Outline

- Semi-discretization
  - Discretizing derivatives
  - Staggered meshes and finite volumes
  - Handling boundary conditions

- Full discretization
  - Order, stability and convergence
  - General stability
Consider the linear initial-value PDE

\[ u_t = Lu + q, \quad x \in \Omega, \ t > 0 \]
\[ u(0, x) = u_0(x). \]

Discretizing on a mesh in space, obtain

\[ \frac{d}{dt} v_j(t) = \sum_{i=-l}^{r} \alpha_i v_{j+i}(t) \]
\[ v_j(0) = u_0(x_j), \quad 1 \leq j \leq J. \]

Leads to a method of lines (MOL), for which techniques from Chapter 2 may be applied.
Semi-discretization

Discretizing derivatives

**Spatial semi-discretization: example**

- **A diffusion problem**

  \[ u_t = u_{xx} + q(x, u), \]
  \[ u(0, x) = u_0(x), \quad u(t, 0) = g_0(t), \quad u(t, 1) = g_1(t). \]

- **Discretize in space using a uniform mesh width** \( h \), obtaining
  \((l = r = 1 \text{ and } v_j(0) = u_0(jh))\)

  \[ \frac{d v_j}{dt} = \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2} + q(x_j, v_j), \quad j = 1, \ldots, J. \]

- **Use boundary conditions to close the system, setting**
  \( v_0(t) = g_0(t), \quad v_{J+1}(t) = g_1(t). \)

  **Obtain a mildly stiff initial-value ODE system of size** \( J \).
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DIFFERENCE OPERATOR NOTATION

Use the following difference operator notation in space or time:

\[ D_+ u_j = u_{j+1} - u_j \quad \text{Forward} \]
\[ D_- u_j = u_j - u_{j-1} \quad \text{Backward} \]
\[ D_0 u_j = u_{j+1} - u_{j-1} \quad \text{Long centered} \]
\[ \delta u_j = u_{j+1/2} - u_{j-1/2} \quad \text{Short centered} \]
\[ \mu u_j = (u_{j+1/2} + u_{j-1/2})/2 \quad \text{Short average} \]
\[ E u_j = u_{j+1} \quad \text{Translation.} \]

Difference operator identities:

\[ D_+ = E - I, \quad D_- = I - E^{-1}, \]
\[ D_+ D_- = D_- D_+ = \delta^2, \]
\[ \mu^2 = 1 + \delta^2/4, \quad \mu \delta = D_0/2, \]
\[ \partial x = h^{-1} \log E \]
**Difference operator notation**

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FORMULAE FOR FIRST DERIVATIVE

● $u_x$, one-sided:

$$u_x = \frac{1}{h} \left( D_+ - \frac{1}{2} D_+^2 \right) u + O(h^2)$$

$$= \frac{1}{h} (u_{j+1} - u_j) - \frac{1}{2h} (u_{j+2} - 2u_{j+1} + u_j) + O(h^2)$$

Just the first term above leads to the 1st order forward difference.

● $u_x$, symmetric, centred:

$$u_x = \frac{D_0}{2h} \left( I - \frac{1}{6} D_+D_- \right) u + O(h^4)$$

$$= \frac{1}{2h} (u_{j+1} - u_{j-1}) - \frac{1}{12h} (u_{j+2} - 2u_{j+1} + 2u_{j-1} - u_{j-2}) + O(h^4)$$

Just the first term above leads to the 2nd order centred difference.
**Formulae for first derivative**

- **$u_x$, one-sided:**

  \[
  u_x = \frac{1}{h} \left( D_+ - \frac{1}{2} D_+^2 \right) u + \mathcal{O}(h^2)
  \]

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  = \frac{1}{h} (u_{j+1} - u_j) - \frac{1}{2h} (u_{j+2} - 2u_{j+1} + u_j) + \mathcal{O}(h^2)
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**Formulae**

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  \[ u_{xx} = \frac{1}{h^2} \left( \delta^2 - \frac{1}{12} \delta^4 \right) u + O(h^4). \]

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- Implicit schemes for discretizing derivatives exist as well, e.g. to obtain 4th order accurate 3-point formulae.

- For explicit scheme, need polynomial of degree $l$ for $l$th derivative. So, at least $l + 1$ points must be used. If exactly $l + 1$ points are used, the scheme is compact. This is a desirable property.
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In general, we want as narrow a discretization stencil as possible, because:

- Generally, boundary conditions are more easily incorporated.
- Occasionally, unwanted spurious solution behaviour is avoided.

