Numerical Solution of Initial Boundary Value Problems

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Lecture 6

Approximations in Time

- Basic theory
- Explicit Runge-Kutta methods
- Dual time-stepping
- Implicit vs explicit
- Summation-by-parts in time

Basic Theory

General linear PDE:

$$u_t = P(\partial/\partial x)u \tag{1}$$

Discretize in space and time separately (method of lines):

$$U_t = QU \tag{2}$$

(Q is obtained by discretizing the PDE in space, including boundary conditions. Coupled space-time discretizations are also possible - e.g. Lax-Wendroff scheme, not the focus here).

<ins>Stability:</ins> Assume that Q can be diagonalized as $T^{-1}QT = \Lambda$.

Test equation:

$$u_t = \lambda u. \tag{3}$$

If a time stepping scheme applied to (3) is stable for all eigenvalues λ of Q, then it is stable also for (2).

Basic Theory

Ex: $\frac{u^{n+1}-u^n}{\Delta t} = \lambda u^n$ (explicit), $\frac{u^{n+1}-u^n}{\Delta t} = \lambda u^{n+1}$ (implicit).

Explicit methods in general stable if

i) $\text{Real}(\lambda) \leq 0$ (Petrowski) and

ii) $|\Delta t \lambda|$ sufficiently small (Von Neumann).

Centered approx. for first order PDE $\Rightarrow \text{Imag}(\lambda) \sim \frac{1}{\Delta x}$
Centered approx. for second order PDE $\Rightarrow \text{Real}(\lambda) \sim \frac{1}{\Delta x^2}$

Implicit methods are often stable for all Δt (A-stability).

A and L stability

Def: A-stability: $|u^{n+1}| < |u^n|$ for all Real$(\lambda) \leq 0$, all $\Delta t > 0$.

Sometimes A-stability is not good enough, no damping of non-physical oscillations.

Def: L-stability: An A-stable method is also called L-stable if

$$\frac{|u^{n+1}|}{|u^n|} \to 0 \quad \text{as} \quad |\Delta t \lambda| \to \infty.$$

A and L stability

Ex: The θ-method

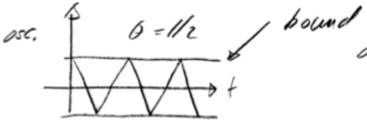
$$\frac{u^{n+1}-u^n}{\Delta t} = \lambda(\theta u^{n+1} + (1-\theta)u^n).$$

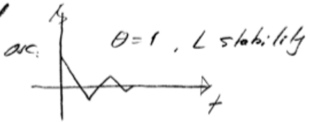
$$u^{n+1} = \underbrace{\frac{1+\Delta t\lambda(1-\theta)}{1-\Delta t\lambda\theta}}_{Z} u^n$$

$|Z(\Delta t\lambda)| \leq 1$ for all Real$(\Delta t\lambda) \leq 0 \quad \Rightarrow$ A-stable, all θ

Let $\Delta t\lambda \to \infty \Rightarrow |Z| = |\frac{1-\theta}{\theta}|$

$\theta = 1$, Backward Euler, $O(\Delta t)$, L-stable
$\theta = 1/2$, Trapezoidal, $O(\Delta t^2)$, not L-stable





Runge-Kutta methods

$$\frac{du}{dt} = F(t,u)$$

- R-K are one-step methods, no start-up problems.
- s intermediate "stages" computed at each time step.
- $F(t,u)$ evaluated in each stage.

