Lecture 2

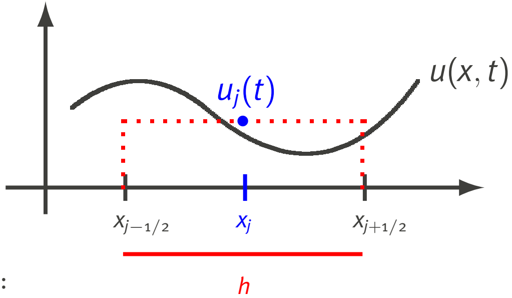
The Heat Equation

Finite Volume Discretization - 1D

Finite Volume Discretization - Preliminaries

- general ideas & notation
- only do space - times discretization later

Continuous case with $x_{j-1/2} = x_j - \frac{h}{2}$ and $x_{j+1/2} = x_j + \frac{h}{2}$:



Cell average:

$$u_j(t) := \frac{1}{h}\int_{C_j} u(x,t)\,dx \qquad \text{with cell } C_j := [x_{j-1/2}, x_{j+1/2}].$$

Finite Volume Discretization - Preliminaries

Interpretation as point approximation

- $u = u(x,t) : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$
- For $x_{j-1/2} = x_j - \frac{h}{2}$ and $x_{j+1/2} = x_j + \frac{h}{2}$ define cell average
$$u_j(t) := \frac{1}{h} \int_{C_j} u(x,t)\, dx \qquad \text{with cell } C_j := [x_{j-1/2}, x_{j+1/2}].$$
- Note: if $u(x,t)$ is smooth, $u_j(t)$ can be seen as 2nd order approx. of $u(x_j,t)$.

Midpoint rule:
$$\int_{C_j} u(x,t)\, dx = h u(x_j,t) + \mathcal{O}(h^3).$$

Hence:
$$u_j(t) = \frac{1}{h} \int_{C_j} u(x,t)\, dx = u(x_j,t) + \mathcal{O}(h^2).$$

Finite Volume Discretization - Motivation

Consider u that fulfills a conservation law, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V u = -\int_{\partial V} \mathbf{F}\cdot\mathbf{n} = -\int_V \nabla\cdot\mathbf{F},$$

for some test volume V and a flux $\mathbf{F}$.

In 1d we can write $\mathbf{F} = f$ for some scalar flux function f.

We have for $V = C_j$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{C_j} u(x,t)\,dx = -\left(f(x_{j+1/2},t) - f(x_{j-1/2},t)\right),$$

We obtain the exact conservation relation on cell C_j with

$$\frac{\mathrm{d}}{\mathrm{d}t}u_j(t) = -\frac{1}{h}\left(f(x_{j+1/2},t) - f(x_{j-1/2},t)\right),$$

Finite Volume Discretization - Motivation

Starting from the exact conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t} u_j(t) = -\frac{1}{h}\left(f(x_{j+\frac{1}{2}}, t) - f(x_{j-+\frac{1}{2}}, t) \right),$$

we introduce a suitable discretization.

- $Q_j(t) \approx u_j(t)$ approximation of cell average.
- $F_{j-\frac{1}{2}}(t) \approx f(x_{j-\frac{1}{2}}, t)$ and $F_{j+\frac{1}{2}}(t) \approx f(x_{j+\frac{1}{2}}, t)$ approximation of flux function.
- Depending on
  - approximation of flux and
  - time discretizations

  we obtain <u>different numerical schemes</u>.

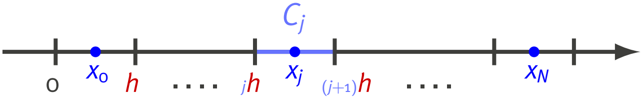
Finite Volume Discretization - Heat equation in 1d

We apply this to the heat equation in 1d:

$$
\begin{aligned}
\partial_t u(x,t) - \partial_x(k(x)\partial_x u(x,t)) &= S(x,t) && \text{for } 0 \le x \le 1, \quad t > 0,\\
u(x,0) &= v(x) && \text{for } 0 \le x \le 1,\\
\partial_{\mathbf{n}} u(0,t) = \partial_{\mathbf{n}} u(1,t) &= 0 && \text{for } t > 0.
\end{aligned}
$$

Flux function $f(x,t) = k(x)\partial_x u(x,t)$.

