Exponential Time Differencing for Nonlinear Advection-Diffusion-Systems

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Design of Lecture

- Overview with simple finite difference example & touch on various application problems
- Brief motivation for the Exponential Time Differencing schemes
- Overview of derivation of ETD schemes
- Mention of advantage of ETD schemes, various splittings for speed-up
- Empirical examples of splitting compared to standard schemes
Introductory Example: Allen-Cahn Eq. (physics)

\[ \frac{\partial u}{\partial t} = \epsilon \frac{\partial u^2}{\partial x^2} + u - u^3, \quad x \in [-1, 1] \]

\[ u(x, 0) = 0.53x + 0.47 \sin(-1.5\pi x), \quad t > 0 \]

\[ u(-1, t) = -1, \quad u(1, t) = 1. \]

A standard test of second order accuracy of new algorithm ‘ETD-RDP.’ Second order rate means error is \( O(h^2 + k^2) \).

\( h = \Delta x \) & \( k = \Delta t \).

<table>
<thead>
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</table>
Standard Example

\[ u_t = \Delta u \]

Centered finite differences for Laplace operator

\[
\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad \Omega = [0, 1] \times [0, 1]
\]

\[
\{x_i, y_j\}_{i,j=1}^{M,N}, \quad \Delta x = 1/(M + 1), \quad \Delta y = 1/(N + 1)
\]

\[ u_{i,j} = \text{approximation for exact } u(x_i, y_j) \]

\[
\Delta u_{i,j} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2}
\]
Standard Baseline Example

\[ \Delta x = \Delta y = h \]

\[ \Delta u_{i,j} \approx \frac{u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1} - 4u_{i,j}}{h^2} \]
Finite Difference Method- matrix form (0 bound. conditions)
Lexicographic ordering of unknowns, partitioned matrix

\[ A = -\frac{1}{h^2} \begin{bmatrix} T & I & \cdots & \cdots \\ I & T & I & \cdots \\ \vdots & \vdots & \ddots & \ddots \\ \vdots & \vdots & \ddots & T & I \\ \cdots & \cdots & \cdots & I & T \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ \vdots \\ u_{N,N} \end{bmatrix} \]

\( T = \text{tridiag}(1, -4, 1) \text{ of size } N \times N \) (also \( I \))

Matrix is order \( N^2 \times N^2 \), very large and sparse
Matrix depends on \( N \) \ldots infinite family, unbounded dimensions
A represents the underlying steady-state elliptic operator; we still have to compute forward in time. Thus, we have an enormous challenge in computational complexity, made much worse by nonlinearities and irregular data.
Standard Crank-Nicolson, time variable is involved

\[ u_{i,j}^\ell = u(x_i, y_j, t^\ell) \quad \text{where } t^\ell = \ell \Delta t = \ell k \]

\[
\frac{u_{i,j}^{\ell+1} - u_{i,j}^\ell}{k} = \frac{1}{2} \left( u_{i+1,j}^\ell + u_{i,j+1}^\ell + u_{i-1,j}^\ell + u_{i,j-1}^\ell - 4u_{i,j}^\ell \right) + \frac{1}{2} h^2 \left( u_{i+1,j}^{\ell+1} + u_{i,j+1}^{\ell+1} + u_{i-1,j}^{\ell+1} + u_{i,j-1}^{\ell+1} - 4u_{i,j}^{\ell+1} \right)
\]

Vector form, in method of lines, time-stepping with \( \ell \)

\[
\frac{u^{\ell+1} - u^\ell}{k} + \frac{1}{2} Au^\ell + \frac{1}{2} Au^{\ell+1} = 0
\]
Crank-Nicolson in Operator Form

\[(I + \frac{1}{2}kA)u^{\ell+1} = (I - \frac{1}{2}kA)u^{\ell}\]

OR

\[u^{\ell+1} = (I + \frac{1}{2}kA)^{-1}(I - \frac{1}{2}kA)u^{\ell}\]