E.g., for \( u_x = \frac{u_{j+1} - u_{j-1}}{2h} \), consider a sinusoidal fluctuation

\[
\{u_j\} = 0, 1, 0, -1, 0, 1, 0, -1, \ldots
\]

Then on a coarser mesh consisting of only the odd mesh points, \( u_x \) is approximated by identically 0.
Compact schemes

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STAGGERED MESHES

To avoid using long differences, consider unknowns corresponding to different solution components to be located at different meshes: It’s all in our head

Example: diffusion equation in 1D

\[ u_t = (a(x)u_x)_x + q(t, x), \quad x \in \Omega, \ t \geq 0. \]

Do not write \((au_x)_x = au_{xx} + a_xu_x\) ! Define flux \(w = au_x\) and discretize:

\[ a(x_{j+1/2}) \frac{v_{j+1} - v_j}{h} = w_{j+1/2}, \]

\[ \frac{dv_j}{dt} = \frac{w_{j+1/2} - w_{j-1/2}}{h} + q(t, x_j). \]

Eliminating \(w\)-values yields the semi-discretization

\[ \frac{dv_j}{dt} = h^{-1} \left[ a(x_{j+1/2}) \frac{v_{j+1} - v_j}{h} - a(x_{j-1/2}) \frac{v_j - v_{j-1}}{h} \right] + q(t, x_j). \]
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\]
Write the diffusion equation as

\[ u_x = a(x)^{-1} w, \]
\[ u_t = w_x + q(t, x). \]

Integrating first equation from \( x_j \) to \( x_{j+1} \) and using midpoint, obtain

\[ v_{j+1} - v_j = h a_{j+1/2}^{-1} w_{j+1/2}. \]

Integrating second equation from \( x_{j-1/2} \) to \( x_{j+1/2} \) and using midpoint, obtain

\[ v'_j = h^{-1} (w_{j+1/2} - w_{j-1/2}) + q_j(t). \]

Substituting, obtain

\[ v'_j \equiv \frac{dv_j}{dt} = h^{-2} \left[ a_{j+1/2} (v_{j+1} - v_j) - a_{j-1/2} (v_j - v_{j-1}) \right] + q_j(t). \]
The finite volume approach becomes important when one of the following occurs:

- The function $a(x)$ has discontinuities.
- The function $q(t, x)$ is a point source, i.e., a $\delta$-function, in $x$.
- We wish to extend the discretization to a nonuniform spatial mesh.
Discontinuous coefficients

\[ \frac{dv_j}{dt} = h^{-1}\left[ a_{j+1/2} \frac{v_{j+1} - v_j}{h} - a_{j-1/2} \frac{v_j - v_{j-1}}{h} \right] + q(t, x_j). \]

As before, but how should \( a_{j+1/2} \) be defined?

Harmonic averaging: define \( a_{j+1/2} \) by

1. Integrating \( u_x = a^{-1}(x)w \), and
2. Discretizing (note \( w \) is smoother than \( a \) and \( u_x \)):

   \[
   \text{ideally } a_{j+1/2} = h \left[ \int_{x_j}^{x_{j+1}} a^{-1} \, dx \right]^{-1} \\
   \text{often must use } a_{j+1/2} = \left[ \frac{a_j^{-1} + a_{j+1}^{-1}}{2} \right]^{-1}
   \]
\[ \frac{dv_j}{dt} = h^{-1} \left[ a_{j+1/2} \frac{v_{j+1} - v_j}{h} - a_{j-1/2} \frac{v_j - v_{j-1}}{h} \right] + q(t, x_j). \]

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If

\[ q(t, x) = \delta(x - x^*_i), \quad x^*_{i-1/2} \leq x^*_i < x^*_{i+1/2} \]

where

\[ q(t, x) = 0 \text{ if } x \neq x^*_i, \quad \int_\Omega q(t, x) dx = 1, \]

then integrating as before, obtain

\[
\frac{dv_j}{dt} = h^{-1} \left[ a_{j+1/2} \frac{v_{j+1} - v_j}{h} - a_{j-1/2} \frac{v_j - v_{j-1}}{h} \right] + hq_j(t)
\]

\[ q_j(t) = \begin{cases} 
1 & \text{if } i = i^*_j, \\
0 & \text{otherwise}.
\end{cases} \]
Discretization principles such as compactness, staggered meshes, and integrate-then-discretize are extended also to 2D and 3D.