1. Discretize in space into N cells of size $h = 1/N$.



Here $x_j = \frac{h}{2} + jh$ for $j = 0, 1, 2, \dots, N-1$.

Finite Volume Discretization - Heat equation in 1d

2. Derive exact update formula as follows.

Conservation law on C_j scaled with $1/h$:

$$\underbrace{\frac{1}{h}\int_{C_j}\partial_t u(x,t)\,dx}_{=\partial_t u_j(t)} - \underbrace{\frac{1}{h}\int_{C_j}\partial_x(k(x)\partial_x u(x,t))\,dx}_{=(*)} = \underbrace{\frac{1}{h}\int_{C_j}S(x,t)\,dx}_{=:S_j(t)} \quad \text{(local mean)}$$

We have:

$$(*) = \frac{1}{h}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}}\partial_x(k(x)\partial_x u(x,t))\,dx = \frac{1}{h}\left(k(x_{j+\frac{1}{2}})\partial_x u(x_{j+\frac{1}{2}},t) - k(x_{j-\frac{1}{2}})\partial_x u(x_{j-\frac{1}{2}},t)\right)$$

With flux function $f_j(t) := -k(x_j)\partial_x u(x_j,t)$ we have

$$(*) = -\frac{1}{h}\left(f_{j+\frac{1}{2}}(t) - f_{j-\frac{1}{2}}(t)\right).$$

Hence:

$$\frac{\mathrm{d}}{\mathrm{d}t}u_j(t) + \frac{1}{h}\left(f_{j+\frac{1}{2}}(t) - f_{j-\frac{1}{2}}(t)\right) = S_j(t).$$

Finite Volume Discretization - Heat equation in 1d

3. Approximation of equation as follows (for smooth u).

$$f_{j+\frac{1}{2}}(t) = -k(x_{j+\frac{1}{2}})\partial_x u(x_{j+\frac{1}{2}}, t) = -k(x_{j+\frac{1}{2}})\frac{u_{j+1}(t) - u_j(t)}{h} + \mathcal{O}(h^2).$$

Approximation: drop $\mathcal{O}(h^2)$ by replacing u_j with approximation Q_j

$$f_{j+\frac{1}{2}}(t) \approx F_{j+\frac{1}{2}}(t) := -\underbrace{k(x_{j+\frac{1}{2}})}_{=:k_{j+\frac{1}{2}}}\frac{Q_{j+1}(t) - Q_j(t)}{h}.$$

Hence from 2., i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}u_j(t) + \frac{1}{h}\left(f_{j+\frac{1}{2}}(t) - f_{j-\frac{1}{2}}(t)\right) = S_j(t),$$

we derive for inner points $j = 1, \ldots, N-2$ the approximation rule

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_j(t) - \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(Q_{j+1}(t) - Q_j(t)) - k_{j-\frac{1}{2}}(Q_j(t) - Q_{j-1}(t))\right) = S_j(t).$$

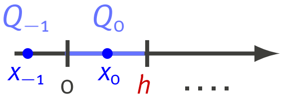
This is a a 2nd order accurate approximation (compare FD).

Finite Volume Discretization - Heat equation in 1*d*

4. **Boundary conditions.**

Approximation $Q_0(t)$ formally requires $Q_{-1}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_j(t) - \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(Q_{j+1}(t) - Q_j(t)) - k_{j-\frac{1}{2}}(Q_j(t) - Q_{j-1}(t))\right) = S_j(t).$$



Boundary does not coincide with nodes $\Rightarrow$ use ghost points.