Issues with accuracy due to steep gradients

Figure 1: Evolution of Allen-Cahn
Example Derivation of Nonlinear PDE... Chemotaxis

rate of change of cell density \( n \) = diffusion of cells + chemotaxis of cells to aspartate + growth and death of cells

rate of change of aspartate concentration \( c \) = diffusion of aspartate + production of aspartate by cells - uptake of aspartate by cells

rate of change of succinate concentration \( s \) = diffusion of succinate - uptake of succinate by cells
Chemotaxis: Nonlinear Reaction-Diffusion System

\[
\begin{align*}
\frac{\partial n}{\partial t} &= D_n \nabla^2 n - \alpha \nabla \left[ \frac{n}{(1 + c)^2} \nabla c \right] + \rho n \left( \delta \frac{s^2}{1 + s^2} - n \right) \\
\frac{\partial c}{\partial t} &= D_c \nabla^2 c + \beta s \frac{n^2}{\gamma + n^2} - nc \\
\frac{\partial s}{\partial t} &= D_s \nabla^2 s - \kappa n \frac{s^2}{1 + s^2}
\end{align*}
\]

where $\nabla^2$ denotes the Laplacian in two dimensions, $\alpha, \beta, \gamma, \delta, \rho$ and $\kappa$ are experimentally determined parameters.
Rogue Wave Model (NLS Eq.): Islas & Schober use our Fourth-order ETD Scheme

A. Islas and C. M. Schober: Rogue waves and downshifting

\[ iu_t + u_{xx} + 2|u|^2u + i\Gamma u \]

\[ + i\epsilon \left( \frac{1}{2}u_{xxx} - 8|u|^2u_x - 2ui(1 + i\beta)\left[ H\left(|u|^2\right)\right]_x \right) = 0, \quad (1) \]

where \( H(f) \) represents the Hilbert transform of \( f \). Throughout this paper “HONLS equation” refers to (1) with \( \Gamma = 0 \) and \( \beta = 0 \). The Hamiltonian for the HONLS equation is given by

\[ H = \int_0^L \left\{ -i|u_x|^2 + i|u|^4 - \frac{\epsilon}{4} (u_x u_{xx} - u_x^* u_{xx}) \right\} \]

\[ + 2\epsilon|u|^2 (u^* u_x - uu_x^*) + i\epsilon|u|^2 \left[ H\left(|u|^2\right)\right]_x \] \quad dx. \quad (2)
Rogue Wave Model (NLS Eq.):

\[ a = 0.5, \quad L = 4\sqrt{2\pi}, \quad \mu_3 = 2\mu_1 \]
Nonlinear Schrödinger Equation Empirical Test

\[ u_t = i \Delta u + 2i |u|^2 u \]

- A. L. Islas, C. M. Schober, M. D. Hederi, K. S. Reger, Univ. of Central Florida
- They test ETDRK4 against a split-step Fourier method of order 4 (SSFM4: Tappert)
- They conclude that ETDRK4 is 5 – 10 times faster
\[ iu_t + u_{xx} + 2|u|^2u + i\Gamma u + \]
\[ i\varepsilon \left( \frac{1}{2} u_{xxx} - 8|u|^2u_x - 2iu(1 + i\beta)H(|u|^2)|_x \right) = 0. \]

- \( H \) is the Hilbert transform, useful to map real signals into an analytic function for Cauchy-Riemann equations
- Investigation uses our ETDRK4 fourth order scheme
Electrochemical Kinetics, Nonlinear Reaction

