Operator Splitting Methods for Approximating Differential Equations

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Overview of Research

The primary focus of my research is the development of efficient and accurate numerical methods for approximating solutions to time-dependent differential equations.

This is a somewhat broad focus, so in particular, I consider the following types of problems.

1. **Singular Problems.**
2. **Nonlinear/Coupled Problems.**
3. **Stochastic Problems.**
4. **Nonlocal Problems.**

A useful approach to each of these problems: **Operator Splitting**

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Why Operator Splitting?

Do rigorous pure mathematics as much as possible. Determine qualitative features of your problem. And then, when exact analysis has reached its limit, resort to computation.

After spending an enormous amount of effort to determine precise qualitative information regarding the behavior of our problem, which often has deep physical significance, we produce numerical solutions that do not respect this qualitative information.

Invariants represent important qualitative information about the problem and it is often advantageous to respect these features when designing numerical methods.

A Nice Example

We can motivate the basic idea of operator splitting by considering the following model problem:

$$u' = Lu, \quad t > 0 \tag{2.1}$$

$$u(0) = u_0 \tag{2.2}$$

$\Longrightarrow$ A system of ordinary differential equations

$\Longrightarrow$ A semidiscretized form of the heat equation

$\Longrightarrow$ An operator problem in an appropriate Banach space

Regardless of the setting, the solution to (2.1)-(2.2) is given by

$$u(t) = \exp(tL)u_0 \tag{2.3}$$

Operator Splitting

If $L = \ell \in \mathbb{C}$, it follows that we can write $\ell = a + b$ and

$$u(t) = \exp(t\ell)u_0 = \exp(t(a+b))u_0 = \exp(ta)\exp(tb)u_0$$

This “splitting" is not guaranteed once L becomes more “complicated."

For general $L = A + B$, we have the following.

$\Longrightarrow$ **Lie-Trotter splitting:** $u(t) = \exp(tA)\exp(tB)u_0 + \mathcal{O}(t^2)$

$\Longrightarrow$ **Strang splitting:** $u(t) = \exp(tA/2)\exp(tB)\exp(tA/2)u_0 + \mathcal{O}(t^3)$

$\Longrightarrow$ **Parallel splitting:**

$$u(t) = \frac{1}{2}\left[\exp(tA)\exp(tB) + \exp(tB)\exp(tA)\right]u_0 + \mathcal{O}(t^3)$$

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Operator Splitting

How do we determine such error bounds?

$\Longrightarrow$ Taylor expansions, of course (in the finite-dimensional setting)

What about more general settings?

$\Longrightarrow$ Variation of parameter methods coupled with appropriate operator conditions

$\Longrightarrow$ The Baker-Campbell-Hausdorff formula (a bit complicated, but extraordinarily useful)

$$\begin{aligned} L &= \log(\exp(A)\exp(B)) \\ &= A + B + \frac{1}{2}[A, B] + \frac{1}{12}\left([A, [A, B]] + [B, [B, A]]\right) \\ &\quad - \frac{1}{24}[B, [A, [A, B]]] + \cdots \end{aligned}$$

Why Do We Like Operator Splitting Methods?

Why would we continue to consider such methods when there are new methods being developed every day?

- These methods allow us to employ methods available for simpler differential equations
- Global error analysis (Splitting methods tend to perform much better than their competitors)
- We are mimicking the structure of the true solution (matrix exponential, semigroup, resolvent family, etc.)
- Exponential splitting methods have nice properties (positive-preserving, monotone, stable, etc.)

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Oh, no! A Nonlinear Problem!

We now set our sights higher and consider the infinitely more interesting problem

$$u' = L(u)u, \quad t > 0 \tag{3.4}$$
$$u(0) = u_0 \tag{3.5}$$

Why is this problem more interesting?

$$u(t) = \exp\left(\int_0^t L(u(s))\,ds\right)u_0 \iff \left[\int_0^{t_1} L(u(s))\,ds, \int_0^{t_2} L(u(s))\,ds\right]$$

In general, this condition is highly unlikely to hold!

Magnus Expansion

Being the stubborn people that we are, we hope that there is a way to "force" an exponential-type solution (even if only locally).

$$\implies u(t) = \exp(\Omega(t,u))u_0, \quad t \in [0, T_*)$$

Surprisingly this works!

