Splitting techniques for solving PDEs

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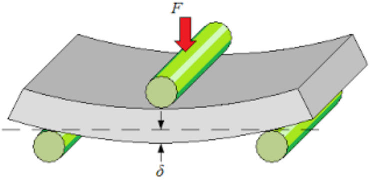
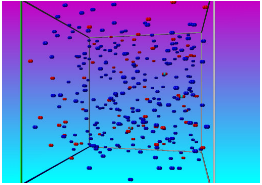
Partial differential equations (PDEs)



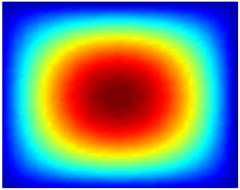


Mathematical model of physical processes

1. Complex movement of leaves in the wind. (Navier-Stokes)
2. Temperature distribution in this room. (Heat equation)
3. Someone leaning at a desk. (Linear elasticity)
4. The molecules floating around us. (Schrödinger)
5. Electromagnetic field allows surfing the web. (Maxwell)
6. Several coupled physical processes. (Systems of PDEs)

Solving PDEs is crucial in industry, academia, environment, ...

Parabolic partial differential equations

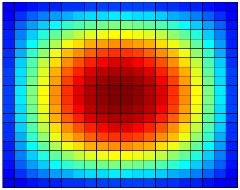


The heat equation:

$$\dot{u} - \Delta u = f, \quad x \in \Omega, \quad u(0) = u_0.$$

1. Heat equation, u is temperature and f heat source.
2. Smoothing property, infinite speed of propagation, as opposed to waves (audio).
3. If $f = f(u)$ the equation is semilinear, leads to different behaviour.
4. Allen-Cahn $f(u) = u - u^3$, phase separation in alloys.

Numerical techniques for solving PDEs



The heat equation:

$$\dot{u} - \Delta u = f(u), \quad \text{in } \Omega, \qquad u(0) = u_0.$$

1. We discretize the domain Ω into finite elements.
2. We discretize in time $\dot{u} \approx \frac{u^{n+1} - u^n}{k}$.

$$\frac{u^{n+1} - u^n}{k} - \Delta_h u^{n+1} = P_h f(u^{n+1}),$$

where $u^0 = P_h u_0$, and P_h is some map into the FE space.

Numerical techniques for solving PDEs

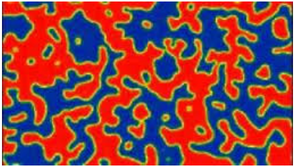
If we were to compute the temperature in a large room of size $16m \times 16m \times 4m$, the algebraic system of equations

$$\frac{u^{n+1} - u^n}{k} - \Delta_h u^{n+1} = P_h f(u^{n+1}),$$

has a huge number of unknowns.

1. Grid on centimeter-scale: size$\Delta_h \approx 10^9 \times 10^9$.
2. A (non)linear system of 10^9 unknowns need to be solved in every time step.
3. This procedure need to be repeated perhaps 10^3 times.
4. This is extremely time consuming (costly) or impossible on many computers.
5. Only development of faster computers is not enough, numerical analysis is needed!

Splitting



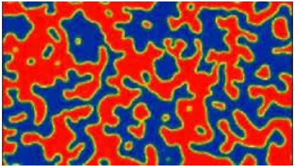
We consider a semilinear heat equation (Allen-Cahn),

$$\dot{u} - \Delta u = f(u), \qquad t \in (0, T]$$

In each time step we wish to,

- first solve a pure diffusion problem, $\dot{u} = \Delta u$,
- then a pure reaction problem, $\dot{u} = f(u)$.

Splitting

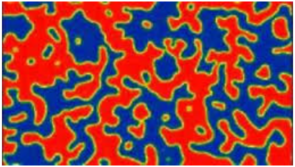


We discretize in time $0 = t_0 < t_1 < \cdots < t_n < \cdots < t_N = T$.
Given $u^s_{n-1} \approx u(t_{n-1})$, on (t_{n-1}, t_n), we solve

$$\begin{cases} \dot{u}^d = \Delta u^d \\ u^d_{n-1} = u^s_{n-1} \end{cases} \qquad \begin{cases} \dot{u}^r = f(u^r) \\ u^r_{n-1} = u^d_n \end{cases} \qquad u^s_n = u^r_n \approx u(t_n).$$

We thereby make a physical split of the equation. This procedure is called exponential splitting or Lie-Trotter splitting (for operators in the 1950s).