\[
\begin{align*}
\frac{\partial c_M}{\partial t} &= \frac{\partial^2 c_M}{\partial x^2} - \kappa_p c_M c_{P_2} - \kappa_p c_M c_{P_1}, \\
\frac{\partial c_{MR}}{\partial t} &= \frac{\partial^2 c_{MR}}{\partial x^2} - 2\left(\frac{\kappa_p}{\xi}\right)c_{MR}^2, \\
\frac{\partial c_{P_0}}{\partial t} &= \frac{\partial^2 c_{P_0}}{\partial x^2} + \left(\frac{\kappa_p}{\gamma}\right)c_{P_1}, \\
\frac{\partial c_{P_1}}{\partial t} &= \frac{\partial^2 c_{P_1}}{\partial x^2} + \kappa_p c_M c_{P_1} - \left(\frac{\kappa_p}{\gamma}\right)c_{P_1} + \left(\frac{\kappa_p}{\gamma}\right)c_{P_2}, \\
\frac{\partial c_{P_2}}{\partial t} &= \frac{\partial^2 c_{P_2}}{\partial x^2} + \left(\frac{\kappa_p}{\xi}\right)c_{MR}^2 + \kappa_p c_M c_{P_2} - \left(\frac{\kappa_p}{\gamma}\right)c_{P_2},
\end{align*}
\]
Nonlinear Transaction Cost Model

\[ V_\tau + \frac{1}{2} \sigma^2 S^2 V_{SS} + \rho S V_S - \rho V = \epsilon S^2 |V_{SS}| \]

\[ \epsilon = \kappa \sigma \sqrt{\frac{2}{\pi \delta \tau}} \]

\( S \) is the price of the underlying asset, \( \rho \) the risk-free interest rate, \( \sigma \) the asset volatility, \( \kappa \) a proportionality constant, and \( V(S, \tau) \) the price of the option written on \( S \)
Typical PDE System of Semilinear Parabolic Type, Advection, Diffusion and Reaction terms.

\[ \frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = D \Delta u + f(t, u) \]

\[ u = \text{vector of reactants (or species, temperature ...)} \]
\[ D = \text{Matrix of Diffusivities, Multi-Scale} \]
\[ \mathbf{v} = \text{drift velocity (} \mathbf{v} \cdot \nabla u = \text{convection flux}) \]
\[ f = \text{nonlinear reaction kinetics} \]
Spatial Mesh, 2-Dimensional Example

$h$ is spatial mesh-size & $k$ is time-step in Method of Lines
May be finite element, finite volume, finite difference, pseudo-spectral methods in space
Convergence Theorem—Simplified

- Nonlinear parabolic initial-boundary value problem:

\[ u_t + Au = f(t, u) \quad \text{for} \quad t \in (0, T), \]
\[ u(\cdot, 0) = u_0 \]

A Convergence Theorem:

\[ \| e_n \| \leq Ck^2 \left( (\log n)(\| A^2 u_0 \| + \| Au_0 \|) + \int_0^{t_n} \| f^{(1)}(\tau) \| d\tau + \int_0^{t_n} \| f^{(2)}(\tau) \| d\tau \right) \]

as \( k \to 0 \) and \( n \to \infty \) with \( nk \leq T \).
Derivation of ETD Using Variation of Constants

\[ E(t) = e^{-tA} \]

Calculate exact one-step time dynamics:

\[ u(t) = E(t)u_0 + \int_{t_0}^{t} E(t - s) f(s, u(s)) \, ds \]

\[ 0 < k \leq k_0, \, t_n = nk, \, 0 \leq n \leq N \]

Basis for ETD. Restrict \( t-t_0 \) to one step, change variables:

\[ u(t_{n+1}) = e^{-kA}u(t_n) + k \int_{0}^{1} e^{-kA(1-\tau)}f(t_n + \tau k, u(t_n + \tau k)) \, d\tau \]
Rational Approximations of $e^{-kA}$

$A$ is a matrix from discretization in the spatial variable

$\quad e^{-z}$ approximated by rational function of $z$ near $0$, $z \geq 0$.
$\quad z$ replaced by $kA$. Examples:

$\quad (0,1)$ - Padé Approximation, Backward Euler:

$$R_{0,1}(-z) = (I + z)^{-1}$$

$\quad (1,1)$ - Padé Scheme (‘Crank-Nicolson Method’):

$$R_{1,1}(-z) = (I + \frac{1}{2}z)^{-1}(I - \frac{1}{2}z)$$
Real-distinct poles (RDP) scheme:

\[ r(-z) = \left( I - \frac{5}{12}z \right) \left( I + \frac{1}{4}z \right)^{-1} \left( I + \frac{1}{3}z \right)^{-1} \]

\[ = 9(I + \frac{1}{3}z)^{-1} - 8(I + \frac{1}{4}z)^{-1} \]

Novel rational approximation. With extra degree of freedom, it is used to design-in L-stability.

