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Lecture 4. Exponential integrators for stiff PDEs

1. Stiff PDEs

$$\boxed{u_t = Lu + N(u)}$$

linear, higher order + nonlinear, lower order

viscous Burgers	shock waves	$u_t = u_{xx} + uu_x$
Korteweg-de Vries	solitons, water waves	$u_t = u_{xxx} + uu_x$
Fisher-KPP	travelling waves	$u_t = u_{xx} + u - u^2$
Allen-Cahn	structure in materials	$u_t = u_{xx} + u - u^3$
Cahn-Hilliard	structure in materials	$u_t = -u_{xx} - u_{xxxx} + (u^3)_{xx}$
Kuramoto-Sivashinsky	flames, turbulence, chaos	$u_t = -u_{xx} - u_{xxxx} + uu_x$
nonlinear Schrödinger	optics, water waves	$u_t = iu_{xx} + i\|u\|^2 u$
complex Ginzburg-Landau	fluids, superconductivity	$u_t = (1 + iA)u_{xx} + u - (1 + iB)u\|u\|^3$
Gray-Scott	pattern formation	$u_t = \epsilon_1 u_{xx} - u + u^2 v,\;\; v_t = \epsilon_2 v_{xx} + a(1 - v) - u^2 v$
Schnakenberg	chemical reactions	$u_t = \epsilon_1 u_{xx} + a - u + u^2 v,\;\; v_t = \epsilon_2 v_{xx} + b - u^2 v$

After discretization in space, this becomes a large stiff system of ODEs.
Spectral discretizations in space are common, since high order is needed to resolve structures.
For efficiency, important to treat the linear and nonlinear terms differently (≈ implicit, explicit).
Order 1 wrt t : easy. Order 2 : can use e.g. Strang splitting. Order >2 : this is the challenge.
Many higher order methods have stiffness problems (i.e. they need excessively small time steps).

3 most important methods: exponential integrators, IMEX = implicit-explicit, spectral deferred correction.

2. Exponential integrators

An integrating factor gives this exact formula:

$$u(t_n + k) = e^{kL}u(t_n) + \int_0^k e^{(k-s)L}\, N\big(u(t_n + s)\big)ds$$

Exponential integrators come from ODE-style discretization of the integral. Here's the simplest, ETD1:

$$u(t_n + k) = e^{kL}u(t_n) + \int_0^k e^{(k-s)L}\, N\big(u(t_n + s)\big)ds$$

The most standard higher-order formula is ETDRK4 (Cox and Matthews 2002).

3. 1D, 2D, and 3D examples

Flexible and powerful for periodic geometries: the `spin/spin2/spin3` codes by Montanelli in Chebfun. Try e.g.
`spin('ac'), spin('ch'), spin('kdv'), spin('ks'), spin2('gl'), spin2('gs'), spin2('gsspots'), spin3('gl').`

4. Comparison of methods

Comparisons by Kassam-T (2002), Buvoli (2015), Montanelli-Bootland (2017). For periodic problems and accuracy <5 digits, no method consistently outperforms ETDRK4. For >5 digits, Buvoli gets better performance with spectral deferred correction up to order 32.

5. Fine points

Non-periodic geometry and order reduction. Hochbruck & Ostermann have highlighted a phenomenon of order reduction. For nonperiodic problems, this makes other methods better than ETDRK4.

Phi functions and rounding errors. Exponential integrators require evaluation of $\varphi_1(z) = \frac{e^z - 1}{z}$, $\varphi_2(z) = \frac{e^z - 1 - z}{z^2}$, etc. The removable singularity at $z = 0$ leads to rounding error trouble for $\varphi_k(z \approx 0)$. One solution (Kassam & T): evaluate $\varphi_k(z_j)$ for points z_j on a circle about z; $\varphi_k(z)$ then comes from a trapezoidal rule approximation to a Cauchy integral.

Non-diagonalizable problems and IMEX methods. Montanelli and Nakatsukasa have looked at exp. integrators on a sphere. Here one cannot diagonalize: the linear algebra is nontrivial. They find that IMEX methods are better. In Chebfun, `spinsphere` .