## **MATH 676**

# Finite element methods in scientific computing

Wolfgang Bangerth, Texas A&M University

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### Lecture 30.25:

### Time discretizations for advectiondiffusion and other problems:

### IMEX, operator splitting, and other ideas

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# Explicit vs implicit time stepping

### Recall (lectures 26-28):

• Parabolic problems, e.g. heat equation:

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

 2<sup>nd</sup> order hyperbolic problems, e.g. wave equation:

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

 1<sup>st</sup> order hyperbolic problems, e.g. transport equation:

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

Implicit time stepping!

Explicit time stepping!

Explicit time stepping!

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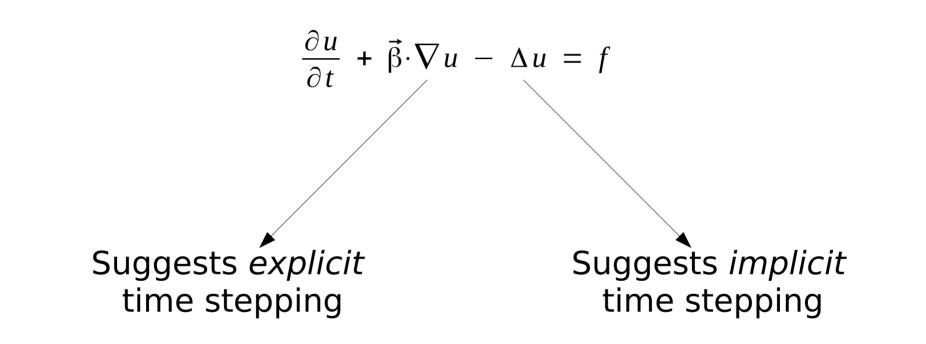
### Questions

**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?



**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

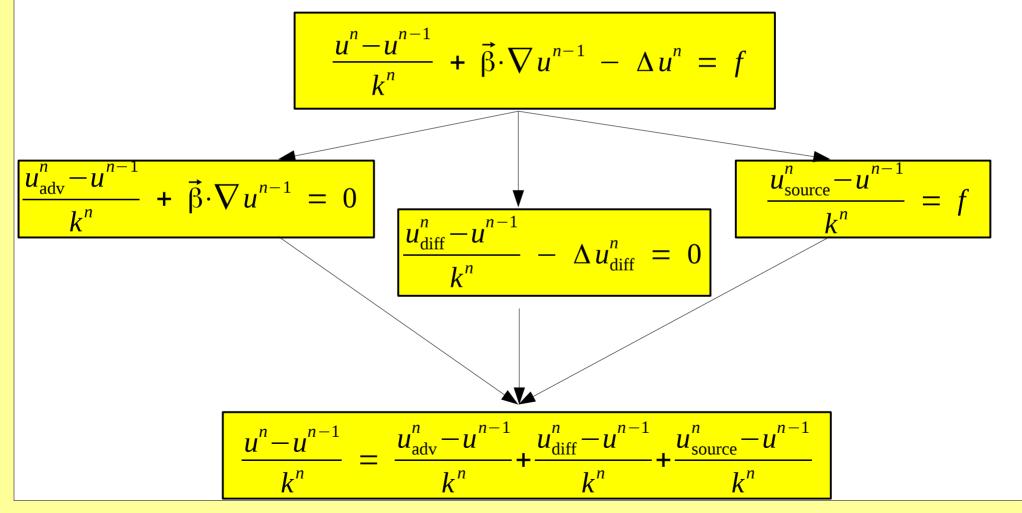
$$\frac{\partial u}{\partial t} + \vec{\beta} \cdot \nabla u - \Delta u = f$$

