More on GIF methods

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Overview

1. The Problem
    - The PDE
    - The ODE
    - The basics
2. GIF methods
    - Krogstad's approach
    - Stiff order conditions
    - Modifying GIF methods
3. Numerical experiments
    - A parabolic example

The PDE

Consider the evolution equation, with an appropriate boundary

$$u_t = \mathcal{L}u + \mathcal{N}(u), \quad u(x,0) = u_0(x)$$

- $\mathcal{L}$ is an unbounded linear operator
- $\mathcal{N}$ is a nonlinear operator

Several well known examples include:

Parabolic	Hyperbolic
Navier–Stokes	Burgers
Kuramoto–Sivasinsky	KdV
Allen–Cahn	Nonlinear Schrödinger

The ODE

After discretization in space we obtain a systems of ODEs

$$u'(t) = Lu(t) + N(u(t)), \quad u(t_{n-1}) = u_{n-1}$$

- L is unbounded either large negative or imaginary eigenvalues
- N is slowly varying

The aim is to exploit the special structure of the ODE

Exponential integrators are most efficient when L has a special structure

Exponential Integrators

All exponential integrators fit into a single framework

An explicit exponential general linear method has the form

$$
\begin{aligned}
U_i &= \sum_{j=1}^{i-1} A_{ij}(hL)hN(U_j) + \sum_{j=1}^{r} U_{ij}(hL)u_j^{[n-1]} \\
u_i^{[n]} &= \sum_{j=1}^{s} B_{ij}(hL)hN(U_j) + \sum_{j=1}^{r} V_{ij}(hL)u_j^{[n-1]}
\end{aligned}
$$

The matrices A, U, B and V are all bounded despite being functions of the unbounded matrix L

Useful Papers

- Lawson, 1967
  - Generalized RK Processes (IF methods), A-stability
- Nørsett, 1969
  - ETD based on Adams–Bashforth methods, A-stability
- Beylkin, Keiser, Vozovoi, 1998
  - ETD methods of Adams type
- Cox and Matthews, 2002
  - ETDRK methods of order 3 and 4
- Krogstad, 2004
  - Generalized IF Methods, connection with CF
- Hochbruck and Ostermann, 2004
  - Stiff order conditions for exponential RK methods

IF (Lawson)

After spatial discretization we obtain a systems of ODEs

$$u' = Lu + N(u), \quad u(t_{n-1}) = u_{n-1}$$

Solve exactly the linear part then make a change of variables

$$\begin{aligned} v(t) &= \mathrm{e}^{(t_{n-1}-t)L} u(t) \\ \underbrace{\mathrm{e}^{(t_{n-1}-t)L}(u' - Lu)}_{v'} &= \mathrm{e}^{(t_{n-1}-t)L} N(u) \\ v' &= \mathrm{e}^{(t_{n-1}-t)L} N(\mathrm{e}^{(t-t_{n-1})L} v) \end{aligned}$$

- Apply a numerical method to the transformed equation
- Transform the approximate solution to the original variable

IF Euler method

The transformed differential equation is

$$v' = \mathrm{e}^{(t_{n-1}-t)L} N(\mathrm{e}^{(t-t_{n-1})L} v), \quad v_{n-1} = u_{n-1}$$

Apply the explicit Euler method

$$v_n = v_{n-1} + hN(v_{n-1}),$$

Transform back with $v_n = \mathrm{e}^{-hL} u_n$, giving the IF Euler method

$$u_n = \mathrm{e}^{hL} u_{n-1} + \mathrm{e}^{hL} N(u_{n-1})$$

High order IF methods

General form of IF Runge–Kutta method is

$$U_i = \sum_{j=1}^{i-1} a_{ij} \mathrm{e}^{(c_i - c_j)hL} hN(U_j) + \mathrm{e}^{c_i hL} u_{n-1}$$

$$u_n = \sum_{i=1}^{s} b_i \mathrm{e}^{(1-c_j)hL} hN(U_i) + \mathrm{e}^{hL} u_{n-1}$$

