Fast solution of stiff PDEs in 1D, 2D and 3D

Industrial and Applied Mathematics Seminar, University of Nottingham

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Stiff PDEs in 1D, 2D and 3D

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with initial condition $u(0,X)$

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  Higher-order terms of the equation are linear: exponential integrators (Section 3)

Trigonometric interpolation (1/3)

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- A periodic (or rapidly decaying) function $u(x)$ on $[0, 2\pi]$ is represented by its trigonometric interpolant on a grid of N points $x_j = 2\pi j/N$, $0 \leq j \leq N-1$,

$$u(x) \approx u_N(x) = {\sum_{k=-N/2}^{N/2}}' u_k e^{ikx}, \quad u_k = \frac{1}{N}\sum_{j=0}^{N-1} u(x_j)e^{-ikx_j} = \texttt{fft}(u(x_j))$$

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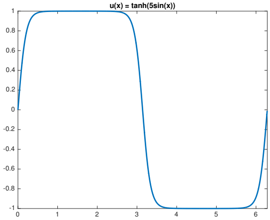
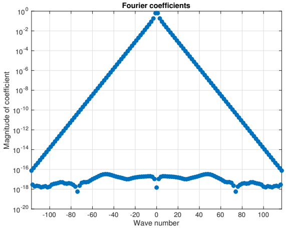
- Example: $u(x) = \tanh(5\sin(x))$, $N = 235$

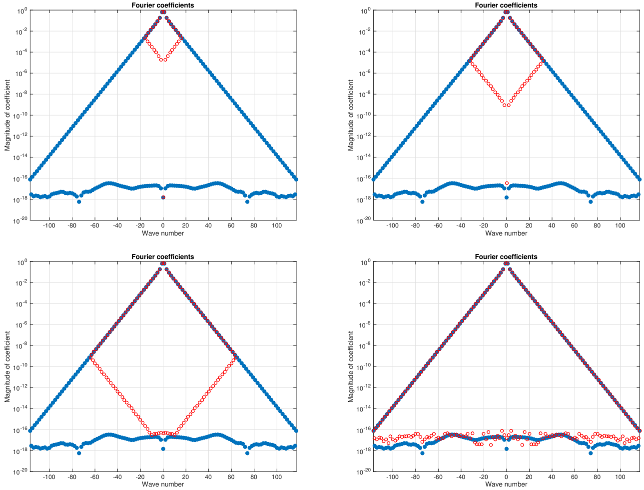
```
u = chebfun(@(x) tanh(5*sin(x)),[0 2*pi],'trig');
```





Trigonometric interpolation (2/3)

- Constructor: evaluates the function on grids of sizes 17, 33, 65, 129, 257, . . ., takes the `fft` and looks at the amplitude of the Fourier coefficients



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- Example in 2D: $u(x, y) = \exp(-5((x-\pi)^2 + (y-\pi)^2))$

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u = chebfun2(@(x,y)exp(-5*((x-pi).^2+(y-pi).^2)),[0 2*pi 0 2*pi],'trig');
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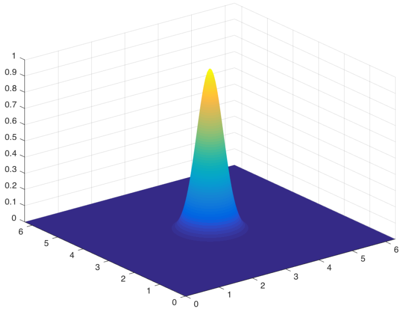

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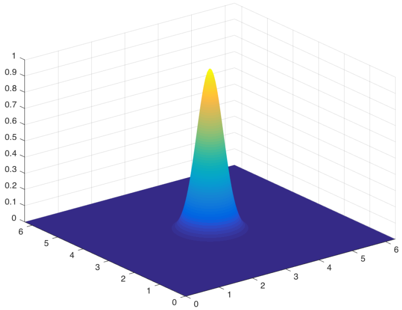

- In 3D, one can type, e.g.,

```
dom = [0 2*pi 0 2*pi 0 2*pi];
u = chebfun3(@(x,y,z)exp(-5*((x-pi).^2+(y-pi).^2+(z-pi).^2)),dom,'trig');
```

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- For discretizing

$$u_t(t,X) = \mathcal{L}u + \mathcal{N}(u), \quad u(0,X) = u_0(X),$$

we use a Fourier spectral method in coefficient space, i.e., we look for a solution of the form (with $N = N_x N_y N_z$ points)

$$u(t,X) \approx \sum_{k_x=-\frac{N_x}{2}}^{\frac{N_x}{2}}{}' \sum_{k_y=-\frac{N_y}{2}}^{\frac{N_y}{2}}{}' \sum_{k_z=-\frac{N_z}{2}}^{\frac{N_z}{2}}{}' u_{k_x k_y k_z}(t) e^{i(k_x x + k_y y + k_z z)}$$

