Operator Splitting in Action: Ideas, Derivations, Global Errors and New Challenges

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structure preserving solvers I

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Preface

Recent trends in highly accurate and structure-preserving numerical methods for partial differential equations

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The development of highly accurate and structure-preserving numerical methods for solving partial differential equations is an ongoing quest even after decades of successful approaches. The research is particularly fuelled by recent demands arising from various applications in sciences and engineering. The significance of its numerical strategies has been universally acknowledged and validated through improvement of discrete methods in diverse branches, including finite difference methods, finite element methods, spectral collocation approaches, spectral Galerkin methods, and so on. In recent years, structure preserving methods, also known as geometric numerical integrators, have also emerged as a central topic in computational mathematics. It has been realized that an integrator should be designed to preserve as much as possible intrinsic features of the underlying problems, such as conservations of the mass, momentum and energy, as well as the symplecticity and multisymplecticity of Hamiltonian systems. Structure-preserving algorithms can be effectively utilized for simulations of a variety of theoretical and application problems, ranging from celestial mechanics, quantum mechanics, fluid dynamics, and geophysics.

This special issue is dedicated to recent advances in aforementioned pursuits for high-accuracy and structure-preserving algorithms when partial differential equations are targeted. We intend to accommodate a broad spectrum of investigations. Contributed papers in this special issue address, in particular, concerns in fields of:

- mass conservation in least-squares finite element methods;
- Fourier pseudo-spectral conservative schemes for Klein–Gordon–Schrödinger equation;
- high-order IMEX-WENO finite volume approximations;
- local discontinuous Galerkin methods for Hamiltonian partial differential equations;
- structure-preserving exponential methods for Burgers–Huxley equation; and
- energy-preserving schemes for 2D Hamiltonian wave equations with Neumann boundary conditions.

The numerical methods proposed by authors of this special issue have demonstrated that highly accurate

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structure preserving solvers II

Geometry, compatibility and structure preservation in computational differential equations

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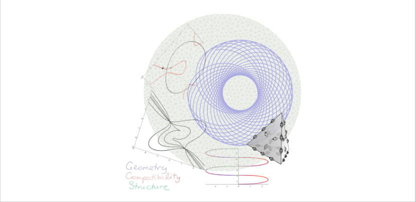

Programme
3rd July 2019 to 19th December 2019
Organisers: Elena Celledoni *(Norwegian University of Science and Technology, Norwegian University of Science and Technology)*

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structure preserving solvers III

Structure preservation and general relativity

Workshop
30th September 2019 to 4th October 2019
Organisers: Douglas Arnold *(University of Minnesota)*
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Workshop Theme

Numerical relativity--the design, implementation, and study of computational methods for the approximate solution of Einstein's equations--is a powerful approach to understanding the complex behavior of gravitational fields. Einstein's equations are statements about the geometry of space times, based on differential geometric structures such as covariance, symmetries, etc. For this reason, structure-preserving numerical methods have the potential to bring enormous benefits to numerical relativity. The development of stable structure-preserving discretization methods for the Einstein equations has thus far proven largely elusive, but it represents a direction with great promise. The successful contribution of numerical relativity to the LIGO observations in 2015 and since has highlighted the important place of numerical relativity in the new world of gravitational wave astronomy. Beyond that, numerical investigations into the behavior of gravity in four and higher dimensions in the highly non-linear regime and computational explorations of holograpy both illustrate the significant role of the field to deciphering the full implications of Einstein's theory of relativity. This role raises many particular challenges, for example, the presence of highly non-linear constraints that must be satisfied for a correct solution, the vast length of time and spatial scales associated to problems of practical interest, the development of singularities, and the necessity to introduce spatial boundaries, which, in turn, require constraint-preserving boundary conditions. All these challenges facing us, together with the recent advances in structure-preserving discretization in other branches of numerical PDE makes this an ideal time to bring together specialists in numerical analysis, computational science, geometry, general relativity, and numerical relativity to discuss and interact in a multidisciplinary environment.

Deadline for applications: 23rd June 2019

GCS programme participants DO NOT need to apply, programme participants with visit dates during GCSW01 will automatically be added to the attendee list.

Please note members of Cambridge University are welcome to turn up and sign in as a non-registered attendee on the day(s) during the workshop and attend the lecture(s). Please note that we cannot provide you with any support including name badge, meals or accommodation.