General form of IF Adams methods is

$$u_n = \mathrm{e}^{hL} u_{n-1} + \sum_{l=0}^{k} \beta_l \mathrm{e}^{lhL} N(u_{n-l})$$

Large error constants and fixed points are not preserved

IF/cRK4

IF/cRK4 of Lawson, where $z = hL$

$$\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & I \\
\frac{1}{2}\mathrm{e}^{\frac{1}{2}z} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}z} \\
0 & \frac{1}{2}I & 0 & 0 & \mathrm{e}^{\frac{1}{2}z} \\
0 & 0 & \mathrm{e}^{\frac{1}{2}z} & 0 & \mathrm{e}^{z} \\
\hline
\frac{1}{6}\mathrm{e}^{z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{6}I & \mathrm{e}^{z}
\end{array}\right]$$

- Reduces to classical order four RK method when $L = 0$
- Does not preserve fixed points
- Has only order one for general parabolic problems
- Is useful for certain problems see Håvard's talk

GIF (Krogstad)

Krogstad viewed the Lawson transformation in another way

As the solution $u(t) = \Phi_{t,\widetilde{F}}(v(t))$, where $\widetilde{F} \approx F$

$$u'(t) = \widetilde{F}(u(t)) = Lu(t)$$

The outcome is the Lawson transformation $u(t) = e^{(t-t_{n-1})L}v(t)$

This idea can be easily extended

Can capture more of the key features with

$$u'(t) = \widetilde{F}(u(t)) = Lu(t) + P(t)$$

where $P(t)$ is some approximation to $N(u(t))$

Krogstad choose $P(t)$ to be a polynomial

GIF

The exact solution is

$$u(t_n) = \mathrm{e}^{hL} u_{n-1} + \sum_{l=1}^{\infty} \phi_l(hL) h^l N_{n-1}^{(l-1)}$$

So the Krogstad transformation is

$$u(t_n) = \mathrm{e}^{hL} v(t_n) + \sum_{l=1}^{\infty} \phi_l(hL) h^l P_{n-1}^{(l-1)}$$

Differentiating gives the transformed ODE

$$v'(t) = \mathrm{e}^{(t_{n-1}-t)L}(N(u(t)) - P(t))$$

Use numerical method on transformed ODE, then back transform

GIF1/cRK4

GIF1/cRK4 with $P(t) = N_{n-1}$ and $z = hL$

$$\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & I \\
\frac{1}{2}\phi_{12} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}z} \\
\frac{1}{2}\phi_{12} - \frac{1}{2}I & \frac{1}{2}I & 0 & 0 & \mathrm{e}^{\frac{1}{2}z} \\
\phi_1 - \mathrm{e}^{\frac{1}{2}z} & 0 & \mathrm{e}^{\frac{1}{2}z} & 0 & \mathrm{e}^{z} \\
\hline
\phi_1 - \frac{2}{3}\mathrm{e}^{\frac{1}{2}z} - \frac{1}{6}I & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{6}I & \mathrm{e}^{z}
\end{array}\right]$$

- Reduces to classical order four RK method when $L = 0$
- Has order two for general parabolic problems
- Preserves fixed points

GIF2/cRK4

GIF2/cRK4 with $P(t) = N_{n-1} + \frac{t - t_{n-1}}{h}(N_{n-1} - N_{n-2})$ and $z = hL$