Explicit R-K (ERK):

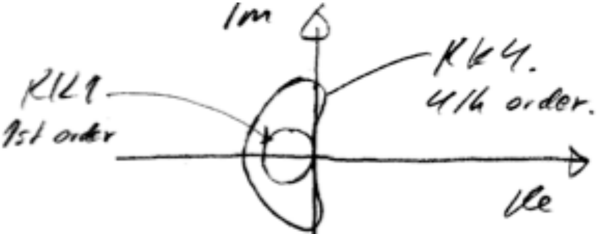
$$\begin{aligned}
k_1 &= F(t_n, u^n) \\
k_2 &= F(t_n + c_2\Delta t, u_n + \Delta t a_{21} k_1) \\
k_3 &= F(t_n + c_3\Delta t, u_n + \Delta t(a_{31}k_1 + a_{32}k_2)) \\
&\dots \\
k_s &= F(t_n + c_s\Delta t + \Delta t(a_{s1}k_1 + \dots + a_{s,s-1}k_{s-1})) \\
u^{n+1} &= u^n + \Delta t(b_1 k_1 + \dots + b_s k_s)
\end{aligned}$$

Runge-Kutta methods

A one-step method applied to test eq. leads to $u^{n+1} = Z(\lambda\Delta t)u^n$. (Z polynomial (explicit) or rational (implicit) appr. of $e^{\lambda\Delta t}$)

Stability region: All μ in the complex plane such that $|Z(\mu)| \leq 1$.

Ex: $u^{n+1} = Z(\mu)u^n = (\underbrace{\underbrace{\underbrace{1+\mu}_{\text{Forward Euler}} + \mu^2/2!}_{\text{Huen's method}} + \mu^3/3! + \mu^4/4!}_{\text{Classical RK4}})u^n$



Dual time-stepping

Assume we want to solve a transient system using an implicit scheme.

$$U_t + Q(U) = F. \tag{4}$$

E.g. Euler backward $\Rightarrow$

$$\frac{U^{n+1} - U^n}{\Delta t} + Q(U^{n+1}) = F^{n+1} \tag{5}$$

How do we solve (5) for U^{n+1} without solving a complicated nonlinear equation? Trick: Let $U^* = U^{n+1}$, add $\frac{\partial U^*}{\partial \tau}$ to (4) $\Rightarrow$

$$\frac{\partial U^*}{\partial \tau} + \underbrace{\frac{U^*}{\Delta t} + Q(U^*)}_{\tilde{Q}(U^*)} = \underbrace{F^{n+1} + \frac{U^n}{\Delta t}}_{\tilde{F}} \tag{6}$$

Can be integrated using a fast steady-state solver.

Explicit vs. Implicit Methods

- Explicit Methods
  - + Simplicity
  - + Easy to program
  - + No system to solve
  - – Small time-steps for stiff problems
- Implicit Methods
  - + Large time-steps allowed
  - + Fast for steady-state
  - – Complicated
- Research fields
  - – IMEX
  - – Implicit for large nonlinear equations
  - – Methods for bounded error growth
  - – SBP-SAT in time

SBP-SAT in time: the first derivative

Consider the scalar constant coefficient problem:

$$u_t + \lambda u = 0, \quad 0 \leq t \leq T, \tag{7}$$

where λ is a real constant. The energy estimate with $u(0) = f$ is

$$u(T)^2 + 2\lambda \|u\|_{L_2}^2 = f^2, \tag{8}$$

where the L_2 norm is defined as $\|u\|_{L_2}^2 = \int_0^T u^2 \mathrm{d}t$.

The fully discrete approximation of (7) becomes

$$\vec{u}_t + \lambda \vec{u} = P^{-1} \tau (u_0 - f) \vec{e}_0, \tag{9}$$

where

$$\vec{u}_t = D_1 \vec{u} = P^{-1} Q \vec{u}. \tag{10}$$

SBP-SAT in time: the first derivative

By choosing $\tau = -1$ and applying the discrete energy method to (9) we find

$$u_N^2 + 2\lambda \|\vec{u}\|_P^2 = f^2 - (u_0 - f)^2, \tag{11}$$

where $\|\vec{u}\|_P^2 = \vec{u}^T P \vec{u}$. The estimate (11) mimics the continuous target (8), only introducing a small additional damping term.

The SBP-SAT first derivative formulation is unconditionally stable (arbitrary Δt) and high order accurate.

The time interval can be divided into an arbitrary number of subdomains, allowing for a multi-stage formulation of the method with reduced number of unknowns.