In addition to visiting the INI, there are multiple ways in which you can participate remotely.

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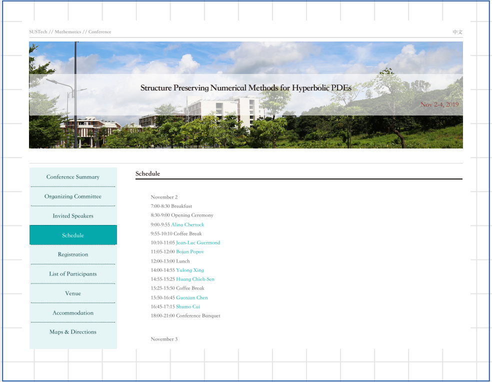

Structure Preserving Numerical Methods for Hyperbolic PDEs, SUSTech, Shenzhen, 2019

structure preserving solvers V

minisymposium on highly accurate and structure-preserving numerical methods

JMM: Denver, CO, USA, January, 2020

but today is for a basic fact

I was sitting in a seminar a few weeks ago. The talk was on deep machine learning for solving an image processing problem. It was outstanding and operator splitting was involved.

Then I asked for a justification for using the splitting. The answer was that it was used before in a reference.

Indeed, proofs in mathematical/numerical analysis have become overwhelmingly complicated. Even the best mathematicians often do not fully comprehend them. Consequently, researchers just keep faith that the underpinnings of a new proof are correct.

Because of this, when mathematicians reference a published result in their work, readers just take their word for it. Kevin Buzzard from Imperial College London Mathematics, is worried about this. There can be a huge possibility that many existing mathematical proofs are incorrect!

©K.B.

Let's now take a look at the legend of splitting methods!

A simple problem

Let $u, u_0 \in \mathbb{C}^n,\ n \geq 1$. Consider the following *initial value problem* (IVP):

$$\frac{\partial u}{\partial t} = \mathcal{L}u, \quad t > t_0, \tag{1}$$

$$u(t_0) = u_0, \tag{2}$$

where

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \cdots + \mathcal{L}_n \tag{3}$$

and $\mathcal{L}_1, \ldots, \mathcal{L}_n$ are operators depending on u and $t > t_0$.

An example of $\mathcal{L}$

An m-dimensional linear partial differential operator may look like

$$\mathcal{L} = \sum_{k=0}^{n} \sum_{\substack{i_1+i_2+\cdots+i_m=k;\\ i_1,i_2,\ldots,i_m\geq 0}} c_{i_1,i_2,\ldots,i_m}(x)\frac{\partial^k}{\partial x_1^{i_1}\partial_2^{i_2}\cdots\partial_m^{i_m}},$$

where $x \in \mathbb{C}^m$.

A formal solution

The formal solution of the IVP is

$$u(t) = \exp\left\{\int_{t_0}^{t} \mathcal{L}(u,\tau)d\tau\right\} u_0 = M(t_0,t)u_0, \tag{4}$$

where

$$M(a,b) = \exp\left\{\int_{a}^{b} \mathcal{L}(u(\tau),\tau)d\tau\right\}.$$

To evaluate (10), the key is to compute M first.

An observation

To this end, let

$$\begin{aligned} M(t_0, t) &= \exp\left\{\int_{t_0}^{t} \mathcal{L}(u,\tau)d\tau\right\} \\ &= \exp\left\{\int_{t_0}^{t} [\mathcal{L}_1(u,\tau) + \mathcal{L}_2(u,\tau) + \cdots + \mathcal{L}_n(u,\tau)]\, d\tau\right\} \\ &= \exp\left\{\int_{t_0}^{t} \mathcal{L}_1(u,\tau)d\tau + \int_{t_0}^{t} \mathcal{L}_2(u,\tau)d\tau + \cdots + \int_{t_0}^{t} \mathcal{L}_n(u,\tau)d\tau\right\} \\ &= \exp\{L_1(t) + L_2(t) + \cdots + L_n(t)\}. \end{aligned}$$

Denote

$$L = L_1 + L_2 + \cdots + L_n.$$

We observe that

$$M = e^{L} = e^{L_1+L_2+\cdots+L_n} \neq e^{L_1} e^{L_2} \cdots e^{L_n}$$

unless $L_1,\ L_2, \ldots, L_n$ commute, *that is,*

$$[L_i, L_j] = [L_j, L_i], \quad i, j \in \{1, 2, \ldots, n\}.$$

But may we wish that

$$M = e^{L} = e^{L_1+L_2+\cdots+L_n} \approx e^{L_1} e^{L_2} \cdots e^{L_n}, \quad t \to t_0^{+}, \tag{5}$$

for making the calculation of M simpler and realistic.