Magnus Expansion

Being the stubborn people that we are, the first attempts were to figure out a way to “force" an exponential-type solution (even if only locally).

$$\implies u(t) = \exp(\Omega(t,u))u_0, \quad t \in [0, T_*)$$

Surprisingly this works! In order for the above to hold true, it can be shown that $\Omega(t,u)$ must satisfy the following differential equation:

$$\Omega_t' = \mathrm{dexp}_\Omega^{-1}(L(u)), \quad \Omega_0 = O$$

where

$$\mathrm{dexp}_\Omega^{-1}(C) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_\Omega^k C,$$

$\{B_k\}_{k\in\mathbb{Z}_+}$ are the Bernoulli numbers, and ad_Ω^k is an iterated Lie bracket, that is,

$$\mathrm{ad}_\Omega^0 C = C, \quad \mathrm{ad}_\Omega^k C = [\Omega, \mathrm{ad}_\Omega^{k-1} C], \quad k \geq 1$$

Magnus Expansion

The Magnus differential equation that must be solved seems to be more complicated than the original problem!

$\Longrightarrow$ Why go through the effort of solving such problems?

Since we are only hoping to approximate the solution, then we only need to solve the Magnus differential equation up to some prescribed accuracy.

$\Longrightarrow$ This is actually a reasonable task!

$\Longrightarrow$ By Picard iteration we have

$$\Omega^{[0]}(t,u) = O, \quad \Omega^{[m+1]}(t,u) = \int_0^t \mathrm{dexp}^{-1}_{\Omega^{[m]}}\left(L(u(s))\right)\, ds,$$

with $\Omega(t,u) - \Omega^{[m]}(t,u) = \mathcal{O}(t^{m+1})$

Magnus Expansion

For instance it can be shown that

$$\exp(\Omega(t))u_0 - \exp(tL(u(t/2))/2)u_0 = \mathcal{O}(t^3)$$

$\Longrightarrow$ The drawbacks are computing matrix exponentials and dealing with iterated commutators for error analysis.

$\Longrightarrow$ Just as before, this method preserves structure! (What do we mean by “structure?")

$\Longrightarrow$ Splitting can now be applied in a similar manner!

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The Kawarada Problem

Consider the following quenching-combustion problem

$$\sigma(x)u_t = \Delta u + f(u), \quad (x,t) \in \Omega \times [0, T_q) \tag{4.6}$$
$$u = 0, \quad (x,t) \in \partial\Omega \times [0, T_q) \tag{4.7}$$
$$u = u_0, \quad (x,t) \in \Omega \times \{0\} \tag{4.8}$$

where f is a positive, monotonically increasing function such that

$$\lim_{u \to c^-} f(u) = +\infty \quad (\text{Think } f(u) = 1/(c-u)).$$

Solutions to (4.6)-(4.8) may only exist locally for certain domains Ω. Further, global and local solutions must be positive and monotonically increasing.

$\Longrightarrow$ In the case of local existence, $u_t \to \infty$ faster than the exponential!

The Kawarada Problem

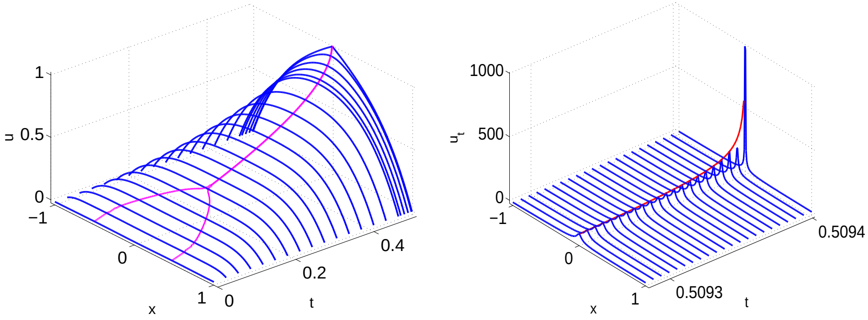

Figure: Three-dimensional curvature views of u, $0 \leq t \leq T^*$, [LEFT] and u_t, $T^0 \leq t \leq T^*$, [RIGHT] where $T^0 = 0.50928649$ and $T^* = 0.50939149$ are used. The magenta and red curves represent functions $\max_{-1 \leq x \leq 1} u$ and $\max_{-1 \leq x \leq 1} u_t$, respectively. The temporal derivative values concentrates about the quenching point with $\max_{-1 \leq x \leq 1} u_t(x, T^*) > 985 \gg 1$.