The multi-stage formulation superconverges at each final multi-stage time. For an SBP-SAT approximation of order (p,2p) with diagonal norm, the full 2p order is obtained.

SBP-SAT in time: the second derivative

We extend the scalar constant coefficient case to the second order equation:

$$u_{tt} + \alpha^2 u_t + \beta^2 u = 0, \quad 0 \leq t \leq T \tag{12}$$

where α^2 and β^2 are positive real constants. Given two initial conditions $u(0) = f$ and $u_t(0) = g$

$$u_t(T)^2 + \beta^2 u(T)^2 + 2\alpha^2 \|u_t\|^2_{L_2} = g^2 + \beta^2 f^2, \tag{13}$$

is found, which is the target for our discrete energy estimate.

We can impose $u_t(0) = g$ in the usual manner. However, implementing $u(0) = f$ is more complicated and needs careful treatment.

SBP-SAT in time: the second derivative

We transform (12) into a system of first order differential equations. Setting $u_t = v$ and applying the SBP-SAT technique for the first derivatives yield

$$
\begin{aligned}
D_1\vec{u} - \vec{v} &= P^{-1}\tau_0(u_0 - f)\vec{e}_0 \\
D_1\vec{v} + \alpha^2\vec{v} + \beta^2\vec{u} &= P^{-1}\tau_{0t}(v_0 - g)\vec{e}_0.
\end{aligned}
\tag{14}
$$

The first equation in (14) above can be used to define a modified discrete first derivative, with the weak SAT condition added to it. Indeed, we let $\tilde{\vec{u}}_t = \vec{v}$, which gives

$$
\tilde{\vec{u}}_t = \vec{u}_t - P^{-1}\tau_0(u_0 - f)\vec{e}_0, \tag{15}
$$

where $\vec{u}_t = D_1\vec{u}$ as in (10). Note also that the modified discrete first derivative $\tilde{\vec{u}}_t$ has the same order of accuracy as $\vec{u}_t$.

SBP-SAT in time: the second derivative

Inserting (15) into the second equation in (14), leads to

$$\tilde{\vec{u}}_{tt} + \alpha^2 \tilde{\vec{u}}_t + \beta^2 \vec{u} = P^{-1} \tau_{0t} ((\tilde{u}_0)_t - g) \vec{e}_0, \tag{16}$$

where the modified discrete second derivative is defined by applying the first derivative operator again on $\tilde{\vec{u}}_t$:

$$\tilde{\vec{u}}_{tt} = D_1 \tilde{\vec{u}}_t. \tag{17}$$

With the choice $\tau_0 = \tau_{0t} = -1$, the discrete energy method gives

$$((\tilde{u}_N)_t)^2 + \beta^2 u_N^2 + 2\alpha^2 \|\tilde{\vec{u}}_t\|_P^2 = h^2 + \beta^2 f^2 - ((\tilde{u}_0)_t - g)^2 - \beta^2 (u_0 - f)^2, \tag{18}$$

which is very similar to the continuous estimate (13).

In a boundary value problem with $u = f$, $u = g$ posed at different boundaries, the standard SBP-SAT technique could have been used.

Summary of SBP-SAT in time

- First derivative
  - + High order accurate
  - + Unconditionally stable
  - + Superconverging at last time step
  - + Fully discrete energy estimates
  - + Preserves nonlinear stability
  - – Large system to solve
- Second derivative
  - + High order accurate
  - + Unconditionally stable
  - + Fully discrete energy estimates
  - – Large system to solve
  - – Wide operators for initial value problems

Exercises/Seminars

- Discretise the advection-diffusion equation, and prove stability, first semi-discrete, next fully discrete, using SBP in time.
- Discretise the initial value problem for the wave equation, and prove stability, first semi-discrete, next fully discrete, using SBP in time.
- Discretise the boundary value problem for the wave equation, and prove stability, first semi-discrete, next fully discrete, using SBP in time.
- Prove that SBP in time preserves semi-discrete stablity.