On splitting methods for nonlinear parabolic evolution equations

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Gray-Scott equation

$$\frac{d}{dt}u = D_1\Delta u - uv^2 + \gamma(1-u)$$
$$\frac{d}{dt}v = D_2\Delta v + uv^2 - (\gamma+\kappa)v$$

$D_1 = 8\cdot 10^{-5}$, $D_2 = 4\cdot 10^{-5}$, $\gamma = 0.024$, $\kappa = 0.06$
Homogeneous Neumann boundary conditions

$$u(x,y,0) = 1 - 2v(x,y,0),$$
$$v(x,y,0) = \begin{cases} \frac{1}{4}\sin^2(4\pi x)\sin^2(4\pi y) & \text{if } 1 \le x, y \le 1.5, \\ 0 & \text{elsewhere} \end{cases}$$

Movie: v-component for $0 \le t \le 3000$

Problem class

Model problem: Fisher equation

Evolution equation of the form

$$\frac{d}{dt}u(t) = A(u(t)) + B(u(t))$$
$$u(0) = u_0$$

where there exist efficient methods for the solution of the subproblems

$$\frac{d}{dt}u(t) = A(u(t)), \quad u(0) = u_0$$
$$\frac{d}{dt}u(t) = B(u(t)), \quad u(0) = u_0$$

Model problem: **Fisher equation**

$$\frac{d}{dt}u = \Delta u + u(1-u)$$

on $\Omega = [0, 1]$ with suitable boundary conditions

Subproblem $\frac{d}{dt}u = \Delta u$ to be solved by "spectral method"

Subproblem $\frac{d}{dt}u = u(1-u)$ to be solved analytically (i.e., exactly)

Proper combination of the methods for the subproblems yields method for the full problem → **Time splitting spectral method**

Spectral method

Model problem: Fisher equation

Exact solution for the nonlinear subproblem

$$\frac{d}{dt}u = B(u) = u(1-u), \;\; u(0) = u_0 :$$

$$u(t,x) = \mathcal{E}_B(t,u_0)(x) = \frac{u_0(x)}{u_0(x) + (1-u_0(x))\mathrm{e}^{-t}}$$

Spectral method for the linear subproblem

$$\frac{d}{dt}u(t) = Au(t) = \Delta u(t), \;\; u(0) = u_0,$$

e.g., with **homogeneous Dirichlet boundary conditions** on $\Omega = [0,1]$: If expansion of initial data u_0 is given

$$u_0(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x)$$

then the solution of $\frac{d}{dt}u(t) = Au(t), \quad u(0) = u_0$ is

$$u(t,x) = \sum_{k=1}^{\infty} e^{-tk^2\pi} c_k \sin(k\pi x)$$

Spectral method

Full discretization

Full discretization:

- For an actual implementation on a computer the solution is computed on a finite set of (equidistant) sample points $\in [0, 1]$ only
- Only finite expansions

$$u(x) = \sum_{k=1}^{N} c_k \sin(k\pi x)$$

  are considered
- Discrete Fourier sine transform: Find finite expansion which coincides ("collocates") with given grid function at sample points
- Inverse discrete Fourier sine transform: Evaluation of finite expansion at sample points

(Inverse) discrete Fourier sine transform implemented by FFT

Time-splitting methods

Strang splitting method

Time splitting spectral method for

$$\tfrac{d}{dt}u(t) = A(u(t)) + B(u(t)),\ \ u(0) = u_0$$

Combine (spectral) methods for the two subproblems
Idea: On a grid $\{t_0 = 0, t_1 = \Delta t, t_2 = 2\Delta t, \ldots\}$ with stepsize Δt compute approximations $\{u_0, u_1 \approx u(t_1), u_2 \approx u(t_2), \ldots\}$ to the solution $u(t)$ iteratively; given u_j compute u_{j+1} by the scheme

$$\text{solve } \tfrac{d}{dt}v(t) = A(v(t)),\ \ v(0) = u_j, \quad \text{set } u_j^* = v(\frac{1}{2}\Delta t)$$

$$\text{solve } \tfrac{d}{dt}v(t) = B(v(t)),\ \ v(0) = u_j^*, \quad \text{set } u_j^{**} = v(t)$$

$$\text{solve } \tfrac{d}{dt}v(t) = A(v(t)),\ \ v(0) = u_j^{**}, \quad \text{set } u_{j+1} = v(\frac{1}{2}\Delta t)$$

