Linearly Stabilized Schemes for the Time Integration of Stiff Nonlinear PDEs

Kevin Chow

December 9, 2016

Table of contents

Introduction

1. Focus on time stepping for stiff nonlinear PDEs.
   - Stability
   - Accuracy
   - Efficiency
   - Simplicity

Example

Consider the heat equation,

$$u_t = u_{xx}, \quad x \in \Omega, t > 0.$$

Discretize in space:

$$U' = LU, \quad U \in \mathbb{R}^N, t > 0.$$

Explicit: $U^{n+1} = G(U^n, U^{n-1}, \dots, LU^n, LU^{n-1}, \dots)$, but $\Delta t \leq Ch^2$.
Implicit: $AU^{n+1} = b$; unconditionally stable, but must solve a linear system.

Example

Now compare with

$$u_t = \frac{u_{xx}}{1+u_x^2} - \frac{1}{u}, \quad x \in \Omega, t > 0.$$

and

$$U' = F(U), \quad U \in \mathbb{R}^N, t > 0.$$

Explicit: $U^{n+1} = G(U^n, U^{n-1}, \dots, F(U^n), F(U^{n-1}), \dots)$, but $\Delta t \leq Ch^2$.
Implicit: $AU^{n+1} = b(U^{n+1})$; unconditionally stable, but must solve a nonlinear system because nonlinearity is in the stiff term.

Example

Comparing side-by-side:

$$u_t = u_{xx}, \quad x \in \Omega, t > 0,$$

Explicit: $\Delta t \leq Ch^2$
Implicit: unconditionally stable; solution to linear system

$$u_t = \frac{u_{xx}}{1+u_x^2} - \frac{1}{u}, \quad x \in \Omega, t > 0,$$

Explicit: $\Delta t \leq Ch^2$
Implicit: unconditionally stable; solution to nonlinear system

Summary: What We Like

Explicit: simple; handles nonlinear terms with no added difficulty.
Implicit: large time steps

Example

Modify the equation,

$$u_t = \frac{u_{xx}}{1+u_x^2} - \frac{1}{u} - u_{xx} + u_{xx}, \quad x \in \Omega, t > 0,$$

$$\downarrow$$

$$U' = F(U) - LU + LU, \quad U \in \mathbb{R}^N, t > 0,$$

and use implicit-explicit time stepping, e.g.

$$\frac{U^{n+1} - U^n}{\Delta t} = F(U^n) - LU^n + LU^{n+1}.$$

Linear Stability

More generally, from $U' = F(U)$, we can modify as

$$U' = \underbrace{F(U) - pLU}_{(\star)} + pLU, \quad p > 0,$$

and apply a time stepping scheme that treats $(\star)$ explicitly.
Key question: Is this unconditionally stable?

Scalar test equation

Standard case:

$$U' = F(U)$$

Linearize $\rightarrow$ Diagonalize $\rightarrow$ Test equation:

$$u' = \lambda u$$

With linear modification:

$$U' = F(U) - pLU + pLU$$

Linearize $\rightarrow$ Diagonalize $\rightarrow$ Test equation:

$$\begin{aligned} u' &= \lambda u - p\lambda u + p\lambda u \\ &= (1-p)\lambda u + p\lambda u \end{aligned}$$

Apply time stepping method:

$$u^{n+1} = \xi(\lambda \Delta t) u^n$$

Stability constraint:

$$|\xi(\lambda \Delta t)| \leq 1$$

Implicit-explicit Euler

Applied to the test equation $u' = (1-p)\lambda u + p\lambda u$, yields

$$\frac{u^{n+1} - u^n}{\Delta t} = (1-p)\lambda u^n + p\lambda u^{n+1}.$$

The amplification factor is

$$\xi_1(\lambda \Delta t) = \frac{1 + (1-p)\lambda \Delta t}{1 - p\lambda \Delta t}.$$

Impose unconditional stability:

$$|\xi_1(\lambda \Delta t)| \leq 1 \text{ for all } \lambda \Delta t < 0 \implies p \geq 1/2.$$

Explicit-implicit-null (EIN)

Use Richardson extrapolation to get second order. The amplification factor is

$$\xi_{EIN}(\lambda\Delta t) = 2\xi_1^2(\lambda\Delta t/2) - \xi_1(\lambda\Delta t).$$

and

$$|\xi_{EIN}(\lambda\Delta t)| \leq 1 \text{ for all } \lambda\Delta t < 0 \implies p \geq 2/3.$$

Implicit-explicit multistep methods

An alternative for second and higher order methods: IMEX multistep methods.

Order	Method	$p \in$
2	SBDF2	$[3/4, \infty)$
	CNAB	$[1, \infty)$
	mCNAB	$[8/9, \infty)$
	CNLF	$[1/2, \infty)$
3	SBDF3	$[7/8, 2]$
4	SBDF4	$[11/12, 5/4]$

Comparing the methods

Do the methods work as advertised?
Examine this with two test problems,

$$u_t = \frac{u_{xx}}{1 + u_x^2} - \frac{1}{u},$$

and

$$u_t = \Delta(u^5).$$

Test Problem 1

First test problem:

$$u_t = \frac{u_{xx}}{1+u_x^2} - \frac{1}{u}, \quad 0 < x < 10, \quad t > 0,$$

with initial condition

$$u(x,0) = 1 + 0.10 \sin\left(\frac{\pi}{5}x\right),$$

and boundary conditions $u(0,t) = 1 = u(10,t)$.

