Lecture 11: Time stepping methods

COMP5930M Scientific Computation

Today

Time stepping for PDE models

Classes of methods

Stability

Implications for nonlinear systems

Time stepping process

Next

Time stepping

- In the Method of Lines framework we define a semi-discrete form of our partial differential equation (PDE) as a coupled system of ordinary differential equations (ODEs)

  For example, a typical discrete 1D PDE at node i is written as:

  $$\dot{\mathbf{u}}_i = \mathbf{f}(\mathbf{u}_{i-1}, \mathbf{u}_i, \mathbf{u}_{i+1})$$

- In this form, many standard numerical methods for ODEs can be applied

First-order accurate methods

- Forward (explicit) Euler:

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = \mathbf{f}(\mathbf{u}^k)$$

- Backward (implicit) Euler:

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = \mathbf{f}(\mathbf{u}^{k+1})$$

Both are $\mathcal{O}(\Delta t)$ accurate (termed, first order)

Implicit or Explicit methods?

Efficiency trade-offs

- Explicit - many short, cheap timesteps

- Implicit - fewer long, expensive timesteps

Accuracy requirements

- Explicit timestep often limited for stability, e.g. $\Delta t < Ch^2$

- Implicit timestep often limited for accuracy, by $\Delta t < Ch$

Higher accuracy in time

- For efficient computation of time-dependent PDE problems we should balance <u>the errors in time and space</u>

- FDM applied to many standard second-order (in space) PDE models leads to <u>a spatial error of $\mathcal{O}(h^2)$</u>

- <u>After applying an approximation in time:</u>
  - An $\mathcal{O}(\Delta t)$ scheme leads to a total error <u>$E \propto \mathcal{O}(\Delta t, h^2)$</u>
  - An $\mathcal{O}(\Delta t^2)$ scheme leads to a total error <u>$E \propto \mathcal{O}(\Delta t^2, h^2)$</u>
    <u>Need to find time-stepping method at least $\mathcal{O}(\Delta t^2)$ accurate</u>

The θ-method

Idea: Linear combination of the implicit and explicit Euler methods

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} \ = \ \theta \, \mathbf{f}(\mathbf{u}^{k+1}) + (1 - \theta) \, \mathbf{f}(\mathbf{u}^k)$$

for $0 \leq \theta \leq 1$

- $\theta = 0$ gives explicit Forward Euler, $\mathcal{O}(\Delta t)$ accurate

- $\theta = 1$ gives implicit Backward Euler, $\mathcal{O}(\Delta t)$ accurate

- $\theta = \frac{1}{2}$ gives an implicit, $\mathcal{O}(\Delta t^2)$ accurate scheme
  - known as the trapezoidal rule or Crank-Nicolson method[1]

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[1]Named after Phyllis Nicolson, a physicist at University of Leeds

Time stepping families

▶ It is possible to define methods of arbitrarily high order

▶ Runge-Kutta family
  ▶ One-step methods:

    $$\mathbf{u}^{k+1} \text{ depends on } \mathbf{u}^k \text{ only}$$

    but $\mathbf{f}(\mathbf{u})$ is evaluated multiple times per step (stages)
  ▶ Commonly explicit methods (RK4), implicit also possible

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- Backward differentiation formulae (BDF)
  - Multi-step methods:

    $$\mathbf{u}^{k+1} \text{ depends on } \mathbf{u}^k, \mathbf{u}^{k-1}, \ldots, \mathbf{u}^{k-m+1}$$

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  - Implicit methods, balance between stability and cost

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Runge-Kutta methods

- Simplest example is Explicit Euler

$$
\begin{aligned}
\mathbf{k}_1 &= \mathbf{f}(\mathbf{u}^k) && \text{(stage 1)} \\
\mathbf{u}^{k+1} &= \mathbf{u}^k + \Delta t\, \mathbf{k}_1
\end{aligned}
$$

- A second-order (explicit) scheme

$$
\begin{aligned}
\mathbf{k}_1 &= \mathbf{f}(\mathbf{u}^k) && \text{(stage 1)} \\
\mathbf{k}_2 &= \mathbf{f}(\mathbf{u}^k + \frac{\Delta t}{2}\mathbf{k}_1) && \text{(stage 2)} \\
\mathbf{u}^{k+1} &= \mathbf{u}^k + \Delta t\, \mathbf{k}_2
\end{aligned}
$$

General Runge-Kutta method with s stages

For the general problem $\mathbf{u}'(t) = \mathbf{f}(t, \mathbf{u}(t))$:

$$\mathbf{k}_i = \mathbf{f}(t_k + c_i \Delta t, \mathbf{u}^k + \Delta t \sum_{j=1}^{s} a_{ij} \mathbf{k}_j), \quad i = 1, \ldots, s \quad \text{(stage } i\text{)}$$

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \Delta t \sum_{i=1}^{s} b_i \mathbf{k}_i \qquad \text{(update)}$$

▶ If $a_{ij} = 0$ for all $i \leq j$ method is explicit, otherwise implicit

▶ Implicit R-K leads to nonlinear system of equations to solve
for $\mathbf{k}_1, \ldots, \mathbf{k}_s$ at each time step $\Rightarrow$ full system is of size $n \times s$!