For this, recall that

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

We have similar operator function expansions

$$\begin{aligned} e^L &= \sum_{k=0}^{\infty} \frac{L^k}{k!} = I + L_1 + L_2 + \cdots + L_n + \frac{1}{2!}[L_1 + L_2 + \cdots + L_n]^2 \\ &\quad + \frac{1}{3!}[L_1 + L_2 + \cdots + L_n]^3 + \cdots ; \\ e^{L_j} &= \sum_{k=0}^{\infty} \frac{L_j^k}{k!} = I + L_j + \frac{L_j^2}{2!} + \frac{L_j^3}{3!} + \cdots , \quad j = 1, 2, \ldots , n. \end{aligned}$$

Continue...

Further,

$$
\begin{aligned}
e^{L_1} e^{L_2} \cdots e^{L_n} &= \left(\sum_{k=0}^{\infty} \frac{L_1^k}{k!} \right) \left(\sum_{k=0}^{\infty} \frac{L_2^k}{k!} \right) \cdots \left(\sum_{k=0}^{\infty} \frac{L_n^k}{k!} \right) \\
&= I + L_1 + L_2 + \cdots + L_n + \frac{1}{2}[L_1^2 + L_2^2 + \cdots + L_n^2 \\
&\quad + 2L_1 L_2 + 2L_1 L_3 + \cdots + 2L_1 L_n + 2L_2 L_3 + \cdots \\
&\quad + 2L_2 L_n + 2L_3 L_4 + \cdots + 2L_{n-1} L_n] + \cdots
\end{aligned}
$$

Continue...

It follows that

$$M(t_0, t) = e^{L_1 + L_2 + \cdots L_n} = e^{L_1} e^{L_2} \cdots e^{L_n} + \mathcal{O}(\tau^2), \quad \tau \to 0^+,$$

if $L_j = \mathcal{O}(\tau), \ j = 1, 2, \ldots, n$, with $\tau = t - t_0$.

There are $n!$ different ways to arrange the product on the right-hand-side of the above equality! Now,

$$u(t) = M(t_0, t) u_0 = e^{L_1(t)} e^{L_2(t)} \cdots e^{L_n(t)} u_0 + \mathcal{O}(\tau^2), \quad \tau \to 0^+.$$

Continue...

Thus,

$$u(t) \approx e^{L_1(t)} e^{L_2(t)} \cdots e^{L_n(t)} u_0.$$

Denote:

$$\begin{aligned} u_n &= e^{L_n} u_0, \\ u_{n-1} &= e^{L_{n-1}} u_n, \\ u_{n-2} &= e^{L_{n-2}} u_{n-1}, \\ \cdots & \quad \cdots, \\ \cdots & \quad \cdots, \\ u_2 &= e^{L_2} u_3, \\ u &= e^{L_1} u_2. \end{aligned}$$

Continue...

They correspond to operator IVPs:

$$
\begin{aligned}
u_n' &= \mathcal{L}_n u_n, \quad u_n(0) = u_0, \\
u_{n-1}' &= \mathcal{L}_{n-1} u_{n-1}, \quad u_{n-1}(0) = u_n, \\
u_{n-2}' &= \mathcal{L}_{n-2} u_{n-2}, \quad u_{n-2}(0) = u_{n-1}, \\
\cdots & \quad \cdots, \\
\cdots & \quad \cdots, \\
u_2' &= \mathcal{L}_2 u_2, \quad u_2(0) = u_3, \\
u_1' &= \mathcal{L}_1 u_1, \quad u_1(0) = u_2, \\
u &= u_1.
\end{aligned}
$$

Continue...