Note: Importance of partial fractions decomposition.
Stability Properties

- $R(z)$ is said to be **A-acceptable** if $|R(z)| < 1$ whenever $\Re(z) > 0$; and **L-acceptable** if, in addition, $|R(z)| \rightarrow 0$ as $\Re(z) \rightarrow \infty$.

- RDP (violet) is L-acceptable, CN (green) is **not** L-acceptable.

![Figure 2](image-url)
Semidiscrete ETD, RDP version

Compute integral exactly ($e^{-kA}$ is a matrix exponential):

$$u(t_{n+1}) \approx e^{-Ak}u(t_n) + A^{-1}(I - e^{-Ak})f(t_n, u(t_n))$$

$$+ k^{-1}A^{-2}(e^{-kA} - I + kA)(f(t_n, u(t_{n+1})) - f(t_n, u(t_n)))$$

Replace $e^{-kA} \approx \left(I - \frac{5}{12}kA\right)\left(I + \frac{1}{4}kA\right)^{-1}\left(I + \frac{1}{3}kA\right)^{-1}$
\[ u_{n+1} = \left( I - \frac{5}{12} Ak \right) \left( I + \frac{1}{4} Ak \right)^{-1} \left( I + \frac{1}{3} Ak \right)^{-1} u_n \]

\[ + \frac{k}{2} \left( I + \frac{Ak}{4} \right)^{-1} \left( I + \frac{Ak}{3} \right)^{-1} f(t_n, u_n) \]

\[ + \frac{k}{2} \left( I + \frac{1}{6} kA \right) \left( I + \frac{1}{4} kA \right)^{-1} \left( I + \frac{1}{3} kA \right)^{-1} f(t_{n+1}, u_{n+1}). \]
Partial Fraction Forms

\[
\left( I - \frac{5}{12}Ak \right) \left( I + \frac{1}{4}Ak \right)^{-1} \left( I + \frac{1}{3}Ak \right)^{-1} = 9 \left( I + \frac{1}{3}Ak \right)^{-1} - 8 \left( I + \frac{1}{4}Ak \right)^{-1}
\]

\[
\left( I + \frac{Ak}{4} \right)^{-1} \left( I + \frac{Ak}{3} \right)^{-1} = 4 \left( I + \frac{1}{3}Ak \right)^{-1} - 3 \left( I + \frac{1}{4}Ak \right)^{-1}
\]

\[
\left( I + \frac{Ak}{6} \right) \left( I + \frac{Ak}{4} \right)^{-1} \left( I + \frac{Ak}{3} \right)^{-1} = 2 \left( I + \frac{1}{3}Ak \right)^{-1} - \left( I + \frac{1}{4}Ak \right)^{-1}
\]
Final Scheme

\[ u^* = (I + Ak)^{-1}[u_n + kf(u_n)], \quad \text{(Estimator for } u_{n+1}) \]

\[ u_{n+1} = \left( I + \frac{1}{3}Ak \right)^{-1} [9u_n + 2kf(u_n) + kf(u^*)] \]
\[ + \left( I + \frac{1}{4}Ak \right)^{-1} [-8u_n - \frac{3k}{2}f(u_n) - \frac{k}{2}f(u^*)]. \]

Each \((-)^{-1}\) is solved efficiently at the point of implemention. These will be sparse matrices, tri- or pentadiagonal.
Implementation of ETD-RDP, stages could be parallelized

1. Solve for $u^*$

\[(I + Ak)u^* = u_n + kf(u_n)\]

2. Solve for $u_{n+1}$

\[
\left(I + \frac{1}{3}Ak\right)v_a = 9u_n + 2kf(u_n) + kf(u^*)
\]

\[
\left(I + \frac{1}{4}Ak\right)v_b = -8u_n - \frac{3}{2}kf(u_n) - \frac{k}{2}f(u^*)
\]

$$u_{n+1} = v_a + v_b$$
After similar calculations...