Backward Differentiation Method (BDF-m)

- ▶ Idea: Use m previous solutions $\mathbf{u}^k, \ldots, \mathbf{u}^{k-m+1}$ to construct Lagrange interpolating polynomial $\mathbf{p}_m(t)$ of degree m s.t.

$$\mathbf{p}_m(t_{k-i+1}) = \mathbf{u}^{k-m+1}, \quad i = 0, \ldots, m$$

  and solve $\mathbf{p}'_m(t_k + \Delta t) = \mathbf{f}(\mathbf{u}^{k+1})$ to find $\mathbf{u}^{k+1}$.

- ▶ Simplest example is Implicit Euler (BDF-1)

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▶ The second order scheme (BDF-2)

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Stability of a time-stepping method

- ▶ There are many different definitions of (numerical) stability

- ▶ Time-stepping method is absolutely stable (A-stable) if the numerical solution applied to the linear test problem:

$$u'(t) = \lambda u(t)$$

approaches zero, $u_k \to 0$ as $k \to \infty$, whenever $\text{Re}(\lambda) < 0$ and for any fixed step size $\Delta t > 0$.

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Example: Stability of Euler methods

Explicit Euler:

$$u^{k+1} = u^k + \lambda\Delta t u^k = (1 + \lambda\Delta t)u^k = R(z)u^k$$

where $R(z) = R(\lambda\Delta t)$ is called the stability function.

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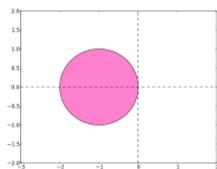Implicit Euler:
$$u^{k+1} = u^k + \lambda \Delta t u^{k+1}$$

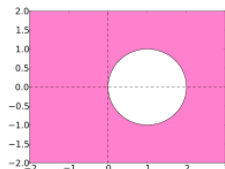so that the stability function is $R(z) = 1/(1-z)$.

Stability region: $|1-z| > 1$

$\Rightarrow$ complex plane except for a disc of radius 1 centered at $z = 1$
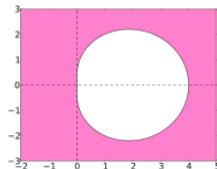
Stability regions of different methods

We can illustrate A-stability by coloring the points $\lambda \Delta t \in \mathbb{C}$ for which different methods are stable for the problem $u'(t) = \lambda u(t)$:
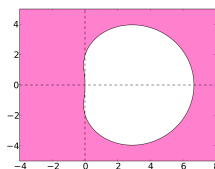

Forward Euler

Backward Euler

BDF-2

BDF-3

Properties of BDF methods

- BDF-m methods can be defined for any $m = 1, 2, 3, \ldots$

- BDF-1 and BDF-2 are A-stable

- BDF-3 almost A-stable (except small region near Im axis)

- BDF-m for $m \geq 6$ is unstable, do not use

Application to nonlinear systems

When choosing the time stepping method, we should consider:

► Computational complexity

  ► Explicit Runge-Kutta method: no nonlinear equation solves

► Stability and accuracy

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The time stepping process

1. $t = t^0$, $\mathbf{u}^0 = \mathbf{U}(x, t^0)$
2. for $k = 0, 1, ...$
   2.1 set initial guess $\mathbf{u}_0^{k+1} = \mathbf{u}^k$
   2.2 $\mathbf{u}^{k+1} = Newton(\mathbf{F}(\mathbf{u}^{k+1}), \mathbf{u}_0^{k+1}, \Delta t, Tol)$
   2.3 $t = t + \Delta t$

▶ For small Δt the initial guess $\mathbf{u}_0^{k+1}$ will be accurate

▶ For very large Δt we may have problems
   with convergence

▶ *Tol* should be chosen sufficiently small so as
   not to compromise the accuracy of the PDE model

Summary

- High-order time stepping methods balance the discretisation error in time and space and outperform first order methods

- Explicit Runge-Kutta methods usually not appropriate for PDEs due to stringent stability requirements ($\Delta t \ll 1$)

- Implicit BDF methods offer a good balance between stability and computational cost

- Time-stepping method should be chosen based on the physics of the specific problem being solved

Next time

► Lecture

  ► Approximation of 2-d nonlinear PDEs

  ► Sparse system structure and efficient algorithms