In other words, the original equation

$$u' = (\mathcal{L}_1 + \mathcal{L}_2 + \cdots + \mathcal{L}_n)u$$

can be split to *n* subequations (each of them is simpler) to solve:

$$\begin{aligned}
u_n' &= \mathcal{L}_n u_n, \\
u_{n-1}' &= \mathcal{L}_{n-1} u_{n-1}, \\
u_{n-2}' &= \mathcal{L}_{n-2} u_{n-2}, \\
\cdots & \quad \cdots, \\
\cdots & \quad \cdots, \\
u_2' &= \mathcal{L}_2 u_2, \\
u' &= \mathcal{L}_1 u.
\end{aligned}$$

Operator splitting:

This is the basic idea of a splitting method!

1. We often call the aforementioned splitting procedure as *Operator Splitting*, since $\mathcal{L}_k,\ k = 1, 2, \ldots, n$, are general operators.
2. If $\mathcal{L}_k,\ k = 1, 2, \ldots, n$, are dimension-related operators, such as an n-dimensional Laplacian $\mathcal{L} = \Delta = \nabla^2$, then the procedure is also called a *Dimensional Splitting*.
3. In general, $\mathcal{L}_k,\ k = 1, 2, \ldots, n$, can be any well-defined operators (not need to be differential operators).
4. The splitting error incurred is of $\mathcal{O}(\tau^{p+1})$ with the order $p = 1$.

A better accuracy?

$$e^{L_1+L_2+\cdots L_n} = e^{L_1} e^{L_2} \cdots e^{L_n} + \mathcal{O}(\tau^{p+1}), \quad p = 1, \ \tau \to 0^+.$$

But, it is found that

$$\begin{aligned} e^{L_1+L_2+\cdots L_n} &= \frac{1}{2}\left(e^{L_1} e^{L_2} \cdots e^{L_n} + e^{L_n} e^{L_{n-1}} \cdots e^{L_1}\right) + \mathcal{O}(\tau^{q+1}); \\ e^{L_1+L_2+\cdots L_n} &= e^{\frac{1}{2}L_1} e^{\frac{1}{2}L_2} \cdots e^{\frac{1}{2}L_{n-1}} e^{L_n} e^{\frac{1}{2}L_{n-1}} \cdots e^{\frac{1}{2}L_2} e^{\frac{1}{2}L_1} + \mathcal{O}(\tau^{q+1}), \end{aligned}$$

with $q = 2$ as $\tau \to 0^+$.

These are second order operator splitting formulae!

Even better?

Do we have even better splitting formulae? Yes.

- Baker-Campbell-Hausdorff formula;
- Zassenhaus formula;
- Magnus expansions;
- Trotter formula;
- Lie algebraic formula;
- Complex coefficient formulas;
- *More importantly, your formula...*

Nonhomogeneous problems?

Not a problem!

For $u, f, u_0 \in \mathbb{C}^n,\ n \geq 1$. Consider the following IVP:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \mathcal{L}u + f, \quad t > t_0, & (6) \\ u(t_0) &= u_0, & (7) \end{aligned}$$

where

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \cdots + \mathcal{L}_n \tag{8}$$

and $\mathcal{L}_1, \ldots, \mathcal{L}_n$ are operators depending on u and $f = f(u, t),\ t > t_0$.

A formal solution

The formal solution of the IVP is

$$\begin{aligned} u(t) &= \exp\left\{\int_{t_0}^{t} \mathcal{L}(u,\tau)d\tau\right\} u_0 + \int_{t_0}^{t} \exp\left\{\int_{\tau}^{t} \mathcal{L}(u,\xi)d\xi\right\} f(u,\tau)d\tau \\ &= M(t_0,t)u_0 + \int_{t_0}^{t} M(\tau,t)f(u,\tau)d\tau. \end{aligned} \tag{9}$$

Apparently,

$$M(\tau,t) = M(t_0,t)M(\tau,t_0),\ \ t_0 \le \tau \le t.$$

So we can play the game of splitting again!

An example

Let $\mathcal{D} = \{(x, y) : \ a < x < b, \ c < y < d\}$. We consider

$$\begin{aligned} u_t &= \alpha^2(x,y)u_{xx} + \beta^2(x,y)u_{yy}, \quad (x,y) \in \mathcal{D}, \ t > 0, \\ u(x,y,t) &= 0, \qquad (x,y) \in \partial\mathcal{D}, \ t \geq 0, \\ u(x,y,0) &= u_0(x,y), \qquad (x,y) \in \mathcal{D}. \end{aligned}$$

A spatial semi-discretization yields

$$v' = (A+B)v, \ t > 0; \ \ v(0) = v_0,$$

where $v \in \mathbb{R}^m$; $A, \ B \in \mathbb{R}^{m \times m}$, $AB \neq BA$.

