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 the errors in time and space

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

- After applying an approximation in time:
  - An $\mathcal{O}(\Delta t)$ scheme leads to a total error $E \propto \mathcal{O}(\Delta t, h^2)$
  - An $\mathcal{O}(\Delta t^2)$ scheme leads to a total error $E \propto \mathcal{O}(\Delta t^2, h^2)$

  Need to find time-stepping method at least $\mathcal{O}(\Delta t^2)$ accurate

The θ-method

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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]

[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)
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- Backward differentiation formulae (BDF)
  - Multi-step methods:
    $$\mathbf{u}^{k+1} \text{ depends on } \mathbf{u}^k, \mathbf{u}^{k-1}, \ldots, \mathbf{u}^{k-m+1}$$
    for a general *m*-step method
  - 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 $\mathbf{u}'(t) = \mathbf{f}(t, \mathbf{u}(t))$:

$$\begin{aligned} \mathbf{k}_i &= \mathbf{f}(t_k + c_i \Delta t, \mathbf{u}^k + \Delta t \sum_{j=1}^{s} a_{ij} \mathbf{k}_j), \quad i = 1, \dots, s \quad \text{(stage } i\text{)} \\ \mathbf{u}^{k+1} &= \mathbf{u}^k + \Delta t \sum_{i=1}^{s} b_i \mathbf{k}_i \qquad \text{(update)} \end{aligned}$$

- If $a_{ij} = 0$ for all $i \le j$ method is explicit, otherwise implicit
- Implicit R-K leads to nonlinear system of equations to solve for $\mathbf{k}_1, \dots, \mathbf{k}_s$ at each time step $\Rightarrow$ full system is of size $n \times s$!

Backward Differentiation Method (BDF-m)

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

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

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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$$\frac{3\mathbf{u}^{k+1} - 4\mathbf{u}^k + \mathbf{u}^{k-1}}{2\Delta t} = \mathbf{f}(\mathbf{u}^{k+1})$$

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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 $\mathrm{Re}(\lambda) < 0$ 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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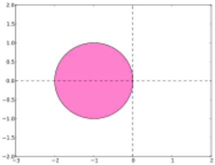
so that the stability function is $R(z) = 1/(1-z)$.

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

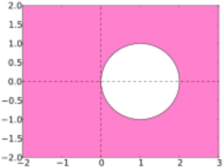
$\Rightarrow$ complex plane except for a disc of radius 1 centered at $z = 1$

Stability regions of different methods

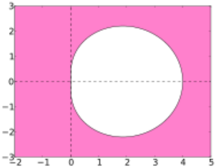
We can illustrate A-stability by coloring the points $\lambda\Delta t \in \mathbb{C}$ for which different methods are stable for the problem $u'(t) = \lambda u(t)$:



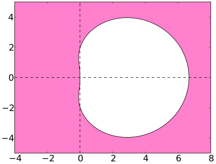
Forward Euler



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

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- Computational complexity
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The time stepping process

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

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- 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

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- 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