Splitting



- The diffusion equation is the standard heat equation for which very efficient methods exists.
- Another advantage is that the reaction equation do not contain spatial derivatives and can be solved cheaply.
- We can allow different time steps for different subproblems.
- However, the accuracy of the splitting must be controlled.

More advanced splitting techniques

In general we consider an equation,

$$\dot{u} = Au + F(u),$$

where $A = \Delta$ in the previous example.
If we let the solution operators to $\dot{v} = Av$ and $\dot{w} = Fw$ be denoted e^{kA} and e^{kF} where k is the time step size. The Lie-Trotter splitting scheme can be written

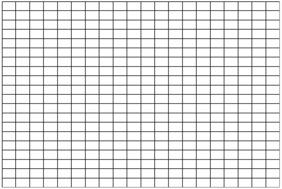
$$u_n^s = e^{kF} e^{kA} u_{n-1}^s$$

A second order (more accurate) splitting scheme is the Strang splitting,

$$u_n^s = e^{\frac{1}{2}kA} e^{kF} e^{\frac{1}{2}kA} u_{n-1}^s,$$

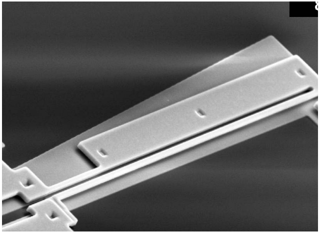
which means half a time step diffusion, a full time step reaction, and half a time step diffusion.

Error analysis



- The error consists of two parts: discretization in space (h) and discretization and splitting in time (k).
- High order methods need high smoothness in the solution.
- The different error sources are not independent.
- Understanding of error is (besides development of the method) the most important task in numerical analysis.

Multiphysics example



We consider temperature (θ), electric potential (ϕ), and displacement ($\mathbf{u}$) in a micro-electro-mechanical system,

$$\left\{\begin{array}{rcl} \dot{\theta} - \Delta\theta & = & \kappa(\theta)|\nabla\phi|^2 - \nabla\cdot\dot{\mathbf{u}} \\ -\nabla\cdot\kappa(\theta)\nabla\phi & = & 0 \\ \ddot{\mathbf{u}} - \nabla\cdot(\epsilon(\mathbf{u}) - \alpha\theta\mathbf{I}) & = & \mathbf{f}. \end{array}\right.$$

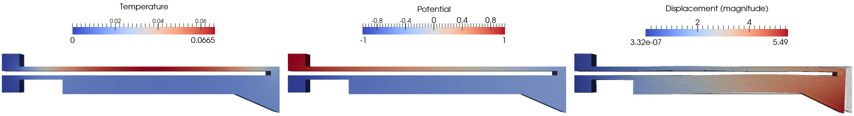
We apply a voltage to the contacts which induces Joule heating giving rise to thermal stresses that bends the device.

Multiphysics example

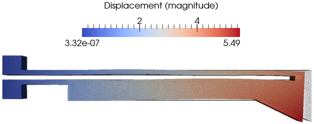
We split the system in each time step into:

- a heat equation,
- an elliptic equation for the electric potential,
- an elastic wave equation.

$$\begin{cases} D_t\theta_n - \Delta\theta_n &= \kappa(\theta_{n-1})|\nabla\phi_{n-1}|^2 - \nabla\cdot D_t\mathbf{u_{n-1}} \\ -\nabla\cdot\kappa(\theta_n)\nabla\phi_n &= 0 \\ D_t^2\mathbf{u_n} - \nabla\cdot(\epsilon(\mathbf{u_n}) - \alpha\theta_n\mathbf{I}) &= \mathbf{f}. \end{cases}$$



Multiphysics example



- Splitting techniques are very natural and necessary.
- The error analysis is complicated, not just splitting errors but discretization in time and space, error in data transfer between solvers (possibly different grids, methods), ...
- Errors may trigger numerical instability which destroys convergence.
- Already existence and uniqueness of solution and regularity of solutions is difficult.
- This situation is typical in real applications.

Erik's contribution

This is an important field of research with direct applications in many areas of science.

- A theoretical framework for analyzing the error due to splitting for semilinear evolution problems (Paper I).
- An analysis of the combined effect of splitting and spatial error for linear parabolic problems (Paper II).
- An analysis of combining physical and spatial splitting (domain decomposition) (Paper III).
- Real applications where splitting reduces the computational cost (Papers IV and V).