Numerical convergence test

Figure: Numerical convergence of linearly stabilized schemes.

Spatial discretization: Uniform grid, centred differences, N=2048.
Final time: $T = 0.35$.
Reference solution: Explicit third order Runge-Kutta, $\Delta t = 1.46 \times 10^{-5}$.
Stabilized by adding and subtracting pu_{xx}.

Failure of SBDF3 and SBDF4

How did we choose p? Consider

$$u' = \lambda u - p\lambda u + p\lambda u$$

and

$$U' = F(U) - pLU + pLU.$$

With the test equation, we derived a restriction on p. More generally, the restriction applies to $p\lambda_L/\lambda_F$. For test problem 1 with centred differences, we find

$$\frac{p\lambda_L}{\lambda_F} \approx p(1 + (D_1\bar{u}_j^n)^2),$$

Failure of SBDF3 and SBDF4

The selection of p for SBDF3 is dictated by

$$\max_{1\leq j\leq N} \frac{7}{8}\frac{1}{1+(D_1\bar{u}_j^n)^2} \leq p \leq \min_{1\leq j\leq N} \frac{2}{1+(D_1\bar{u}_j^n)^2}.$$

Figure: Development of instabilities using SBDF3, $p = 1.625$.

Test Problem 2

Second test problem:

$$u_t = \Delta(u^5), \quad (x, y) \in [0, 1]^2, \quad t > 0,$$

with initial and boundary conditions set such that the exact solution is

$$u(x, y, t) = \left(\frac{4}{5}(2t + x + y)\right)^{1/4}.$$

Numerical convergence test

Figure: Numerical convergence of linearly stabilized schemes.

Spatial discretization: second order centred differences; N=2048.
Final time: $T = 0.40$.
Reference solution: explicit third order Runge-Kutta, $\Delta t = 6.25 \times 10^{-6}$.
Stabilized using $p\Delta u$, and

$$\frac{p\lambda_L}{\lambda_F} \approx \frac{p}{8(1+t)}.$$

Error constant

Discretizing $u' = (1-p)\lambda u + p\lambda u$, we observe that the discretization error grows with p.
We examine this behaviour by applying the time stepping method and finding the series expansion of the amplification factor at $\Delta t = 0$.
For second order methods, leading order error term is Δt^3. The coefficient indicates how the method behaves.

Table: Coefficient of leading order error term as applied to the test equation.

Method	Coefficient
EIN	$\frac{1}{2}(p - p^2)$
SBDF2	p
CNAB	
mCNAB	
CNLF	

Amplification factor as $\Delta t \to \infty$

Methods performing well at large time step-sizes have small amplication factor as $\Delta t \to \infty$.

Figure: Amplification factor as $\Delta t \to \infty$.

Image Inpainting

In Schönlieb and Bertozzi (2011), the authors proposed the fourth order inpainting model

$$u_t = -\Delta\nabla \cdot \left(\frac{\nabla u}{\sqrt{|\nabla u|^2 + \epsilon^2}} \right) + \lambda(u_0 - u),$$

and numerical solution by the first order accurate method

$$\frac{u^{n+1} - u^n}{\Delta t} = -\Delta\nabla \cdot \left(\frac{\nabla u^n}{\sqrt{|\nabla u^n|^2 + \epsilon^2}} \right) + \lambda(u_0 - u^n) + p_0\lambda u^n + p_1\Delta^2 u^n$$

$$- p_0\lambda u^{n+1} - p_1\Delta^2 u^{n+1}.$$

Image inpainting

Figure: A vandalized photograph.

Table: Iteration counts for TV-H^{-1} image restoration.

	Δt	Iterations
SBDF1	0.30	1002
SBDF2	0.54	401
CNAB	0.64	347

Motion by mean curvature

We evolve the level set equation for motion by mean curvature,

$$u_t = \kappa\,|\nabla u| = |\nabla u|\,\nabla\cdot\left(\frac{\nabla u}{|\nabla u|}\right)$$

on an initial dumbbell-shaped curve in 3D. We solve to time $T = 0.75$ on a $256 \times 128 \times 128$ periodic grid.

On a machine with an Intel® Core™ i5-4570 CPU@3.20GHz running MATLAB 2014b:

- Forward Euler: 3000 time steps $\rightarrow$ over 28 minutes.
- SBDF2: 75 time steps $\rightarrow$ under 100 seconds.

Motion by mean curvature

Figure: Dumbbell-shaped curve under mean curvature flow.

Conclusion

Contributions of this thesis mainly fall into two categories:

1. Further developed linearly stabilized schemes.
   - Set out a framework for developing new methods of this type.
   - Identified properties necessary for effective schemes.
2. Proposed new methods that outperform existing ones.
   - IMEX multistep methods and exponential time differencing methods.

Future work:

1. Development higher order methods without the deficiencies exhibited by ETD methods.
2. Detailed comparison with popular algorithms for nonlinear stiff PDEs.