MATH 676

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Finite element methods in scientific computing

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Lecture 30.25:

Time discretizations for advection-diffusion and other problems:

IMEX, operator splitting, and other ideas

Explicit vs implicit time stepping

Recall (lectures 26-28):

- Parabolic problems, e.g. heat equation:

$$\frac{\partial u}{\partial t} - \Delta u = f$$

Implicit time stepping!

- 2nd order hyperbolic problems, e.g. wave equation:

$$\frac{\partial^2 u}{\partial t^2} - \Delta u = f$$

Explicit time stepping!

- 1st order hyperbolic problems, e.g. transport equation:

$$\frac{\partial u}{\partial t} + \vec{\beta} \cdot \nabla u = f$$

Explicit time stepping!

Questions

Questions for this lecture:

- What do we do for problems that do not fall into these neat categories?
- What are common approaches?

Explicit vs implicit time stepping

Example: What to do with advection-diffusion problems?

$$\frac{\partial u}{\partial t} + \vec{\beta}\cdot\nabla u - \Delta u = f$$

Suggests *explicit* time stepping

Suggests *implicit* time stepping

Note: Advection-diffusion equations describe processes where material/energy is transported and diffuses (water, atmosphere, etc). Diffusion is often small.

IMEX schemes

Example: What to do with advection-diffusion problems?

Answer 1: Implicit/explicit (*IMEX*) schemes

- treat transport explicitly
- treat diffusion implicitly

$$\frac{\partial u}{\partial t} + \vec{\beta}\cdot\nabla u - \Delta u = f$$

$$\downarrow$$

$$\frac{u^n - u^{n-1}}{k^n} + \vec{\beta}\cdot\nabla u^{n-1} - \Delta u^n = f \qquad \left(k^n = t^n - t^{n-1}\right)$$

$$\downarrow$$

$$u^n - k^n\,\Delta u^n = u^{n-1} - k^n\,\vec{\beta}\cdot\nabla u^{n-1} + k^n\,f$$

IMEX schemes

Reformulation: Such schemes are often *approximated* in a way that separate the physical effects:

$$\frac{u^n - u^{n-1}}{k^n} + \vec{\beta}\cdot\nabla u^{n-1} - \Delta u^n = f$$

$$\frac{u^n_{\text{adv}} - u^{n-1}}{k^n} + \vec{\beta}\cdot\nabla u^{n-1} = 0$$

$$\frac{u^n_{\text{diff}} - u^{n-1}}{k^n} - \Delta u^n_{\text{diff}} = 0$$

$$\frac{u^n_{\text{source}} - u^{n-1}}{k^n} = f$$

$$\frac{u^n - u^{n-1}}{k^n} = \frac{u^n_{\text{adv}} - u^{n-1}}{k^n} + \frac{u^n_{\text{diff}} - u^{n-1}}{k^n} + \frac{u^n_{\text{source}} - u^{n-1}}{k^n}$$

IMEX schemes

Reformulation: Such schemes are often *approximated* in a way that separate the physical effects:

$$\frac{u^n - u^{n-1}}{k^n} + \vec{\beta} \cdot \nabla u^{n-1} - \Delta u^n = f$$

$$\delta u^n_{\text{adv}} = -k^n \; \vec{\beta} \cdot \nabla u^{n-1}$$

$$\delta u^n_{\text{diff}} = k^n \; \Delta \left(u^{n-1} + \delta u^n_{\text{diff}} \right)$$

$$\delta u^n_{\text{source}} = k^n \; f$$

$$u^n = u^{n-1} + \delta u^n_{\text{adv}} + \delta u^n_{\text{diff}} + \delta u^n_{\text{source}}$$

IMEX schemes

Reformulation: Such schemes are often *approximated* in a way that separate the physical effects:

$$u^n = u^{n-1} + \delta u^n_{\text{adv}} + \delta u^n_{\text{diff}} + \delta u^n_{\text{source}}$$

- Computing increments can be done independently:
  – concurrently (in parallel)
  – by separate codes
- Source contribution may be included into the other solves
- Scheme can be generalized to higher order

Operator splitting schemes

Example: What to do with advection-diffusion problems?

Answer 2: Operator splitting schemes solve for one physical effect *after* the other.

With operator splitting, we can also
- treat transport explicitly
- treat diffusion implicitly

Note: IMEX treats terms concurrently, operator splitting sequentially.

Operator splitting schemes

Formulation: Operator splitting schemes separate the physical effects:

$$\frac{u^n - u^{n-1}}{k^n} + \vec{\beta}\cdot\nabla u^{n-1} - \Delta u^n = f$$

$$\frac{u^n_{\text{adv}} - u^{n-1}}{k^n} + \vec{\beta}\cdot\nabla u^{n-1} = 0$$

$$\frac{u^n_{\text{diff}} - u^n_{\text{adv}}}{k^n} - \Delta u^n_{\text{diff}} = 0$$

$$\frac{u^n_{\text{source}} - u^{n-1}_{\text{diff}}}{k^n} = f$$

$$u^n = u^n_{\text{source}}$$

This method is called “Lie” splitting

Operator splitting schemes

Formulation: Operator splitting schemes separate the physical effects.