$\rightarrow$ second order **Strang splitting**, characterized by list of coefficients

$$\frac{1}{2}, 1, \frac{1}{2}$$

Time-splitting methods

Higher order schemes

Lie-Trotter (1st order):

$$1, 1$$

Strang (2nd order):

$$\frac{1}{2}, 1, \frac{1}{2}$$

3rd order scheme:

$$\frac{7}{24}, \frac{2}{3}, \frac{3}{4}, -\frac{2}{3}, -\frac{1}{24}, 1$$

Yoshida (4th order):

$$\frac{1}{2(2-2^{1/3})}, \frac{1}{2-2^{1/3}}, \frac{1-2^{1/3}}{2(2-2^{1/3})}, \frac{-2^{1/3}}{2-2^{1/3}}, \frac{1-2^{1/3}}{2(2-2^{1/3})}, \frac{1}{2-2^{1/3}}, \frac{1}{2(2-2^{1/3})}$$

Note: Schemes of order 3 or higher necessarily contain negative coefficients

- Suitable for evolution equation of (time-symmetric) *Schrödinger* type
- *Not* suitable for evolution equation of *parabolic* type
- Remedy: Schemes with complex coefficients with positive real part

Time-splitting methods

Higher order schemes with complex coefficients

4th order scheme (see Castella, Chartier, Descombes, Vilmart (2009)):

$$\omega_1 = \frac{1}{2 - 2^{1/3} e^{2i\pi/3}} = 0.324396404020171183 + 0.134586272490806697i$$

$$\omega_2 = 1 - 2\omega_1 = 0.351207191959657634 - 0.269172544981613394i$$

i	a_i	b_i
1	$\omega_1/2$	ω_1
2	$(\omega_1 + \omega_2)/2$	ω_2
3	$(\omega_1 + \omega_2)/2$	ω_1
4	$\omega_1/2$	

http://www.asc.tuwien.ac.at/~winfried/splitting/index.php

Numerical experiments

No order reduction for periodic boundary conditions

Periodic boundary conditions, $N = 256$

Consistent initial condition

$$u_0(x) = \sin(2\pi x)$$

Global error at $t_{\mathrm{end}} = 0.1$:

dt	err	p
0.100E+00	0.318E-02	
0.500E-01	0.456E-03	2.80
0.250E-01	0.385E-04	3.57
0.125E-01	0.262E-05	3.88
0.625E-02	0.167E-06	3.97
0.313E-02	0.105E-07	3.99
0.156E-02	0.658E-09	4.00
0.781E-03	0.412E-10	4.00
0.391E-03	0.257E-11	4.00
0.195E-03	0.161E-12	4.00

Numerical experiments

Massive order reduction for homogeneous Dirichlet boundary conditions

Homogeneous Dirichlet boundary conditions, $N = 256$

Consistent initial condition

$$u_0(x) = \sin(2\pi x)$$

Global error at $t_{\text{end}} = 0.1$:

dt	err	p
0.100E+00	0.946E-03	
0.500E-01	0.119E-03	2.99
0.250E-01	0.941E-05	3.66
0.125E-01	0.628E-06	3.91
0.625E-02	0.400E-07	3.97
0.313E-02	0.253E-08	3.98
0.156E-02	0.174E-09	3.86
0.781E-03	0.187E-10	3.22
0.391E-03	0.340E-11	2.46
0.195E-03	0.702E-12	2.28

Numerical experiments

Massive order reduction for homogeneous Dirichlet boundary conditions

Homogeneous Dirichlet boundary conditions, $N = 256$

Inconsistent initial condition

$$u_0(x) = \cos(2\pi x)$$

Global error at $t_{\text{end}} = 0.1$:

dt	err	p
0.100E+00	0.116E-02	
0.500E-01	0.325E-03	1.83
0.250E-01	0.396E-04	3.04
0.125E-01	0.303E-05	3.71
0.625E-02	0.204E-06	3.89
0.313E-02	0.143E-07	3.83
0.156E-02	0.155E-08	3.21
0.781E-03	0.283E-09	2.45
0.391E-03	0.629E-10	2.17
0.195E-03	0.221E-10	1.51

Error analysis

$$\frac{\mathrm{d}}{\mathrm{d}t} u = \Delta u + F(u)$$

Abstract setting

$$\frac{\mathrm{d}}{\mathrm{d}t} u(t) = H(u(t)) = Au(t) + B(u(t)), \quad t \in (0, T]$$

Dirichlet boundary conditions:

$$A : D(A) \to L_2(\Omega), \quad D(A) = H^2(\Omega) \cap H_0^1(\Omega), \quad Au = \Delta u,\; u \in D(A)$$

B defined point-wise, at least well defined on $H^d(\Omega)$:

$$B : D(B) \to L_2(\Omega), \quad H^d(\Omega) \subset C^0(\Omega) \subset D(B), \quad B(u)(x) = F(u(x)),\, x \in \Omega$$