Mesh subintervals are now replaced by mesh cells in 2D or 3D.

Not everything extends smoothly and effortlessly!

Consider examples in 2D.
Anisotropic diffusion in 2D

\[ u_t = (au_x)_x + (au_y)_y + q \equiv \nabla \cdot (a \nabla u) + q \]

on a square domain \( \Omega : 0 \leq x, y \leq 1 \).

- If \( a \) is constant, easy:
  \[
  \frac{dv_{i,j}}{dt} = \frac{a}{h^2} [-4v_{i,j} + v_{i-1,j} + v_{i+1,j} + v_{i,j-1} + v_{i,j+1}] + q_{i,j}, \quad 1 \leq i, j \leq J
  \]

- More generally, rewrite as 1st order system
  \[
  u_t = w_x^x + w_y^y + q = \nabla \cdot w + q, \\
  w = a \nabla u.
  \]

Integrate first DE over a control volume
\[
\frac{dv_{i,j}}{dt} = h^{-1} [w_{i+1/2,j}^x - w_{i-1/2,j}^x + w_{i,j+1/2}^y - w_{i,j-1/2}^y] + q_{i,j}.
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Semi-discretization

Staggered meshes and finite volumes

Anisotropic diffusion in 2D cont.

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\[
w_{i+1/2,j}^x = \int_{y_{j-1/2}}^{y_{j+1/2}} w^x(x_{i+1/2}, y) dy, \quad 1 \leq i, j \leq J.
\]

- For 2nd eqn, e.g. \( u_x = a^{-1} w^x, (w = (w^x, w^y)) \), integrate in \( x \), but where in \( y \)?!
- Obtain

\[
\frac{d v_{i,j}}{dt} = h^{-2} \left[ a_{i+1/2,j} (v_{i+1,j} - v_{i,j}) - a_{i-1/2,j} (v_{i,j} - v_{i-1,j}) \right.
\]
\[
+ a_{i,j+1/2} (v_{i,j+1} - v_{i,j}) - a_{i,j-1/2} (v_{i,j} - v_{i,j-1}) \right] + q_{i,j},
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where, e.g.,

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Anisotropic diffusion in 2D cont.

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**Example: isotropic denoising**

- An image is polluted by noise, resulting in $u_0(x, y)$.
- Want to denoise it, i.e., recover $u$ – something close to the original (unavailable) image.
- **Isotropic diffusion:** Solve
  
  $$u_t = u_{xx} + u_{yy},$$
  $$u(0, x, y) = u_0(x, y),$$

  for appropriate $t$ not too small and not too large!

- Difficulty: image edges are indiscriminantly smoothed, too. (Recall integration of heat equation starting with a step function, Fig. 1.4.)
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INSTANCE: CAMERA MAN

True model

Data with 20% noise

Modified TV - fixed $\epsilon = 4$

Modified TV - fixed $\epsilon = 3000$
Anisotropic denoising

- Smooth only in directions where $u$ does not vary too abruptly!
- One way: total variation (TV).

$$u_t = \nabla \cdot \left( \frac{\nabla u}{|\nabla u|} \right),$$

$$u(0, x, y) = u_0(x, y).$$

- “Like before” with

$$a = a(u) = 1 / |\nabla u|,$$

where $|\nabla u| = \sqrt{u_x^2 + u_y^2}$.

(The latter expression is modified in regions where $u$ is very flat.)

- Common choice

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- Does not always look great, but often works well.
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(The latter expression is modified in regions where $u$ is very flat.)

- Common choice

$$a_{i+1/2,j} = a_{i,j+1/2} = h \left[ (u_{i+1,j} - u_{i,j})^2 + (u_{i,j+1} - u_{i,j})^2 \right]^{-1/2}.$$

- Does not always look great, but often works well.
Outline

- Semi-discretization
  - Discretizing derivatives
  - Staggered meshes and finite volumes
  - Handling boundary conditions
- Full discretization
  - Order, stability and convergence
  - General stability
Boundary conditions (BC)

- In 1D

\[ u_t = u_{xx}, \quad 0 \leq x \leq 1, \ t > 0, \]
\[ u(0, x) = u_0(x). \]

- Dirichlet BC: \( u(t, 1) = g_1(t) \)
- Neumann BC: \( \frac{\partial u}{\partial x}(t, 0) = g_0(t) \).