Example 1

Let $\mathcal{D} = \{(x,y) : \ a < x < b, \ c < y < d\}$. We consider

$$
\begin{aligned}
u_t &= \alpha^2(x,y)u_{xx} + \beta^2(x,y)u_{yy}, \quad (x,y) \in \mathcal{D}, \ t > 0, \\
u(x,y,t) &= 0, \qquad (x,y) \in \partial\mathcal{D}, \ t \geq 0, \\
u(x,y,0) &= u_0(x,y), \qquad (x,y) \in \mathcal{D}.
\end{aligned}
$$

A spatial semi-discretization yields

$$v' = (A+B)v, \ t > 0; \ \ v(0) = v_0,$$

where $v \in \mathbb{R}^m$; $A, \ B \in \mathbb{R}^{m\times m}$, $AB \neq BA$.

OR, in operator splitting,

split the operators

$$v' = (\mathcal{A} + \mathcal{B})v, \ t > 0; \ \ v(0) = v_0,$$

where

$$\begin{aligned} \mathcal{A} &= \alpha^2(x,y)\frac{\partial^2}{\partial x^2}, \\ \mathcal{B} &= \beta^2(x,y)\frac{\partial^2}{\partial y^2}. \end{aligned}$$

To solve a 2-dimensional PDE is to solve two 1-dimensional PDEs!

Example 2

Let $\tilde{\mathcal{D}} = \{(\tilde{x}, \tilde{y}) : 0 < \tilde{x} < a, \ 0 < \tilde{y} < b\}$. We consider

$$\begin{aligned} u_t &= \nabla(a(\tilde{x}, \tilde{y})\nabla u) + f(u), \quad (\tilde{x}, \tilde{y}) \in \tilde{\mathcal{D}}, \ t > 0, \\ u(\tilde{x}, \tilde{y}, t) &= 0, \quad (\tilde{x}, \tilde{y}) \in \partial\tilde{\mathcal{D}}, \ t \geq 0, \\ u(\tilde{x}, \tilde{y}, 0) &= u_0(\tilde{x}, \tilde{y}), \quad (\tilde{x}, \tilde{y}) \in \tilde{\mathcal{D}}, \end{aligned}$$

where the ∇ is the two-dimensional gradient vector, coefficient a is bounded, positive and continuously differentiable over $\mathcal{D}$. The source function $f(u)$ has the following properties:

$$f(0) = f_0 > 0;$$

$$f(u) \text{ is strictly increasing for } 0 \leq u < 1;$$

$$\lim_{u \to 1^-} f(u) = \infty.$$

continue...

A semidiscrization leads to

$$
\begin{aligned}
(v_t)_{i,j} \quad = \quad & \frac{1}{b^2h^2}\left[a_{i-1/2,j}v_{i-1,j} + a_{i+1/2,j}v_{i+1,j} - (a_{i-1/2,j} + a_{i+1/2,j})v_{i,j}\right. \\
& \left. + a_{i,j-1/2}v_{i,j-1} + a_{i,j+1/2}v_{i,j+1} - (a_{i,j-1/2} + a_{i,j+1/2})v_{i,j}\right] \\
& + f(v_{i,j}), \quad 1 \le i,j \le N.
\end{aligned}
$$

The above is apparently a second order approximation of the IBVP at any mesh point (x_i, y_j), $1 \le i,j \le N$. Thus,

$$
\begin{aligned}
v' \quad &= \quad (P+Q)v + f(v), \quad t > 0, \\
v(0) \quad &= \quad u_0,
\end{aligned}
$$

Again, a formal solution

The formal solution of the IVP is

$$\begin{aligned} u(t) &= \exp\left\{\int_{t_0}^{t}(P+Q)d\tau\right\}u_0 + \int_{t_0}^{t}\exp\left\{\int_{\tau}^{t}(P+Q)d\xi\right\}f(u,\tau)d\tau \\ &= M(t_0,t)u_0 + \int_{t_0}^{t}M(\tau,t)f(u,\tau)d\tau. \end{aligned} \tag{10}$$

Apparently,

$$M(\tau,t) = M(t_0,t)M(\tau,t_0),\ \ t_0 \le \tau \le t.$$

So we can play the game of splitting again!