$$\left[\begin{array}{cccc|cc}
0 & 0 & 0 & 0 & I & 0 \\
\frac{1}{2}\phi_{12} + \frac{1}{4}\phi_{22} & 0 & 0 & 0 & e^{\frac{1}{2}z} & -\frac{1}{4}\phi_{22} \\
\frac{1}{2}\phi_{12} + \frac{1}{4}\phi_{22} - 3I & \frac{1}{2}I & 0 & 0 & e^{\frac{1}{2}z} & -\frac{1}{4}\phi_{22} + \frac{1}{2}I \\
\phi_1 + \phi_2 - \frac{3}{2}e^{\frac{1}{2}z} & 0 & e^{\frac{1}{2}z} & 0 & e^{z} & -\phi_2 + \frac{1}{2}e^{\frac{1}{2}z} \\
\hline
\phi_1 + \phi_2 - e^{\frac{1}{2}z} - \frac{1}{3}I & \frac{1}{3}e^{\frac{1}{2}z} & \frac{1}{3}e^{\frac{1}{2}z} & \frac{1}{6}I & e^{z} & -\phi_2 + \frac{1}{3}e^{\frac{1}{2}z} + \frac{1}{6}I \\
I & 0 & 0 & 0 & 0 & 0
\end{array}\right]$$

- Reduces to classical order four RK method when $L = 0$
- Has order three for general parabolic problems
- Preserves fixed points

Stiff order conditions

The GIF methods in matrix form, with $u_i = u_{n-i-1}$ are

$$\begin{aligned} U =& A(hL)hN(U) + U(hL)hN(u) + \mathrm{e}^{chL}u_{n-1} \\ u_n =& B(hL)hN(U) + V(hL)hN(u) + \mathrm{e}^{hL}u_{n-1} \end{aligned}$$

Substitute exact solution and expand in Taylor series, with $w_i = i$

$$u(t_n) = \sum_{k=0}^{\infty} \left[B(hL)c^k + V(hL)(-w)^k \right] h^{k+1} \frac{N_{n-1}^{(k)}}{k!} + \mathrm{e}^{hL}u(t_{n-1}) + r$$

The output approximations must satisfy

$$r = \left[\phi_{k+1}(chL) - B(hL)\frac{c^k}{k!} + V(hL)\frac{(-w)^k}{k!} \right] h^{k+1} N_{n-1}^{(k)}$$

Stiff order conditions

The internal stages and output approximation must satisfy

$$\begin{aligned} c^{k+1}\phi_{k+1}(chL) =& A(hL)\frac{c^k}{k!} + U(hL)\frac{(-w)^k}{k!} \\ \phi_{k+1}(chL) =& B(hL)\frac{c^k}{k!} + V(hL)\frac{(-w)^k}{k!} \end{aligned}$$

- If $P(t)$ is of order q
- GIF methods have stiff stage order and order q

Hochbruck and Ostermann proved stiff order p is guaranteed if stiff order $p-1$ conditions are satisfied and non-stiff order p conditions.

GIF methods have overall stiff order $q+1$

Modifying GIF methods

The GIF methods satisfy stiff stage and overall order q

- Asymptotically correct error estimates
- Uniform continuous extensions

Most exponential integrators use fixed stepsizes

- Difficult to change stepsize as for LMS methods
- Aim to satisfy stiff stage order q and stiff order $q+1$
- Only need to modify the solution component

$$\sum_{i=1}^{s} B_i(hL)\frac{c_i^j}{j!} + \sum_{i=1}^{q} V_i(hL)\frac{(-1)^j}{j!} = \phi_{j+1}(hL)$$

Modifying GIF methods

Satisfy conditions while only modifying $B_s(z)$

The GIF1m/cRK4

$$B(z) = \begin{bmatrix} \phi_1 - \phi_2 - \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \phi_2 - \frac{1}{2}\mathrm{e}^{\frac{1}{2}z} \end{bmatrix}$$

$$V(z) = [e^z]$$

The GIFm2/cRK4 is

$$B(z) = \begin{bmatrix} \phi_1 - 2\phi_3 - \frac{1}{2}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}z} & \frac{1}{2}\phi_2 + \phi_3 - \frac{1}{4}\mathrm{e}^{\frac{1}{2}z} \end{bmatrix}$$

$$V(z) = \begin{bmatrix} e^z & \frac{1}{2}\phi_2 + \phi_3 - \frac{1}{4}\mathrm{e}^{\frac{1}{2}z} \end{bmatrix}$$