- Discretization:

\[
\frac{dv_j}{dt} = \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2}, \quad j = 0, 1, \ldots, J, \\
v_{J+1} = g_1(t), \\
v_{1} - v_{-1} \quad \frac{2h}{2h} = g_0(t).
\]

- How to handle the ghost unknown \( v_{-1} \)?
**Boundary conditions (BC)**

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\[ \frac{v_1 - v_{-1}}{2h} = g_0(t). \]

- How to handle the ghost unknown \( v_{-1} \)?
**Handling Neumann BC**

- Concentrate on Neumann BC at the left interval end:
  \[
  \frac{dv_0}{dt} = \frac{v_1 - 2v_0 + v_{-1}}{h^2},
  \]
  \[
  \frac{v_1 - v_{-1}}{2h} = g_0(t).
  \]

- Eliminate ghost unknown: \( v_{-1} = v_1 - 2hg_0(t) \). Substitute into difference eqn at \( j = 0 \):
  \[
  \frac{dv_0}{dt} = \frac{2v_1 - 2v_0 - 2hg_0(t)}{h^2}.
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- Alternatively, do not eliminate: solve differential-algebraic equations DAE in time.
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\]

- Alternatively, do not eliminate: solve differential-algebraic equations (DAE) in time.
Consider example: simplest heat equation

\[ u_t = u_{xx} + u_{yy}. \]

- Dirichlet, boundary part of grid: extend directly.
- Neumann, boundary part of grid: extend in finite volume fashion. (Often in practice BC is on the flux, \( w \).)
Natural and essential BC

- Consider Ritz formulation of elliptic PDE

\[
\min_u \int_{\Omega} \left[ a|\nabla u|^2 + bu^2 - 2uq \right] \, dxdy,
\]

\(a(x, y) > 0, \ b(x, y) \geq 0.\)

- Necessary condition for minimum are the Euler-Lagrange equations

\[-\nabla \cdot (a \nabla u) + bu = q, \quad \text{in} \ \Omega,\]

\[\frac{\partial u}{\partial n}|_{\partial \Omega} = 0.\]

So Neumann BC are natural!

- More generally, given Neumann (natural) conditions on part of the boundary and Dirichlet (essential) on the rest, in the functional minimization formulation only the essential BC must be explicitly imposed.
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- More generally, given **Neumann** (natural) conditions on part of the boundary and **Dirichlet** (essential) on the rest, in the functional minimization formulation only the essential BC must be explicitly imposed.
Can discretize first and only then optimize:

\[
\min_v \sum_{i,j=0}^{J} \frac{1}{2}[a_{i+1/2,j}(v_{i+1,j} - v_{i,j})^2 + a_{i+1/2,j+1}(v_{i+1,j+1} - v_{i,j+1})^2 \\
+ a_{i,j+1/2}(v_{i,j+1} - v_{i,j})^2 + a_{i+1,j+1/2}(v_{i+1,j+1} - v_{i+1,j})^2] \\
+ \frac{h^2}{4} \sum_{i,j=0}^{J} [b_{i,j}v_{i,j}^2 - 2q_{i,j}v_{i,j} + b_{i+1,j}v_{i+1,j}^2 - 2q_{i+1,j}v_{i+1,j} \\
+ b_{i,j+1}v_{i,j+1}^2 - 2q_{i,j+1}v_{i,j+1} + b_{i+1,j+1}v_{i+1,j+1}^2 - 2q_{i+1,j+1}v_{i+1,j+1}]
\]

Necessary conditions - equate gradient to 0: obtain previous 5-point discretization plus Neumann BC automatically.

Essential BC are used to move known boundary values to right hand side of linear system.

Advantage: the obtained matrix is symmetric positive definite!
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OUTLINE

- Semi-discretization
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Full discretization (linear PDE) order, stability, convergence

**Full discretization**

- **Explicit one-step** scheme

\[ v_j^{n+1} = \sum_{i=-l}^{r} \beta_i v_{j+i}^{n}. \]

- Can write this in (potentially infinite) matrix-vector notation

\[ v^{n+1} = Qv^n \]

- **Implicit one-step** scheme

\[ \sum_{i=-l}^{r} \gamma_i v_{j+i}^{n+1} = \sum_{i=-l}^{r} \beta_i v_{j+i}^{n}, \]

- Can write concisely as

\[ Q_1 v^{n+1} = Q_0 v^n \]
Full discretization (linear PDE) order, stability, convergence