ETD-CN

\[
\begin{align*}
  \nu_{n+1} &= u^* + \frac{1}{2} kR_{0,1} \left( \frac{1}{2} kA \right) \left[ f(t_{n+1}, u^*) - f(t_n, \nu_n) \right], \\
  u^* &= R_{1,1}(kA) \nu_n + kR_{0,1} \left( \frac{1}{2} kA \right) f(t_n, \nu_n) \\
  R_{0,1}(-z) &= (1 + z)^{-1}
\end{align*}
\]

Implementation

\[
\begin{align*}
  (2I + kA) N_b &= 4 \nu_n + 2k f(t_n, \nu_n) \\
  b_n &= -\nu_n + N_b \\
  (2I + kA) N_v &= k \left[ f(t_{n+1}, b_n) - f(t_n, \nu_n) \right] \\
  \nu_{n+1} &= b_n + N_v.
\end{align*}
\]
Reaction-Diffusion System Example

One spatial variable describes a chemical reaction with two components:

\[
\frac{\partial u}{\partial t} = A + u^2 v - (B + 1)u + \alpha \frac{\partial^2 u}{\partial x^2}
\]

\[
\frac{\partial v}{\partial t} = Bu - u^2 v + \alpha \frac{\partial^2 v}{\partial x^2}
\]

with \(0 \leq x \leq 1\), \(A = 1\), \(B = 3\), \(\alpha = 1/50\), bound. cond.

\[
\begin{align*}
  u(0, t) &= u(1, t) = 1 \\
  v(0, t) &= v(1, t) = 3
\end{align*}
\]

and initial conditions

\[
\begin{align*}
  u(x, 0) &= 1 + \sin(2\pi x) \\
  v(x, 0) &= 3.
\end{align*}
\]
<table>
<thead>
<tr>
<th>$k = h$</th>
<th>Error ETD-CN</th>
<th>CPU</th>
<th>Error CN</th>
<th>CPU</th>
<th>Error BDF-2</th>
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<td>22.078</td>
<td>$6.34 \times 10^{-5}$</td>
<td>22.437</td>
</tr>
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</table>

Table 1: Numerical errors ($l_2$) and CPU-time (sec) using ETD-CN, regular Crank-Nicolson, and the second order Backward Differentiation Formula (BDF2).
Splitting ETD Schemes

Abstract Cauchy problem

\[ \frac{dU}{dt} + \mathcal{A}(U) = 0, \quad U(0) = U_0 \]

Write \( \mathcal{A} \) as a sum of more elementary operators, say

\[ \mathcal{A} = \mathcal{A}_l + \cdots + \mathcal{A}_1. \]

Decomposition is natural, e.g., \( \mathcal{A}_j \) represents differentiation in a spatial direction, or could model a composition of phenomena like convection, reaction, or diffusion.