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- The linear part $\mathcal{L}$ is discretized with Fourier differentiation matrices $\Rightarrow$ matrix $\mathbf{L}$
- This leads to a system of N ODEs for the coefficients $u(t) = \{u_{k_x k_y k_z}(t)\}$,

$$u'(t) = \mathbf{L}u + \mathbf{N}(u), \quad u(0) = u_0$$

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- First three Fourier differentiation matrices (even N):

$$D = \begin{pmatrix} 0 \\ (-\frac{N}{2}+1)i \\ \vdots \\ -2i \\ -i \\ 0 \\ i \\ 2i \\ \vdots \\ (\frac{N}{2}-1)i \end{pmatrix}, \quad D^{(2)} = \begin{pmatrix} -\frac{N^2}{4} \\ \vdots \\ -4 \\ -1 \\ 0 \\ -1 \\ -4 \\ \vdots \\ -(\frac{N}{2}-1)^2 \end{pmatrix}, \quad D^{(3)} = \begin{pmatrix} 0 \\ -(-\frac{N}{2}+1)^3 i \\ \vdots \\ 8i \\ i \\ 0 \\ -i \\ -8i \\ \vdots \\ -(\frac{N}{2}-1)^3 i \end{pmatrix}$$

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- 3D: $\mathcal{L}u = u_{xx} + u_{yy} + u_{zz} \Rightarrow \mathbf{L} = I \otimes I \otimes D^{(2)} + I \otimes D^{(2)} \otimes I + D^{(2)} \otimes I \otimes I$

Exponential integrators (1/10)

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- **Method:** Time-stepping with exponential integrators, e.g.,

$$u_{n+1} = e^{h\mathbf{L}}u_n + h\varphi_1(h\mathbf{L})\mathbf{N}(u_n), \quad h = t_{n+1} - t_n, \quad \varphi_1(z) = \frac{e^z - 1}{z}$$

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- **How to derive this scheme?** Consider the linearized version of the system of ODEs on $[t_n, t_{n+1}]$,

$$u'(t) = \mathbf{S}(u_n) + (u - u_n)\mathbf{S}_u(u_n), \quad u(t_n) = u_n$$

with exact solution at t_{n+1}

$$u_{n+1} = u_n + h\varphi_1(h\mathbf{S}_u(u_n))\mathbf{S}(u_n),$$

and approximate $\mathbf{S}_u(u_n)$ by $\mathbf{L}$

Exponential integrators (2/10)

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For given starting values $u_0, u_1, \ldots, u_{q-1}$ at times $t = 0, h, \ldots, (q-1)h$, the numerical approximation u_{n+1} at time $t_{n+1} = (n+1)h$, $n+1 \geq q$, is given by

$$u_{n+1} = e^{hL}u_n + h\sum_{i=1}^{s} B_i(hL)\mathbf{N}(v_i) + h\sum_{i=1}^{q-1} V_i(hL)\mathbf{N}(u_{n-i}),$$

with *steps* u_{n-i} and *stages* $v_1 = u_n$ and, for $2 \leq i \leq s$,

$$v_i = e^{C_i hL}u_n + h\sum_{j=1}^{i-1} A_{i,j}(hL)\mathbf{N}(v_j) + h\sum_{j=1}^{q-1} U_{i,j}(hL)\mathbf{N}(u_{n-j})$$

Exponential integrators (3/10)

Method	Type	Order	Stages s	Steps q
ABNørsett4	ETD Adams-Bashforth	4	1	4
ABNørsett5	ETD Adams-Bashforth	5	1	5
ABNørsett6	ETD Adams-Bashforth	6	1	6
Friedli (VRK4)	ETD Runge-Kutta	4	4	1
Strehmel-Weiner	ETD Runge-Kutta	4	4	1
Cox-Matthews (ETDRK4)	ETD Runge-Kutta	4	4	1
Krogstad (ETDRK4-B)	ETD Runge-Kutta	4	4	1
Minchev	ETD Runge-Kutta	4	4	1
Hochbruck-Ostermann	ETD Runge-Kutta	4	5	1
Luan-Ostermann (EXPRK5S8)	ETD Runge-Kutta	5	8	1
(Mod)GenLawson41	(Mod.) Gen. Lawson	4	4	1
(Mod)GenLawson42	(Mod.) Gen. Lawson	4	4	2
(Mod)GenLawson43	(Mod.) Gen. Lawson	4	4	3
(Mod)GenLawson44	(Mod.) Gen. Lawson	5	4	4
(Mod)GenLawson45	(Mod.) Gen. Lawson	6	4	5
PEC423	Predictor-corrector	4	2	3
PECEC433	Predictor-corrector	4	3	3
PEC524	Predictor-corrector	5	2	4
PECEC534	Predictor-corrector	5	3	4
PEC625	Predictor-corrector	6	2	5
PECEC635	Predictor-corrector	6	3	5
PEC726	Predictor-corrector	7	2	6
PECEC736	Predictor-corrector	7	3	6