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  \[ Q_1 v^{n+1} = Q_0 v^n \]
Order of accuracy

Local truncation error:

\[ \tau(t, x) = k^{-1} \left[ \sum_{i=-l}^{r} \gamma_i u(t + k, x + ih) - \sum_{i=-l}^{r} \beta_i u(t, x + ih) \right]. \]

Pretend grid function \( v \) is defined at every point. Difference method is

- **accurate of order** \((p_1, p_2)\) if

  \[ \|\tau(t)\| = \|\tau(t, \cdot)\| \leq c(t) (k^{p_1} + h^{p_2}) \]

- **consistent** if \( \|\tau(t)\| \to 0 \) as \( k, h \to 0 \).
**Example: Heat Equation**

For heat equation \( u_t = u_{xx} \), discretize in space by centred \( O(h^2) \) scheme. Next, discretize in time:

- **Forward Euler**

  \[
  \frac{1}{k}(v_j^{n+1} - v_j^n) = \frac{1}{h^2}(v_{j+1}^n - 2v_j^n + v_{j-1}^n)
  \]

  – order \((1, 2)\).

- **Crank-Nicolson**: apply trapezoidal

  \[
  \frac{1}{k}(v_j^{n+1} - v_j^n) = \frac{1}{2h^2}(v_{j+1}^{n+1} - 2v_j^{n+1} + v_{j-1}^{n+1} + v_{j+1}^n - 2v_j^n + v_{j-1}^n)
  \]

  – order \((2, 2)\) and better stability properties, but *implicit*: must solve a tridiagonal linear system at each time step.

- **Backward Euler**? – at first glance, combines worst of both worlds, but...
Set $\mu = k/h^2$.

**Forward Euler:**

$$v_{j}^{n+1} = v_{j}^{n} + \mu D_+ D_- v_{j}^{n}$$

**Trapezoidal (CN):**

$$v_{j}^{n+1} = v_{j}^{n} + \frac{\mu}{2} D_+ D_- (v_{j}^{n} + v_{j}^{n+1})$$

**Backward Euler:**

$$v_{j}^{n+1} = v_{j}^{n} + \mu D_+ D_- v_{j}^{n+1}$$
Stability and Convergence

Method is

- **stable** if there are constants \( \tilde{K} \) and \( \tilde{\alpha} \) such that
  \[
  \|v(t)\| \leq \tilde{K} e^{\tilde{\alpha} t} \|v(0)\|.
  \]

- **convergent** if
  \[
  u(t, x) - v(t, x) \to 0, \quad k, h \to 0.
  \]

Lax Equivalence Theorem:
If the linear evolutionary PDE is well-posed and the difference method is consistent then

\[
\text{convergence} \iff \text{stability}.
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In fact, if the method is stable then the solution error inherits the order of accuracy.
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**Lax Equivalence Theorem:**
If the linear evolutionary PDE is well-posed and the difference method is consistent then

convergence $\iff$ stability.

In fact, if the method is stable then the solution error inherits the order of accuracy.
**General linear stability**

- Generally, with $Q = Q_1^{-1}Q_0$, can write
  \begin{align*}
  v^{n+1} &= Q(nk, h)v^n = \cdots = \prod_{l=0}^n Q(lk, h)v^0 = S_{k,h}(t_{n+1}, 0)v^0.
  \end{align*}

- The stability condition is
  \[
  \|\prod_{l=0}^n Q(lk, h)\| \leq \tilde{K}e^{\tilde{\alpha}nk} \quad \forall n, k, \ nk \leq t_f.
  \]

- If $Q$ does not depend on $t$
  \[
  \|Q(h)^n\| \leq \tilde{K}e^{\tilde{\alpha}nk}.
  \]

- This is satisfied if for all $k$ and $h$ small enough,
  \[
  \|Q\| \leq e^{\tilde{\alpha}k} = 1 + O(k).
  \]
Difficult in general to show that $\|Q^n\| \leq \bar{K}$. Fortunately, can sometimes ignore lower order derivatives:

**Theorem:** If the scheme

$$v^{n+1} = \hat{Q}v^n$$

is stable and $\tilde{Q}$ is a bounded operator then the scheme

$$v^{n+1} = (\hat{Q} + k\tilde{Q})v^n$$

is stable as well.

Good for $u_t = u_x + b(x)u$ and for $u_t = u_{xx} + bu$, but not for $u_t = u_{xx} + au_x$. 
Low order terms

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