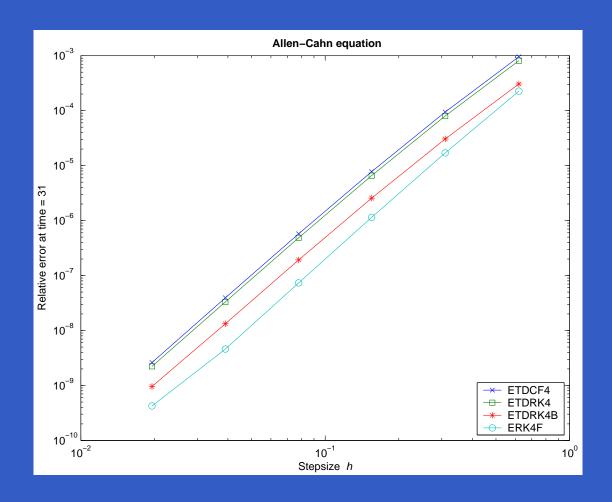
where  $\mathbf{L} = \varepsilon D^2$ ,  $\mathbf{N}(u(t)) = u - u^3$  and D is the Chebyshev differentiation matrix

# Allen-Cahn equation





# Allen-Cahn equation



## Numerical experiments

#### **Example 3:** Korteweg de Vries equation

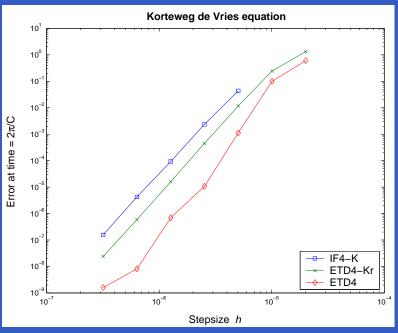
$$u_t = -u_{xxx} - uu_x, \qquad x \in [-\pi, \pi],$$

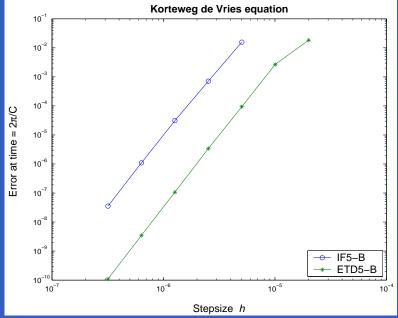
with periodic boundary conditions and with initial condition

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

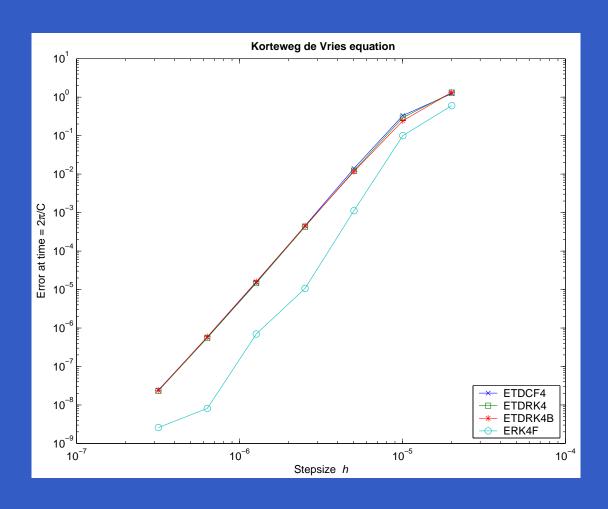
where C=625. The exact solution is  $2\pi/C$  periodic and is given by u(x,t)=u(x-Ct,0). We use a 256-point Fourier spectral discretization in space. In this case the matrix L is again diagonal. The integration in time is done for one period.

# KdV equation





# **KdV** equation



## Generalized IF Methods

Consider the semi discretised problem (1)

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

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

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)

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

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

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

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

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

Now apply a numerical method to the transformed equation.