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- Predictor-Corrector methods of order ≥ 5 more accurate but often unstable

Exponential integrators (4/10)

Example 1: ETD RK schemes for KdV equation from $t = 0$ to $t = 0.005$

We plot relative error $= \frac{\|u_{\mathbf{approx}} - u_{\mathbf{exact}}\|_\infty}{\|u_{\mathbf{exact}}\|_\infty}$ vs relative time-step $= \frac{dt}{0.005}$ and time

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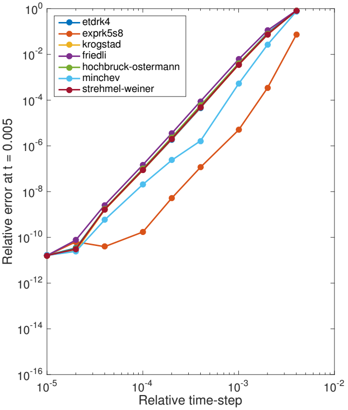
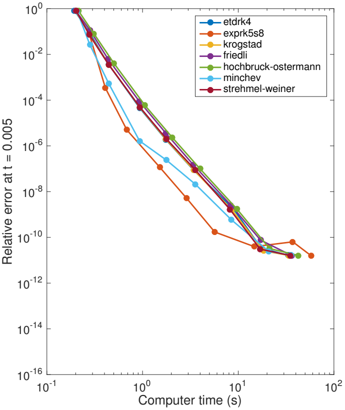
Example 1: ETD RK schemes for KdV equation from $t = 0$ to $t = 0.005$

We plot relative error $= \frac{\|u_{\text{approx}} - u_{\text{exact}}\|_\infty}{\|u_{\text{exact}}\|_\infty}$ vs relative time-step $= \frac{dt}{0.005}$ and time





Exponential integrators (5/10)

Example 2: ETD RK schemes for KdV equation from $t = 0$ to $t = 0.015$

Exponential integrators (5/10)

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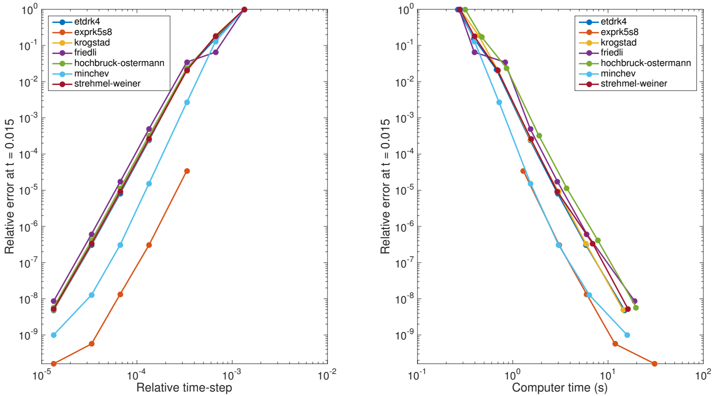
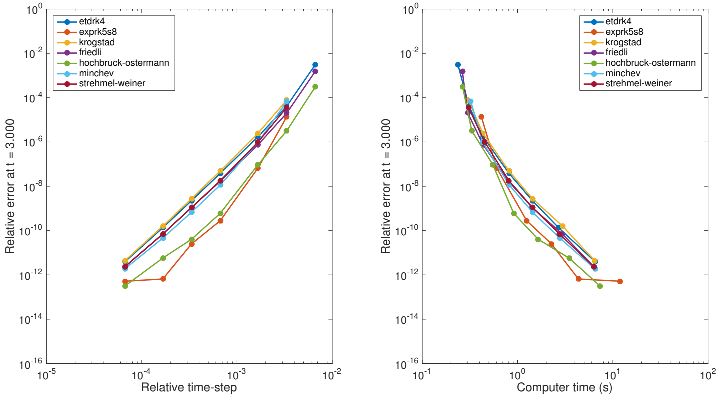


Exponential integrators (6/10)

Example 3: ETD RK schemes for Cahn-Hilliard equation from $t = 0$ to $t = 3$

Exponential integrators (6/10)