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

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

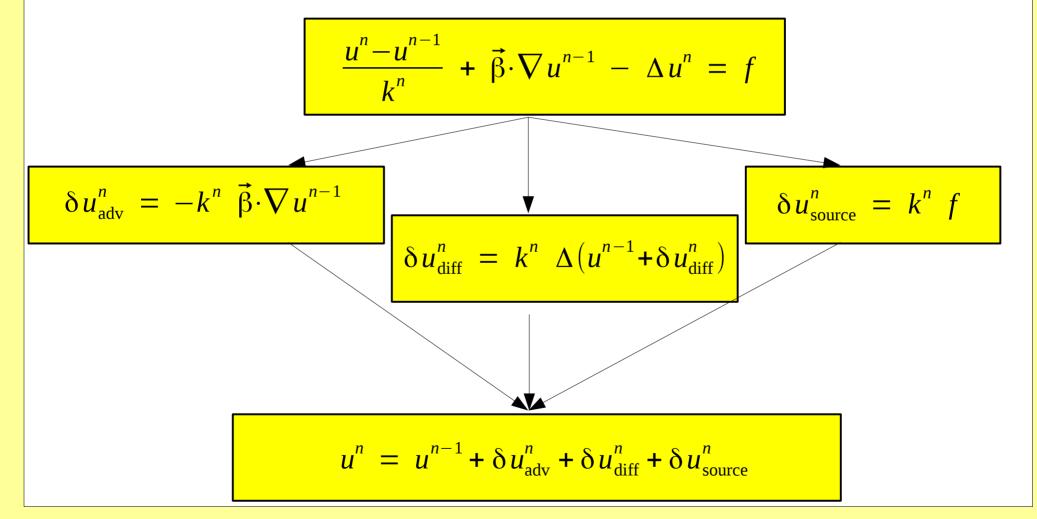
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**Reformulation:** Such schemes are often *approximated* in a way that separate the physical effects:



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

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

- 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

**Example:** What to do with advection-diffusion problems?

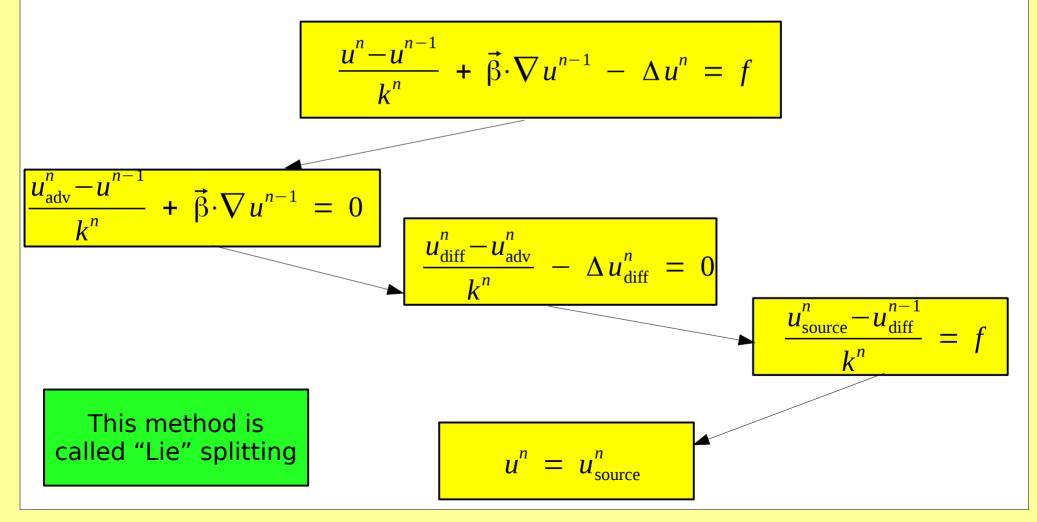
**Answer 2:** Operator splitting schemes solve for one physical effect *after* the other.

With operator splitting, we can also

- treat transport explicitly
- treat diffusion implicitly

**Note:** IMEX treats terms concurrently, operator splitting sequentially.

**Formulation:** Operator splitting schemes separate the physical effects:



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**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")

**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:** •  $\vec{f}(\vec{u}) = \begin{pmatrix} -ku_A u_B \\ -ku_A u_B \\ +ku_A u_B \end{pmatrix}$ 

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**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

**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.

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**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:

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

• Half diffusion step:

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

• The order of sub-steps can be reversed.

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**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, ...)

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

• BDF-2

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

**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

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

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# 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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