$\Longrightarrow H = A + B$ at least well defined on

$$H^{\max(2,d)} \cap H_0^1(\Omega) \subset D(A) \cap D(B) = D(H)$$

Error analysis

Flows A . . . unbounded linear operator generating semi-group $(e^{tA})_{t\geq 0}$
Flow with respect to A given by

$$\mathcal{E}_A(t, u) = e^{tA}u, \quad t \geq 0$$

Flow with respect to B given using flow Φ of scalar ODE $\frac{\mathrm{d}}{\mathrm{d}t}u(t) = F(u(t))$:

$$\mathcal{E}_B(t, u)(x) = \Phi(t, x, u(x)), \quad x \in \Omega, \ t \in (T_{\min}(u), T_{\max}(u)).$$

Error analysis

Lie/Trotter:

$$\mathcal{S}(t,u) = \mathcal{E}_B(t, \mathrm{e}^{tA}u)$$

Defect:

$$\mathcal{D}(t,u) = \frac{\partial}{\partial t}\mathcal{S}(t,u) - H(\mathcal{S}(t,u))$$

Local error:

$$\mathcal{L}(t,u) = \mathcal{S}(t,u) - \mathcal{E}_H(t,u)$$

Estimate local error by defect (L_F ... Lipschitz constant for F):

$$\|\mathcal{L}(t,u)\| \le \mathrm{e}^{tL_F} \int_0^t \|\mathcal{D}(\tau,u)\| \,\mathrm{d}\tau$$

Integral representation of defect:

$$\mathcal{D}(t,u) = \int_0^t \partial_2 \mathcal{E}_B(t-\tau, \mathcal{E}_B(\tau, \mathrm{e}^{tA}u)) \cdot [B,A](\mathcal{E}_B(\tau, \mathrm{e}^{tA}u)) \,\mathrm{d}\tau$$

Error analysis

To obtain an estimate for the local error we have to estimate

$$[B, A](\mathcal{E}_B(\tau, \mathrm{e}^{tA} u)),$$

where

$$[B, A](v) = -F''(v)\nabla v \cdot \nabla v$$

By stability estimates for F and Φ and thus for B and $\mathcal{E}_B$:

$$\begin{aligned} \|[B, A](\mathcal{E}_B(\tau, \mathrm{e}^{tA} u))\| &\leq \mathcal{C}\|\nabla\mathcal{E}_B(\tau, \mathrm{e}^{tA} u) \cdot \nabla\mathcal{E}_B(\tau, \mathrm{e}^{tA} u)\| \\ &\leq \mathcal{C}\left(\|\mathrm{e}^{tA} u\|^2 + \|\mathrm{e}^{tA} u\|\|\nabla\mathrm{e}^{tA} u\| + \|\nabla\mathrm{e}^{tA} u \cdot \nabla\mathrm{e}^{tA} u\|\right) \end{aligned}$$

Here

$$\|\mathrm{e}^{tA} u\| \leq \|u\|$$

$$\|\nabla\mathrm{e}^{tA} u\| \leq \mathcal{C} t^{s-\frac{1}{2}} \|u\|_{H^{2s}(\Omega)} \quad \text{if } u \in D((-A)^s) \text{ with } s \leq \frac{1}{2}$$

$$\|\nabla\mathrm{e}^{tA} u \cdot \nabla\mathrm{e}^{tA} u\| \leq \mathcal{C} t^{\min\{s-\frac{1}{2}, 2s-1\}-\frac{d}{4}-\varepsilon} \|u\|^2_{H^{2s}(\Omega)} \quad \text{if } u \in D((-A)^s) \text{ with } s \leq \frac{1}{2} + \frac{d}{4}$$

$$\Longrightarrow$$

$$\|[B, A](\mathcal{E}_B(\tau, \mathrm{e}^{tA} u))\| \leq \mathcal{C} t^{\min\{s-\frac{1}{2}, 2s-1\}-\frac{d}{4}-\varepsilon} \|u\|^2_{H^{2s}(\Omega)} \quad \text{if } u \in D((-A)^s) \text{ with } s \leq \frac{1}{2} + \frac{d}{4}$$

Error analysis

Fujiwara (1967):
Dirichlet boundary conditions:

$$u \in H^1(\Omega) \quad \Rightarrow \quad u \in D((-A)^{\frac{1}{4}-\varepsilon}) \quad \Rightarrow \text{choose } s = \frac{1}{4} - \varepsilon$$

$\Longrightarrow$ estimate for the local error

$$\|\mathcal{L}(t,u)\| \le \mathcal{C} t^{\frac{3}{2}-\frac{d}{4}-\varepsilon} = \mathcal{C} t^{\frac{5}{4}-\varepsilon} \quad (d = 1)$$

Numerical experiment: Fisher equation on $[0,1]$, $N = 8192$, inconsistent initial condition

$$u_0(x) = \cos(2\pi x)$$

Local error:

dt	err	p
0.156E-02	0.135E-03	
0.781E-03	0.539E-04	1.33
0.391E-03	0.228E-04	1.24
0.195E-03	0.972E-05	1.23
0.977E-04	0.414E-05	1.23
0.488E-04	0.176E-05	1.24
0.244E-04	0.742E-06	1.24
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