Example 3

We consider the Schrödinger equation

$$ih\frac{\partial\psi}{\partial t} = -\frac{h^2}{2\mu}\frac{\partial^2\psi}{\partial x^2} + U(\psi, x, t)\psi$$

together with suitable initial-boundary conditions. Apparently, the above can be written as

$$ih\frac{\partial\psi}{\partial t} = \mathcal{A}\psi + \mathcal{B}\psi.$$

This indicates another round of operator splitting!

The LOD solution

We denote

$$\mathcal{L}_1 = A, \ \mathcal{L}_2 = B.$$

Thus, instead of solving the original IVP, we consider the following:

$$\text{Subproblem 1:} \qquad w_2' = Bw_2, \quad w_2(0) = v_0; \tag{11}$$

$$\text{Subproblem 2:} \qquad w_1' = Aw_1, \quad w_1(0) = w_2. \tag{12}$$

We expect the convergence:

$$\|w_1 - v\| = \mathcal{O}(t^2), \quad t \to 0^+.$$

The above is also called a Local One-Dimensional (LOD) method.

The LOD solution

The solutions to (11) and (12) are

$$w_2 = e^{tB} v_0, \; w_1 = e^{tA} w_2, \quad t > 0,$$

respectively. To secure our convergence, we take a temporal step size $1 \gg \tau > 0$ such that for grids $\{t_0 = 0, \; t_1 = \tau, \; t_2 = 2\tau, \ldots, t_k = k\tau, \ldots\}$, we have

$$w_2(t_{k+1}) = e^{\tau B} w_2(t_k), \; w_1(t_{k+1}) = e^{\tau A} w_1(t_k), \quad k = 0, 1, 2, \ldots,$$

with $w_2(t_0) = v_0, \; w_1(t_0) = w_2(t_1)$.

But, how to evaluate matrix exponentials $e^{\tau B}, \; e^{\tau A}$?

Three most essential schemes

$$
\begin{aligned}
\text{Forward Euler:} \quad & e^{\tau M} \approx I + \tau M; \\
\text{Backward Euler:} \quad & e^{\tau M} \approx (I - \tau M)^{-1}; \\
\text{Crank-Nicolson:} \quad & e^{\tau M} \approx (I + \frac{\tau}{2} M)(I - \frac{\tau}{2} M)^{-1} \\
\text{[2/2] Padé:} \quad & e^{\tau M} \approx (I + \frac{\tau}{2} M + \frac{\tau^2}{12} M^2)(I - \frac{\tau}{2} M + \frac{\tau^2}{12} M^2)^{-1}.
\end{aligned}
$$

where $I, \ M \in \mathbb{R}^{m \times m}$.

Global error estimate:

Let $A, B \in \mathbb{C}^{m\times m}$. What is the error of splitting, say,

$$\varepsilon_1(t) = e^{t(A+B)} - e^{tA}e^{tB} \quad \text{for } t > 0?$$

Notice that $\varepsilon_1(0) = O$. Differentiate ε_1 :

$$\begin{aligned}
\varepsilon_1'(t) &= (A+B)e^{t(A+B)} - Ae^{tA}e^{tB} - e^{tA}Be^{tB} \\
&= (A+B)(e^{(A+B)} - e^{tA}e^{tB}) + (Be^{tA} - e^{tA}B)e^{tB} \\
&= (A+B)\varepsilon_1(t) + [B, e^{tA}]e^{tB}.
\end{aligned}$$

Global error estimate:

Recall the solution formula, we have

$$\varepsilon_1(t) = \int_0^t e^{(t-\tau)(A+B)}[B, e^{\tau A}]e^{\tau B} d\tau.$$

Let

$$S(\tau) = [B, e^{\tau A}], \quad \tau > 0, \quad S(0) = O.$$

A differentiation yields

$$\begin{aligned} S'(\tau) &= A[B, e^{\tau A}] + [B, A]e^{\tau A} \\ &= AS(\tau) + [B, A]e^{\tau A}. \end{aligned}$$

Global error estimate:

By the same token,

$$S(\tau) = \int_0^\tau e^{(\tau-\xi)A}[B, A]e^{\xi A} d\xi.$$

A substitution leads to

$$\varepsilon_1(t) = \int_0^t e^{(t-\tau)(A+B)} \int_0^\tau e^{(\tau-\xi)A}[B, A]e^{\xi A} e^{\tau B} d\xi d\tau.$$

Theorem 1.

$$\|\varepsilon_1(t)\|_2 \le \frac{t^2}{2!} \|[A, B]\|_2 \max\{e^{t\mu(A+B)}, e^{t(\mu(A)+\mu(B))}\},$$

where $\mu(M)$ is the logarithmic norm of M.

Strang's splitting:

For

$$\varepsilon_2(t) = e^{t(A+B)} - e^{\frac{t}{2}A}e^{tB}e^{\frac{t}{2}A}, \quad t \geq 0.$$

Theorem 2.

$$\begin{aligned} \|\varepsilon_2(t)\|_2 \quad \leq \quad & \frac{2t^3}{4!}\,\|A+2B\|_2\,\|[A,B]\|_2 \\ & \times \max\left\{e^{t\left(\frac{1}{2}\mu(A)+\mu(\frac{1}{2}A+B)\right)},\, e^{t\mu(A+B)}\right\} \\ & \times \max\left\{e^{\theta\left(\frac{1}{2}\mu(A)+\mu(B)\right)},\, e^{\theta\mu\left(\frac{1}{2}A+B\right)}\right\}, \quad 0 < \theta < t. \end{aligned}$$

Parallel splitting:

For

$$\varepsilon_3(t) = e^{t(A+B)} - \frac{1}{2}\left(e^{tA}e^{tB} + e^{tB}e^{tA}\right), \quad t \geq 0.$$

Theorem 3.

$$\|\varepsilon_3(t)\|_2 \leq \frac{t^3}{3!}\|A - B\|_2\|[A, B]\|_2 \max\left\{e^{t\mu(A+B)}, e^{t(\mu(A)+\mu(B))}\right\}.$$

A question:

Now, for

$$\varepsilon_4(t) = e^{tA}e^{tB} - e^{tB}e^{tA}, \quad t \geq 0.$$

Theorem 4.

$$\|\varepsilon_4(t)\|_2 \leq ??$$

Another one:

Now, for

$$\varepsilon_5(t) = e^{\frac{t}{2}A}e^{tB}e^{\frac{t}{2}A} - e^{\frac{t}{2}B}e^{tA}e^{\frac{t}{2}B}, \quad t \geq 0.$$

Theorem 5.

$$\|\varepsilon_5(t)\|_2 \leq ???$$

An application:

As we know,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \epsilon^2 \mathcal{L}_m u + \frac{\psi(\theta)}{1-u}, \quad x \in \mathcal{D}_m \subset \mathbb{R}^m,\ t > t_0, \\ u &= 0, \quad x \in \partial\mathcal{D}_m,\ t > 0, \\ u(x,t) &= \phi_0^2(x) \ll 1, \end{aligned}$$

is a typical m-dimensional stochastic Kawarada problem.

Theorem 6. *There is an effective operator splitting method such that the numerical solution of the stochastic Kawarada problem is structurely preservative.*

More questions:

How about splitting involving

- multiple operators?
- general linear operators?
- nonlinear operators?
- singular operators?
- symplecticity and Sobolev spaces?
- quantum and gravitational computing?
- AI/ML?

Some references

1. S. Blanes, F. Casas and A. Murua, Splitting methods with complex coefficients, Bol. Soc. Esp. Mat. Apl., 50 (2010), 47-60.
2. R. I. McLachlan and G. Reinout W. Quispel, Splitting methods, Acta Numerica, 11 (2002), 341-434.
3. Q. Sheng, Solving linear partial differential equations by exponential splitting, IMA J. Numer. Anal., 9 (1989), 199-212.
4. Q. Sheng, Global error estimate for exponential splitting, IMA J. Numer. Anal., 14 (1993), 27-56.
5. Q. Sheng, The ADI Method, Encyclopedia of Applied and Computational Mathematics, Springer Verlag GmbH, Heidelberg, 2015.

Appreciations!

Thank you all, and

have a very successful and productive 2020!