Solving stiff PDEs on the sphere

Numerical Analysis Group, Mathematical Institute

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Introduction

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- **Problem:** Stiff PDEs of the form

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

$u(t,x,y,z)$ is a function of time t and (x,y,z) with $x^2+y^2+z^2=1$
$\mathcal{L}$ is a linear differential operator, e.g., $\mathcal{L} = \alpha\Delta$ with $\alpha \in \mathbf{R}$ or $\alpha \in i\mathbf{R}$
$\mathcal{N}$ is a nonlinear operator, e.g., $\mathcal{N}(u) = u|u|^2$

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- **Method:** Double Fourier Sphere (DFS) method in space with mn points,

$$u(t,\lambda,\theta) \approx \sum_{j=-m/2}^{m/2-1} \sum_{k=-n/2}^{n/2-1} \hat{u}_{jk}(t) e^{ij\theta} e^{ik\lambda}$$

  This leads to a system of mn ODEs for $\hat{u}(t) = \{\hat{u}_{jk}(t)\}$,

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- **Observations:**
Multiplication matrices in coefficient space: no pole singularity
Special structure of the discrete Laplacian: optimal $O(mn\log mn)$ complexity
Implicit-explicit schemes and exponential integrators: no severe CFL restrictions

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$$x = \cos\lambda \sin\theta, \;\; y = \sin\lambda \sin\theta, \;\; z = \cos\theta,$$

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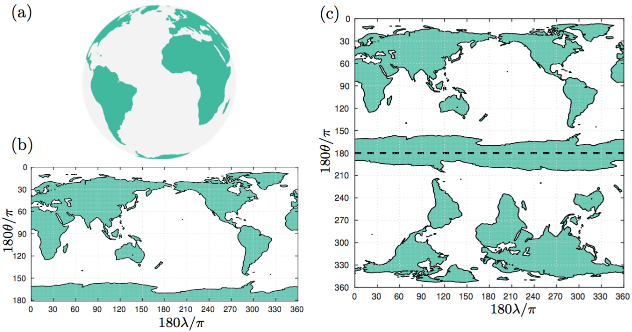
- Key idea: double up $u(\lambda, \theta)$ and flip it to make it periodic in both directions



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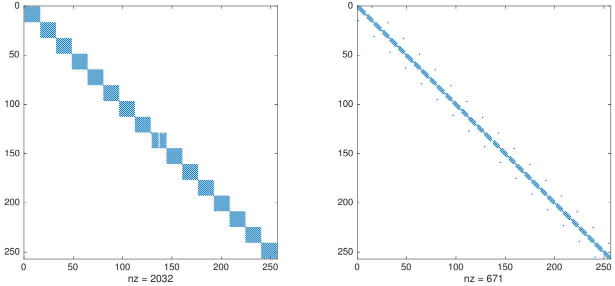
- Null space of $\tilde{\mathbf{M}}_{\sin^2}$: spurious modes 1 and ± 1 because it doesn't handle correctly the extreme wavenumbers
- The correct matrix, $\mathbf{M}_{\sin^2}$, is nonsingular (row diagonally dominant and irreducible)

The Double Fourier Sphere method (3/3)

- Sparsity patterns of $\mathbf{L}$ (left) and $\mathbf{M}_{\sin^2}\mathbf{L}$ (right):



- Each $m \times m$ block of $\mathbf{L}$: dense
- Each $m \times m$ block of $\mathbf{M}_{\sin^2}\mathbf{L}$: "pentadiagonal plus rank two"
- Consequence:

$$(z\mathbf{I} + h\mathbf{L})x = b$$

can be solved in $O(mn)$ operations since it is equivalent to solving

$$(z\mathbf{M}_{\sin^2} + h\mathbf{M}_{\sin^2}\mathbf{L})x = \mathbf{M}_{\sin^2} b$$

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- Exponential integrators: **L** integrated exactly with matrix exponential, numerical scheme for **N**, e.g.,

$$\textbf{ETDRK1} \qquad \hat{u}^{n+1} = e^{h\mathbf{L}}\hat{u}^n + \mathbf{L}^{-1}(e^{h\mathbf{L}} - \mathbf{I})\mathbf{N}(\hat{u}^n)$$

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- IMEX: implicit scheme for **L**, explicit formula for **N**, e.g.,

$$\textbf{IMEX} - \textbf{BDF2} \qquad (3\mathbf{I} - 2h\mathbf{L})\hat{u}^{n+1} = 4\hat{u}^n - \hat{u}^{n-1} + 4h\mathbf{N}(\hat{u}^n) - 2h\mathbf{N}(\hat{u}^{n-1})$$

Fourth-order time-stepping on the sphere (2/3)

- Dozens of exponential integration formulas of order four and higher have been proposed over the last 15 years
- Hard to do much better than the ETDRK4 scheme of Cox and Matthews