Example 3: ETD RK schemes for Cahn-Hilliard equation from $t = 0$ to $t = 3$

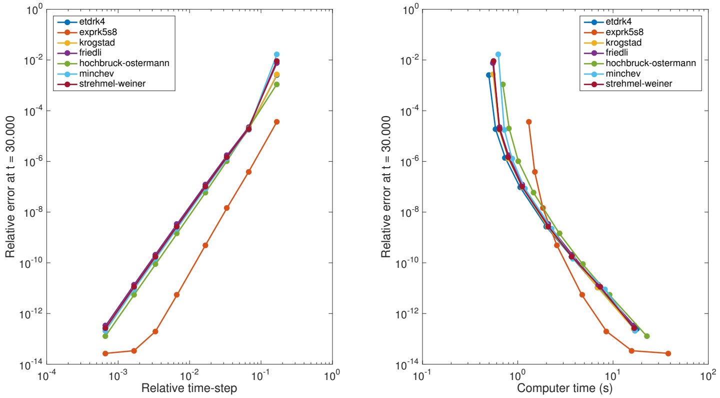


Exponential integrators (7/10)

Example 4: ETD RK schemes for Gray-Scott equations in 2D from $t = 0$ to $t = 30$

Exponential integrators (7/10)

Example 4: ETD RK schemes for Gray-Scott equations in 2D from $t = 0$ to $t = 30$



Exponential integrators (8/10)

Example 5: PEC schemes for KdV equation from $t = 0$ to $t = 0.015$

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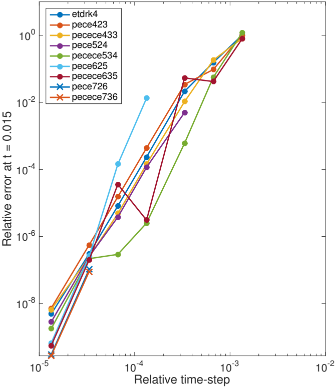
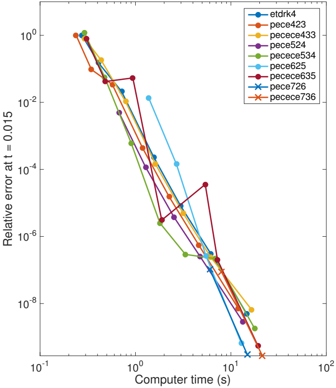


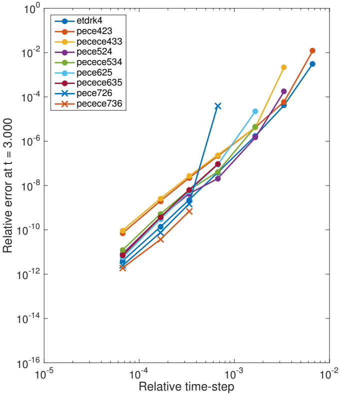


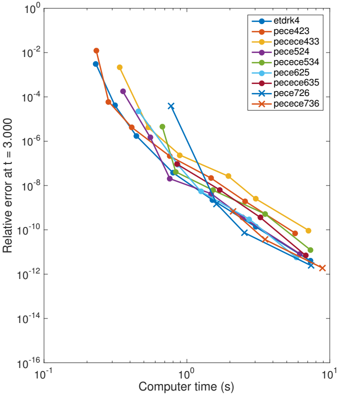
Exponential integrators (9/10)

Example 6: PEC schemes for Cahn-Hilliard equation from $t = 0$ to $t = 3$

Exponential integrators (9/10)

Example 6: PEC schemes for Cahn-Hilliard equation from $t = 0$ to $t = 3$



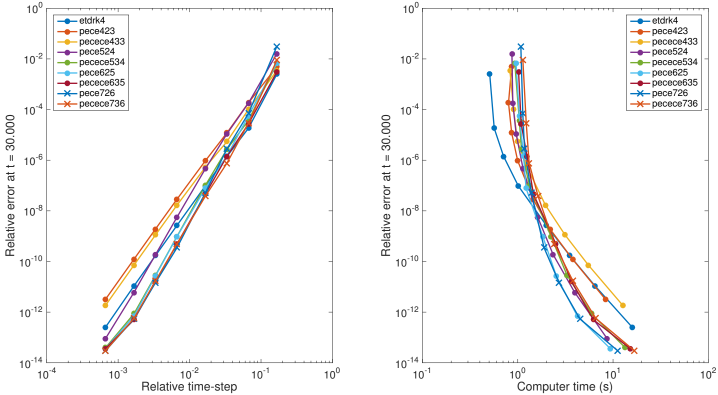


Exponential integrators (10/10)

Example 7: PEC schemes for Gray-Scott equations in 2D from $t = 0$ to $t = 30$

Exponential integrators (10/10)

Example 7: PEC schemes for Gray-Scott equations in 2D from $t = 0$ to $t = 30$



Conclusion

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- Future work includes PDEs on the sphere (with `spherefun`)