Choose a decomposition so that \( \mathcal{A}_j \) give simpler equations,

\[ \frac{dU_j}{dt} + \mathcal{A}_j(U_j) = 0, \quad U^1(0) = U_0 \quad j = 1 \cdots l. \]

With \( U_j(t) = S^j_t U_{j-1} \) the fundamental solution split equation, solve sub-equations sequentially:
\[ U(n\Delta t) \approx [S_{\Delta t}^l \cdots S_{\Delta t}^1]^n U_0. \]

\[ U(t) = \lim_{\Delta t \to 0, n \to \infty, t = n\Delta t} [S_{\Delta t}^l \cdots S_{\Delta t}^1]^n U_0. \]
Novel Integrating Factor Splitting for ETD

\[ u_t + Au = F(u), \quad u(0) = u_0 \]

Change of variable

\[ v = e^{Bt} u. \]

Differentiate

\[ v_t = e^{Bt} u_t + Be^{Bt} u. \]

\[ v_t = e^{Bt} F(u) - e^{Bt} Au + Be^{Bt} u \]

assuming \( A \) and \( B \) commute

\[ v_t + (A - B)e^{Bt} u = e^{Bt} F(u) \]

\[ v_t + (A - B)v = e^{Bt} F(e^{-Bt} v) \]
Find a special $B$ to enhance convergence speed \ldots Working in a two dimensional domain, use dimensional splitting

$$A = A_1 + A_2$$

where $A_1$ and $A_2$ give the action of the discrete Laplace operator in the $x$ and $y$ direction. Choose $B = A_1$:

$$v_t + A_2 v = e^{A_1 t} F(e^{-A_1 t} v).$$

Set $e^{A_1 t} F(e^{-A_1 t} v) = \tilde{F}(v)$

We arrive at:

$$v(t_{n+1}) = e^{-kA_2} v(t_n) + e^{-kA_2} \int_0^k e^{A_2 \tau} \tilde{F}(v(t_n + \tau)) d\tau$$
Figure 3: Solution of 2D enzyme kinetics (irregular data top right, Crank-Nicolson). Log-log efficiency and convergence plots.
Numerical Tests of Split Scheme Performance

Evaluate convergence & efficiency for two-dimensional problem:

\[
\frac{\partial u}{\partial t} = d \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{u}{(1 + u)} \quad 0 < x, y < 1, t > 0
\]

with homogeneous Dirichlet boundary conditions and initial condition

\[
u(x, y, 0) = 1 \quad 0 \leq x, y \leq 1.\]
Figure 4: Efficiency plots for Dimensional Splitting on Enzyme Kinetics Equation with nonsmooth data.
Generalized Nonlinear Schrödinger Equation

\[ iu_t + u_{xx} + f(|u|^2)u = 0 \]

Use ETD-CN with two spatial discretizations: central differences and quartic splines.

A splitting method (Linear-Nonlinear parts split):

\[ u_t = (\mathcal{L} + \mathcal{N})u \]

where

\[ \mathcal{L}u = i \cdot u_{xx} \]
\[ \mathcal{N}u = i \cdot f(|u|^2)u \]

- Linear operator \( \mathcal{L} \) provides a governing law for the propagation of dispersive waves.
- Non-linear term \( \mathcal{N} \) helps dismiss dispersion of waves.
Energy Conservation of the Solitons

Comparison of total energy of $u_1$ and $u_2$ calculated by ETD-CN ($h = 0.05$ and $k = 0.01$) w/ the exact energy. We calculate to $T = 40$ for a long time period.

<table>
<thead>
<tr>
<th>Time</th>
<th>$|u_1|_2$</th>
<th>Exact energy of $u_1$</th>
<th>$|u_2|_2$</th>
<th>Exact energy of $u_2$</th>
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<td>1.302711</td>
</tr>
</tbody>
</table>

The greatest difference with exact energy occurs at time 40, which is 0.000037.
Open Challenges

1. Develop theory & best practice for 2D & 3D problems using GMRES or other Krylov subspace method
2. Develop parallel versions, theory and practice
3. Resolve the very challenging issues with advection and diffusion together
4. Resolve the multi-scale challenges of widely varying diffusion rates
5. Further study issues with discontinuities in the forcing term
6. Develop theory & best practice for meshless methods (in space) with ETD schemes
7. Experiment with domain decomposition in spatial domain, coupled with ETD
8. Develop further into fractional PDE and nonlocal boundary conditions & nonlocal operators
9. Sharper proofs using semi-group theory