MA5233 Computational Mathematics

Lecture 22: Time-dependent PDEs

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Time-dependent PDEs

Introduction

Last two topics:

- ODEs $\approx$ differential equations in time.
- PDEs $\approx$ differential equations in space.

New topic: differential equations in both space and time.

Heat equation

Given $u_0 : [0,1] \to \mathbb{R}$, find $u : [0,1] \times [0,T] \to \mathbb{R}$ such that for all $x \in [0,1]$ and $t \in [0,T]$ it holds

$$\begin{cases} \frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t), & \text{(PDE)} \\ u(x,0) = u_0(x), & \text{(initial conditions)} \\ u(0,t) = u(1,t) = 0. & \text{(boundary conditions)} \end{cases}$$

Heat equation is the simplest time-dependent PDE and serves as a role model for more complicated equations.

See Lecture 5 for physical interpretation of this equation.

Time-dependent PDEs

Discretisation of time-dependent PDEs

Most numerical methods for time-dependent PDEs are derived according to the following scheme.

0. Original PDE:

$$\text{Find } u : [0,1] \times [0,T] \to \mathbb{R} \text{ such that } \tfrac{\partial u}{\partial t}(x,t) = \tfrac{\partial^2 u}{\partial x^2}(x,t). \tag{1}$$

1. Discretise in space using finite differences / Galerkin method.
   This replaces (1) with

$$\text{Find } u : [0,T] \to \mathbb{R}^n \text{ such that } \tfrac{\partial u}{\partial t}(t) = Au(t). \tag{2}$$

   where $u(t) \in \mathbb{R}^n$ is the vector of point values for finite differences or vector of expansion coefficients for Galerkin's method.

2. Discretise in time using Runge-Kutta / multistep method.
   This replaces (2) with

$$\text{Find } (u_k \in \mathbb{R}^n)_{k=0}^m \text{ such that } u_{k+1} = u_k + B\, u_k\, \tfrac{T}{m}.$$

   where $u_k \approx u(T\,\frac{k}{m})$.

The next slides demonstrate this procedure using FD and explicit Euler.

Time-dependent PDEs

Finite difference and explicit Euler discretisation of heat equation

0. Original PDE: $\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t)$
1. Finite difference discretisation (assuming $(x_k := \frac{k}{n+1})_{k=0}^{n+1}$):

$$\tfrac{\partial u}{\partial t}\big(x_k, t\big) \approx (n+1)^2 \Big(u(x_{k-1}, t) - 2\, u(x_k, t) + u(x_{k+1}, t)\Big).$$

   Let us write this as $\frac{\partial u}{\partial t}(t) = Au(t)$.

2. Explicit Euler time-stepping (assuming $(t_\ell := T\,\frac{\ell}{m})_{\ell=0}^{m}$) :

$$u\big(t_{\ell+1}\big) \approx u(t_\ell) + Au(t_\ell)\,\tfrac{T}{m}.$$

See `example()` in `22_time_dependent_pdes.jl`.

Time-dependent PDEs

Error analysis

Same setup as for Runge-Kutta methods:

- Exact time propagator $\Phi_t : u(x,0) \mapsto u(x,t)$.
- Numerical time propagator $\tilde{\Phi}_t : u(x_k,0) \mapsto \tilde{u}(x_k,t)$.

Note that Φ_t maps functions to functions, while $\tilde{\Phi}_t$ maps point-values to point-values. As before, we assume that functions are implicitly converted to point-values if this is required by context.

Assumptions on numerical propagator:

- Consistency: $\|\tilde{\Phi}_t(u) - \Phi_t(u)\| = \mathcal{O}\big(t\,(t^p + n^{-q})\big)$ for some $p, q > 0$.
- Stability: $\|\tilde{\Phi}_t(u_2) - \tilde{\Phi}_t(u_1)\| \leq (1 + \tilde{L}\,t)\,\|u_2 - u_1\|$ for some $\tilde{L} > 0$.

Main new ingredient:

- space-discretised ODE $\frac{\partial u}{\partial t} = Au(t)$ is only an approximation to the exact equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}(t)$.
- Hence, consistency error involves a spatial component $\mathcal{O}\big(t\,n^{-q}\big)$ and a temporal component $\mathcal{O}\big(t^{p+1}\big)$.

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Theorem

Under the assumptions on previous slide, we have

$$\|\tilde{u}(T) - u(T)\| = \mathcal{O}\big(m^{-p} + n^{-q}\big)$$

where $u(T)$ denotes the vector of point-values of the exact solution and $\tilde{u}(T)$ is the numerically computed approximation using m equidistant steps in time and n equispaced grid points in space.

Proof. The proof is a minor modification of what we have done for the Runge-Kutta schemes in Lecture 16. As before, let us introduce the shorthand notation

$$\Phi(u) := \Phi_{T/m}(u), \quad \tilde{\Phi}(u) := \tilde{\Phi}_{T/m}(u), \quad u_k := u(\tfrac{Tk}{m}), \quad \tilde{u}_k := \tilde{u}(\tfrac{Tk}{m}).$$

Both u_k and $\tilde{u}_k$ are vectors of point values.