The Kawarada Problem

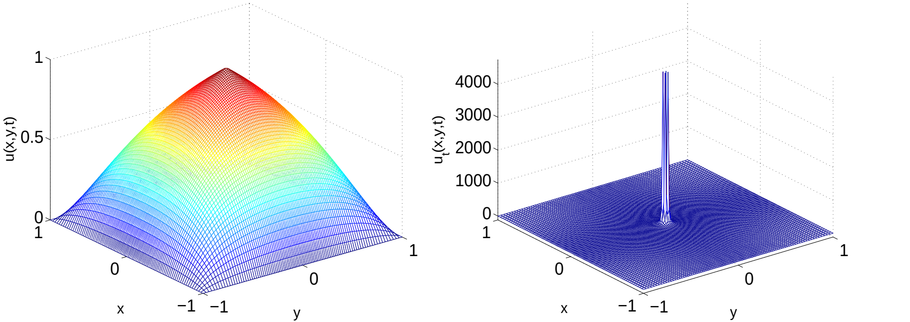

Figure: Solution u [LEFT] and its temporal derivative u_t [RIGHT] immediately prior to quenching.

The Kawarada Problem

We can use our previously discussed methods to solve this problem efficiently!

$\Longrightarrow$ Standard splitting methods (via variation of constants):

$$u(t) = S_t u_0 + \frac{t}{2}(S_t f(u_0) + f(u(t)))$$

where $S_t = \exp(tA/2)\exp(tB)\exp(tA/2)$.

$\Longrightarrow$ Magnus Expansion:

$$u(t) = T_t u_0$$

where $T_t = \exp(tf/2)\exp(tA/2)\exp(tB)\exp(tA/2)\exp(tf/2)$.

Both methods are stable and preserve positivity and monotonicity!

Predator-Prey Model

Consider the following generalized SKT predator-prey model:

$$u_t - \Delta \left(d_1 u + s_1 u^2 + c_{12} vu \right) = f(u, v) \quad (4.9)$$

$$v_t - \Delta \left(d_2 v + s_2 v^2 + c_{21} uv \right) = g(u, v) \quad (4.10)$$

defined on an appropriate domain with appropriate boundary conditions.

$\Longrightarrow$ How to handle the self-diffusion term, Δu^2?

$\Longrightarrow$ How to handle the nonlinear coupling?

Predator-Prey Model

Let's demonstrate a possibility with just (4.9):

$$\begin{aligned}
&\left(I - \frac{d_1\tau_k}{2}P\right)\left(I - \frac{d_1\tau_k}{2}R\right)\left(I - \frac{s_1\tau_k}{2}PD_{k+1}^{(u)}\right)\left(I - \frac{s_1\tau_k}{2}RD_{k+1}^{(u)}\right)\\
&\quad\times\left(I - \frac{c_{12}\tau_k}{2}PD_{k+1}^{(v)}\right)\left(I - \frac{c_{12}\tau_k}{2}RD_{k+1}^{(v)}\right)u_{k+1}\\
&= \left(I + \frac{d_1\tau_k}{2}P\right)\left(I + \frac{d_1\tau_k}{2}R\right)\left(I + \frac{s_1\tau_k}{2}PD_{k}^{(u)}\right)\left(I - \frac{s_1\tau_k}{2}RD_{k}^{(u)}\right)\\
&\quad\times\left(I + \frac{c_{12}\tau_k}{2}PD_{k}^{(v)}\right)\left(I + \frac{c_{12}\tau_k}{2}RD_{k}^{(v)}\right)u_k + \frac{\tau_k}{2}(f_{k+1} + f_k),
\end{aligned}$$