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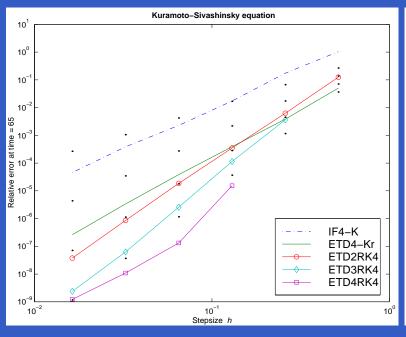
#### GIF like GLMs

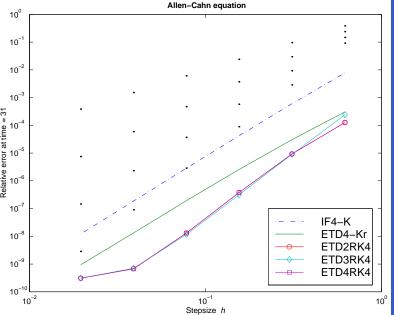
- Information from past was used to capture key features of F.
- These methods reduced to a methods with maximum stage order when L=0.
- This is at the cost of smaller stability regions.
- When L=0 the GIF methods are GLMs.

#### GIF like GLMs

The GIF showed significant improvements over all other methods.

# More Experiments





We can rewrite the equation  $u' = \mathbf{L}u + \mathbf{N}(u(t), t), \ u(t_0) = u_0$  in the form

$$\dot{y} = (\mathbf{A}_{u,t}, a).y = \tilde{F}_{u,t}(y)$$
$$y(0) = y_0$$

where

$$\mathbf{A}_{u,t} = \begin{pmatrix} \mathbf{L} & \frac{\mathbf{N}(u,t) - \mathbf{N}_0}{t} \\ 0 & 0 \end{pmatrix}, a = \begin{pmatrix} \mathbf{N}_0 \\ 1 \end{pmatrix},$$

$$y = \begin{pmatrix} u \\ v \end{pmatrix}, y_0 = \begin{pmatrix} u_0 \\ 0 \end{pmatrix}, \mathbf{N}_0 = \mathbf{N}(u_0, 0)$$

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

$$\tilde{F}_{\hat{u},\hat{t}}(u) = (\mathbf{A}_{\hat{u},\hat{t}}, a).y = \mathbf{A}_{\hat{u},\hat{t}} y + a,$$

where

$$\mathbf{A}_{\hat{u},\hat{t}} = \begin{pmatrix} \mathbf{L} & \frac{\hat{\mathbf{N}} - \mathbf{N}_0}{\hat{t}} \\ & & \\ 0 & 0 \end{pmatrix}, \quad \hat{\mathbf{N}} = \mathbf{N}(\hat{u},\hat{t})$$

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The flow of such vector field is the solution of  $\dot{y} = \tilde{F}_{\hat{u},\hat{t}}(y), \quad y(0) = y_0$ 

$$\phi_{t,\tilde{F}}(y_0) = \operatorname{Exp}(t\tilde{F}_{\hat{u},\hat{t}}).y_0 = \begin{pmatrix} \exp(t\mathbf{L})u_0 + t\phi^{[1]}(t\mathbf{L})\mathbf{N}_0 + t^2\phi^{[2]}(t\mathbf{L})\frac{\hat{\mathbf{N}} - \mathbf{N}_0}{\hat{t}} \\ t \end{pmatrix}$$

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and satisfies

$$\phi_{\alpha t,\tilde{F}} \,=\, \phi_{t,\alpha\tilde{F}} \qquad \phi_{\alpha t,\tilde{F}} \circ \phi_{\beta t,\tilde{F}} \,=\, \phi_{(\alpha+\beta)t,\tilde{F}} \qquad \text{Exp}^3 \text{ Integrators for semiline}$$

### Conclusion

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- The order theory were rederived in a more general settings.
- The IF, ECM (ETDRK) methods are special cases of these methods.

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