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Proof (continued). We compute

$$\begin{aligned}
\|\tilde{u}(T) - u(T)\| &= \|\tilde{\Phi}(\tilde{u}_{m-1}) - \Phi(u_{m-1})\| \\
&\leq \|\tilde{\Phi}(\tilde{u}_{m-1}) - \tilde{\Phi}(u_{m-1})\| + \|\tilde{\Phi}(u_{m-1}) - \Phi(u_{m-1})\| \\
&\leq (1 + \tfrac{\tilde{L}T}{m})\,\|\tilde{u}_{m-1} - u_{m-1}\| + \mathcal{O}\big(m^{-1}\,(m^{-p} + n^{-q})\big) \\
&\leq \dots \\
&\leq 0 + \left(\sum_{k=0}^{m-1} (1 + \tfrac{\tilde{L}T}{m})^k\right)\, \mathcal{O}\big(m^{-1}\,(m^{-p} + n^{-q})\big) \\
&\leq (1 + \tfrac{\tilde{L}T}{m})^{m-1}\, \mathcal{O}\big(m^{-p} + n^{-q}\big)
\end{aligned}$$

Claim follows after observing that since $1 + x \leq \exp(x)$, we have

$$(1 + \tfrac{\tilde{L}T}{m})^{m-1} \leq \exp\big(\tilde{L}\,T\,\tfrac{m-1}{m}\big) \leq \exp\big(\tilde{L}\,T\big).$$

Time-dependent PDEs

Consistency of FD + explicit Euler

$$\begin{aligned}\tilde{u}(t) &= u(0) + Au(0)\,t \\ u(t) &= u(0) + \tfrac{\partial u}{\partial t}(0)\,t + \mathcal{O}(t^2)\end{aligned}$$

Since

$$\tfrac{\partial u}{\partial t}(x_k, 0) = \tfrac{\partial^2 u}{\partial x^2}(x_k, 0) = (Au)_k + \mathcal{O}\big(n^{-2}\big),$$

we have $\tilde{u}(t) - u(t) = \mathcal{O}\big(t\,(t + n^{-2})\big)$.

Stability of FD + explicit Euler

$$\begin{aligned}\|\tilde{\Phi}_t(u_2) - \tilde{\Phi}_t(u_1)\| &\leq \|u_2 - u_1\| + t\,\|Au_2 - Au_1\| \\ &\leq \big(1 + \|A\| t\big)\,\|u_2 - u_1\|.\end{aligned}$$

Conclusion

Error for finite difference and explicit Euler discretisation with m equidistant time-steps and n mesh points is given by

$$\text{error} = \mathcal{O}\big(m^{-1} + n^{-2}\big).$$

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Discussion

- Solving time-dependent PDEs involves two limits $m, n \to \infty$.
- Analysis shows that error can effectively be decomposed into temporal and spatial components.
- Optimal efficiency is achieved if these two components are of equal magnitude, i.e. if $m^{-p} \approx n^{-q}$.

Concrete examples (assuming finite difference discretisation in space):

- For explicit or implicit Euler, choose $m \propto n^2$.
- For explicit or implicit midpoint, choose $m \propto n$.

See `convergence()`.

Observation

For explicit methods, solution blows up if m is too small compared to n.

Time-dependent PDEs

Asymptotic behaviour of heat equation

Physical intuition: $u(x,t) \to 0$ for $t \to \infty$ due to boundary conditions.

Mathematical analysis:

- If $u_0(x) = \sin(\pi k x)$, then $u(x,t) = \sin(\pi k x)\exp\big(-(\pi k)^2 x\big)$.
- Heat equation is linear: if $u_k(x,t)$ solves heat equation with initial conditions $u_{0,k}(x)$ for $k \in \{1,2\}$, then $u_1(x,t) + u_2(x,t)$ solves heat equation for initial conditions $u_{0,1}(x) + u_{0,2}(x)$.
- Fourier theory: any (reasonable) $u_0(x)$ can be written as

$$u_0(x) = \sum_{k=1}^{\infty} \hat{u}_k \sin(\pi k x).$$

Conclusion:

$$u(x,t) = \sum_{k=1}^{\infty} \hat{u}_k \sin(\pi k x)\exp\big(-(\pi k)^2 t\big),$$

i.e. solutions decay exponentially in time.

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Asymptotic behaviour of Runge-Kutta methods

Runge-Kutta with time-step Δt applied to the ODE $\dot{u} = Au$ produces solutions $\tilde{u}_k$ which go to zero for $k \to \infty$ if and only if the stability function $R(z)$ satisfies $|R(\lambda\,\Delta t)| < 1$ for all eigenvalues λ of A.

Time step constraint for FD + explicit Runge-Kutta method

- We showed in Lecture 5 that the eigenvalues of the finite difference matrix A satisfy $\lambda_k \in \big(-4\,(n+1)^2, 0\big)$.
- We showed in Lecture 17 that stability functions $R(z)$ for explicit Euler and midpoint rule satisfy $|R(z)| \geq 1$ for $z \in \mathbb{R} \setminus (-2, 0)$.

Conclusion: stability constraint $|R(\lambda\Delta t)| < 1$ is satisfied if and only if

$$4\,(n+1)^2\,\Delta t \leq 2 \quad \iff \quad \Delta t \leq \tfrac{1}{2}\,(n+1)^{-2}.$$

Discussion

- Time step constraint is acceptable for explicit Euler method since convergence anyway requires $\Delta t \propto n^{-2}$.
- Time step constraint means explicit midpoint offers no advantage over explicit Euler: for convergence, $\Delta t \propto n^{-1}$ would be enough, but stability imposes $\Delta t \propto n^{-2}$.