Predator-Prey Model

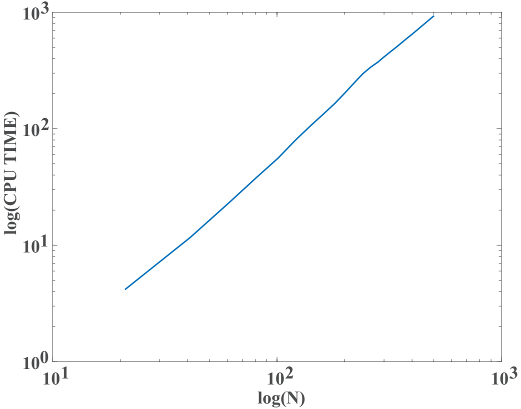

Figure: A log-log plot of the computational time, in seconds, versus N after 1000 iterations. The temporal step is held constant, $\tau = 10^{-6}$, while $h = 1/(N-1)$. A linear least squares approximates the slope of the line to be 1.75681. This indicates that the computational time is proportional to $N^{1.75681}$. Since this is slower than N^2, then the proposed nonlinear splitting scheme is highly efficient.

Semilinear Stochastic Problem

Consider the following stochastic differential equation

$$X_t = [A + f(X_t)]\, X_t\, dt + g(X_t) dW_t, \quad t > 0 \tag{4.11}$$
$$X_0 = \xi_0 \tag{4.12}$$

where $\{W_t\}_{t \geq 0}$ is a standard Brownian motion on an appropriate probability space.

$\Longrightarrow$ These problems are of great interest!

$\Longrightarrow$ In general, numerical algorithms for (4.11)-(4.12) are limited (low convergence rates, high computational cost, etc.)

Semilinear Stochastic Problem

Typically to improve convergence rates for approximations to (4.11)-(4.12), we must keep higher-order derivatives.

By using Magnus expansion methods, we can derive schemes of higher-order, by only using the simplest approximations!

⟹ Let $B = f(X_0)$ and $C = \Delta W_t g(X_0)$.

⟹ In general, C is only a 1/2-order approximation of $\int g(X_t)\, dW_t$!

⟹ By using the approximation

$$X_t = S_t X_0$$

where $S_t = \exp(C/2)\exp(t(A+B))\exp(C/2)$, we increase the accuracy to first-order!

Fractional Cauchy Problem

Consider the following fractional Cauchy problem:

$$ {}_0^C D_t^\alpha u = (A+B)u, \quad t > 0 \tag{4.13} $$

$$ u(0) = u_0 \tag{4.14} $$

$\Longrightarrow$ $${}_0^C D_t^\alpha u(t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s)\, ds, \quad 0 < \alpha < 1$$

$\Longrightarrow$ The solution to (4.13)-(4.14) is given by $u(t) = E_{\alpha,1}(t^\alpha(A+B))u_0$, where

$$ E_{\alpha,\beta}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta + \alpha k)}. $$

Fractional Cauchy Problem

The approximation of solutions to (4.13)-(4.14) are complicated by the nonlocal features of the problem!

$\Longrightarrow$ In particular, standard splitting procedures do not apply (well).

$\Longrightarrow$ The convergence rates are of the form $\mathcal{O}(t^{m\alpha})$ (degenerates as $\alpha \to 0^+$)

We are able to bypass these issues by considering

$$
{}^{C}_{t_n}D^{\alpha}_{t} u = (A + B)u - \underbrace{\frac{1}{\Gamma(1-\alpha)} \int_0^{t_n} (t_{n+1} - s)^{-\alpha} u'(s)\, ds}_{:= Lu(t_n)}, \quad t_n < t < t_{n+1}
$$

$\Longrightarrow$ This can yield “non-degenerate" convergence rates!

Fractional Cauchy Problem

The previous reformulation yields a solution of the form

$$u(t) = E_{\alpha,1}(h^\alpha(A+B))u_n - \int_{t_n}^{t_{n+1}} \boldsymbol{e}_\alpha(s) Lu(s)\, ds, \tag{4.15}$$

where

$$\boldsymbol{e}_\alpha(s) := (t_{n+1}-s)^{\alpha-1} E_{\alpha,\alpha}((t_{n+1}-s)^\alpha(A+B)).$$

From (4.15), it can be shown that the solution to (4.13)-(4.14) is given by

$$u(t) = E_{\alpha,1}(h^\alpha A)E_{\alpha,1}(h^\alpha B)u_n - Lu(t_n) + \mathcal{O}(h).$$

$\Longrightarrow$ I am currently working on further improving these results via a Strang-type splitting approximation.

THANK YOU!

Questions?