ETDRK4

$$
\begin{aligned}
\hat{a}^n &= e^{h\mathbf{L}/2}\hat{u}^n + (h/2)\varphi_1(\mathbf{L}h/2)\mathbf{N}(\hat{u}^n),\\
\hat{b}^n &= e^{h\mathbf{L}/2}\hat{u}^n + (h/2)\varphi_1(\mathbf{L}h/2)\mathbf{N}(\hat{a}^n),\\
\hat{c}^n &= e^{h\mathbf{L}/2}\hat{a}^n + (h/2)\varphi_1(\mathbf{L}h/2)\big[2\mathbf{N}(\hat{b}^n) - \mathbf{N}(\hat{u}^n)\big],\\
\hat{u}^{n+1} &= e^{h\mathbf{L}}\hat{u}^n + hf_1(h\mathbf{L})\mathbf{N}(\hat{u}^n) + hf_2(h\mathbf{L})\big[\mathbf{N}(\hat{a}^n) + \mathbf{N}(\hat{b}^n)\big] + hf_3(h\mathbf{L})\mathbf{N}(\hat{c}^n)
\end{aligned}
$$

- In general: precompute $e^{h\mathbf{L}}$ by diagonalizing $\mathbf{L}$ and using contour integrals, $O(nm^3)$, then $O(nm^2)$ per time-step (dense blocks)
- Real eigenvalues: no precomputation, $e^{h\mathbf{L}}\hat{u}^n$ products can be evaluated directly using Carathéodory-Fejér (CF) approximations, $O(mn)$ per time-step

Fourth-order time-stepping on the sphere (3/3)

- We consider two IMEX schemes
- Multistep and stable for diffusive PDEs only:

$$\textbf{IMEX}-\textbf{BDF4} \qquad \begin{aligned}(25\mathbf{I}-12h\mathbf{L})\hat{u}^{n+1} = {} & 48\hat{u}^{n}-36\hat{u}^{n-1}+6\hat{u}^{n-2}-3\hat{u}^{n-3} \\ & +48h\mathbf{N}(\hat{u}^{n})-72h\mathbf{N}(\hat{u}^{n-1}) \\ & +48h\mathbf{N}(\hat{u}^{n-2})-2h\mathbf{N}(\hat{u}^{n-3})\end{aligned}$$

- One-step with six stages and stable for both diffusive and dispersive PDEs:

LIRK4

$$\hat{v}_1 = \hat{u}^n,$$

$$(\mathbf{I}-a_{ii}h\mathbf{L})\hat{v}^i = \hat{u}^n + h\sum_{j=2}^{i-1} b_j\mathbf{L}\hat{v}_j + h\sum_{j=1}^{i-1}\tilde{a}_{ij}\mathbf{N}(\hat{v}_j), \quad 2\leq i\leq 6,$$

$$\hat{u}^{n+1} = \hat{u}^n + h\sum_{i=2}^{6} b_i\mathbf{L}\hat{v}_i + h\sum_{i=1}^{6}\tilde{b}_i\mathbf{N}(\hat{v}_i)$$

- Both have a $O(mn)$ cost per time-step

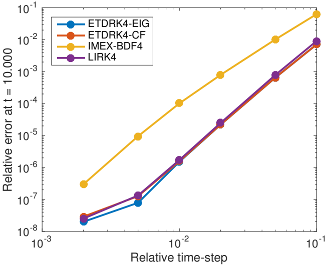
Numerical comparisons (1/3)

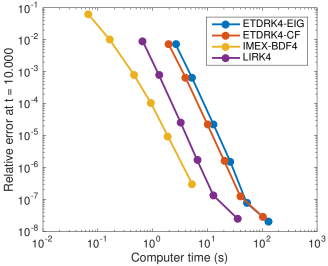
Allen-Cahn equation:

$$u_t = 10^{-2}\Delta u + u - u^3,$$

with $u_0(\lambda,\theta) = Y_8^2(\lambda,\theta)$, $m = n = 200$ and up to $t = 10$

Diffusive PDE: we can use ETDRK4-CF, ETDRK4-EIG, IMEX-BDF4, LIRK4





IMEX-BDF4 the most efficient for diffusive PDEs

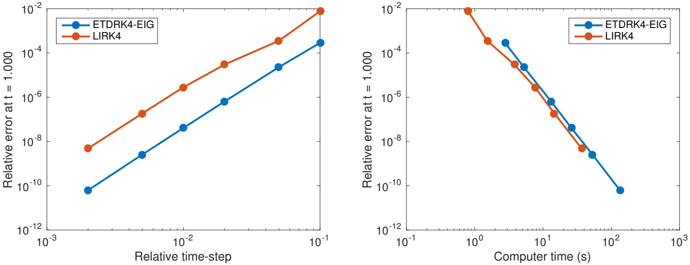
Numerical comparisons (2/3)

Nonlinear Schrödinger equation:

$$u_t = i\Delta u + iu|u|^2,$$

with $u_0(x,y,z) = \exp(-x^2 - y^2 - (z-1)^2)$, $m = n = 200$ and up to $t = 1$

Dispersive PDE: we can only use ETDRK4-EIG and LIRK4



LIRK4 the most efficient for dispersive PDEs

Numerical comparisons (3/3)

IMEX − BDF4

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\end{aligned}$$

	IMEX		ETDRK4	
	BDF4	LIRK4	CF	EIG
# FFTs $O(2mn\log mn)$	2	12	8	8
# backslashes $O(12mn)$	1	6	90	0
# dense mat-vec × $O(nm^2)$	0	0	0	9
diffusive PDEs	✓	✓	✓	✓
dispersive PDEs	×	✓	×	✓

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- Future work includes PDEs on the disk and inside the unit ball