- Computing 3 increments can be done
  – independently
  – by separate codes
- Source contribution may be included into the other solves

- The Lie scheme is only first order in k^n
- Scheme can be generalized to second order (“Strang splitting”)

Operator splitting schemes

Example: Consider the reaction of 3 species

$$A + B \rightarrow C$$

in a reactor. A simple model would be

- Solution variable: $u(x,t) = \{u_A(x,t), u_B(x,t), u_C(x,t)\}$
- Equation: $$\frac{\partial \vec{u}}{\partial t} - \Delta \vec{u} = \vec{f}(\vec{u})$$
- Reaction terms: $$\vec{f}(\vec{u}) = \begin{pmatrix} -k u_A u_B \\ -k u_A u_B \\ +k u_A u_B \end{pmatrix}$$

Operator splitting schemes

Example: Consider the equation

$$\frac{\partial \vec{u}}{\partial t} - \Delta \vec{u} = \vec{f}(\vec{u})$$

Here:

- One term is a spatial process (diffusion, a PDE)
- One term is a local process (reaction, an ODE)

- We may have different codes that are specialized in each process

Operator splitting schemes

Example: Consider the equation

$$\frac{\partial \vec{u}}{\partial t} - \Delta \vec{u} = \vec{f}(\vec{u})$$

First order operator splitting ("Lie splitting"):

- First account for the effect of one time step's worth of diffusion (implicit):

$$\frac{\vec{u}^{*} - \vec{u}^{n-1}}{k^n} - \Delta \vec{u}^{*} = 0$$

- Then account for one time step's worth of reactions (local ODE):

$$\frac{\partial \vec{u}^{**}}{\partial t} = \vec{f}(\vec{u}^{**}), \quad \vec{u}^{**}(t_{n-1}) = \vec{u}^{*} \quad \rightarrow \quad \vec{u}^{n} = \vec{u}^{**}(t_n)$$

- The order could of course be reversed.

Operator splitting schemes

Example: Consider the equation

$$\frac{\partial \vec{u}}{\partial t} - \Delta \vec{u} = \vec{f}(\vec{u})$$

Second order operator splitting ("Strang splitting"):

- Half diffusion step:

$$\frac{\vec{u}^{*} - \vec{u}^{n-1}}{k^n/2} - \Delta \vec{u}^{*} = 0$$

- Full reaction step:

$$\frac{\partial \vec{u}^{**}}{\partial t} = \vec{f}(\vec{u}^{**}), \qquad \vec{u}^{**}(t_{n-1}) = \vec{u}^{*} \qquad \rightarrow \text{solve for } \vec{u}^{**}(t_n)$$

- Half diffusion step:

$$\frac{\vec{u}^{n} - \vec{u}^{**}(t_n)}{k^n/2} - \Delta \vec{u}^{n} = 0$$

- The order of sub-steps can be reversed.

More accuracy

Background, part 1: Both IMEX and Operator Splitting schemes need to discretize the time derivative

$$\frac{\partial \vec{u}}{\partial t}$$

This can be done in many ways, for example:

- Simplest approximation (Euler, BDF-1, ...)

$$\frac{\partial u}{\partial t} \approx \frac{u^{\mathrm{n}} - u^{n-1}}{k}$$

- BDF-2

$$\frac{\partial u}{\partial t} \approx \frac{\frac{3}{2} u^{\mathrm{n}} - 2 u^{n-1} + \frac{1}{2} u^{n-2}}{k}$$

More accuracy

Background, part 2: We need to approximate *explicit terms* in equations such as

$$\frac{\partial u}{\partial t} + \vec{\beta} \cdot \nabla u - \Delta u = f$$

This can be done in many ways, for example:

- Explicit Euler

$$\frac{u^n - u^{n-1}}{k^n} + \vec{\beta} \cdot \nabla u^{n-1} - \Delta u^n = f$$

- Two-step (explicit) extrapolation

$$\frac{u^n - u^{n-1}}{k^n} + \vec{\beta} \cdot \nabla \left(u^{n-1} + k^n \frac{u^{n-1} - u^{n-2}}{k^{n-1}} \right) - \Delta u^n = f$$

Summary

Many important, time-dependent equations are not purely

- parabolic
- Hyperbolic.

For these equations, one often wants to treat

- some terms explicitly
- some terms implicitly
- treat different physical effects separately.

There are many ways of doing this (e.g., IMEX, Operator Splitting) and many variations to achieve higher order accuracy.

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