Significant performance improvement over GIF methods

GIF overview

Usually $P(t)$ is some interpolating polynomial

- If degree of $P(t)$ equals degree of the Adams method
    - ETD Adams method
- If degree of $P(t)$ is greater than degree of Adams method
    - new type of exponential Adams method
- If a Runge–Kutta method is used on transformed equation
    - exponential general linear method

If q is the order of $P(t)$, then stiff order $q+1$ is guaranteed

High stiff stage order is achieved at the cost of stability

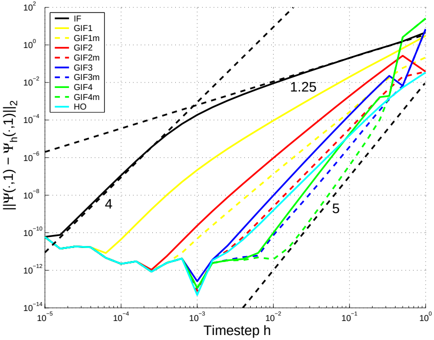
A modification increases order and overcomes loss of stability

A parabolic example

Use a 64-point standard finite difference discretization with Dirichlet boundary on

$$u_t = u_{xx} + \frac{1}{1+u^2} + \Phi, \quad x \in [0,1]$$

where Φ ensures $u(x,t) = x(1-x)\mathrm{e}^t$ and integrate over $t = [0,1]$

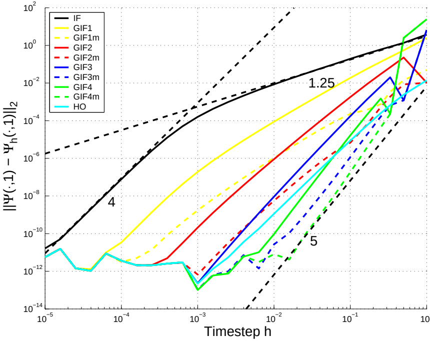


A parabolic example

Use a 64-point standard finite difference discretization with Dirichlet boundary on

$$u_t = u_{xx} + \int_0^1 u \, \mathrm{d}x + \Phi, \quad x \in [0, 1]$$

where Φ ensures $u(x, t) = x(1 - x)\mathrm{e}^t$ and integrate over $t = [0, 1]$



Other exponential GLMs

Another exponential GLM in Nordsieck type form is

$$\begin{aligned} U &= A(hL)hN(U) + U(hL)u^{[n-1]} \\ u^{[n]} &= B(hL)hN(U) + V(hL)u^{[n-1]} \end{aligned}$$

To satisfy stiff stage order and order simply satisfy

$$\begin{aligned} U(hL) &= C(hL) - A(hL)C(0)K \\ V(hL) &= E(hL) - B(hL)C(0)K \end{aligned}$$

where $K = \delta_{i,j+1}$, $C(hL)$ and $E(hL)$ are

$$C(hL) = \begin{bmatrix} e^{hL} & c\phi_1(chL) & c^2\phi_2(chL) & \dots \end{bmatrix}$$

$$E(hL) = \begin{bmatrix} e^{hL} & \phi_1(hL) & \phi_2(hL) & \dots \\ 0 & 1 & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Other exponential GLMs

The stiff stage order and order conditions are easily satisfied

The matrices $A(hL)$ and $B(hL)$ are free parameters

Use freedom to

- obtain good stability
- reduce higher order error
- construct methods easily

Currently trying to work how to do this

Discussion

- GIF methods generalize ETD Adams methods
- Easy to construct GIF methods with high stiff order
- GIF methods perform very well, but we hopefully can do better

- *Thank you for your attention*

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