- Example 1. Dirichlet BC $u(0,t) = 0$:

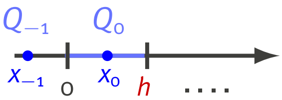
$$u(0,t) \approx \frac{Q_0 + Q_{-1}}{2} = 0 \qquad \Rightarrow \qquad Q_{-1} = -Q_0.$$

Finite Volume Discretization - Heat equation in 1d

4. Boundary conditions.

Approximation $Q_0(t)$ formally requires $Q_{-1}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_j(t) - \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(Q_{j+1}(t) - Q_j(t)) - k_{j-\frac{1}{2}}(Q_j(t) - Q_{j-1}(t))\right) = S_j(t).$$



Boundary does not coincide with nodes $\Rightarrow$ use ghost points.

- Example 2. Neumann BC $\partial_x u(0,t) = 0$:

$$\partial_x u(0,t) = \frac{u(x_0,t) - u(x_{-1},t)}{h} + \mathcal{O}(h^2) \approx \frac{Q_0 - Q_{-1}}{h} = 0$$

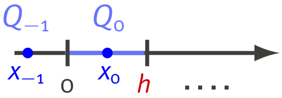
$$\Rightarrow Q_{-1} = Q_0.$$

Finite Volume Discretization - Heat equation in $1d$

4. Boundary conditions.

Approximation $Q_0(t)$ formally requires $Q_{-1}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_j(t) - \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(Q_{j+1}(t) - Q_j(t)) - k_{j-\frac{1}{2}}(Q_j(t) - Q_{j-1}(t))\right) = S_j(t).$$



Boundary does not coincide with nodes $\Rightarrow$ use ghost points.

- Example 3. Neumann BC $\partial_x u(0,t) = -1$:

$$\partial_x u(0,t) \approx \frac{Q_0 - Q_{-1}}{h} = -1$$

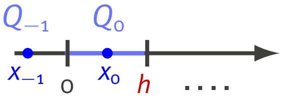
$\Rightarrow Q_{-1} = Q_0 + h.$

Finite Volume Discretization - Heat equation in 1d

4. Boundary conditions.

Approximation $Q_0(t)$ formally requires $Q_{-1}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_j(t) - \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(Q_{j+1}(t) - Q_j(t)) - k_{j-\frac{1}{2}}(Q_j(t) - Q_{j-1}(t))\right) = S_j(t).$$



Ghost points for the case Neumann BC $\partial_x u(0,t) = 0$.

We derived: $Q_{-1} = Q_0$. Hence

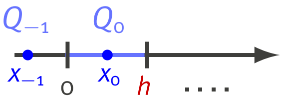
$$\frac{\mathrm{d}}{\mathrm{d}t}Q_0(t) = \frac{1}{h^2}\left(k_{\frac{1}{2}}(Q_1(t) - Q_0(t)) - k_{-\frac{1}{2}}(Q_0(t) - Q_{-1}(t))\right) + S_0(t)$$
$$= \frac{k_{\frac{1}{2}}}{h^2}(Q_1(t) - Q_0(t)) + S_0(t).$$

Finite Volume Discretization - Heat equation in 1d

4. Boundary conditions.

Approximation $Q_{N-1}(t)$ formally requires $Q_N(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_j(t) - \frac{1}{h^2}\left(k_{j+\frac{1}{2}}(Q_{j+1}(t) - Q_j(t)) - k_{j-\frac{1}{2}}(Q_j(t) - Q_{j-1}(t))\right) = S_j(t).$$



Ghost points for the case Neumann BC $\partial_x u(1,t) = 0$.

Analogously: $Q_N = Q_{N-1}$. Hence

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_{N-1}(t) = \frac{k_{N-\frac{3}{2}}}{h^2}(Q_{N-2}(t) - Q_{N-1}(t)) + S_{N-1}(t).$$

Finite Volume Discretization - Heat equation in 1d

5. Assemble linear system of ordinary differential equations for $Q_j(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Q} = \mathbf{A}\mathbf{Q} + \mathbf{S},$$

where

$$\mathbf{Q}(t) = \begin{pmatrix} Q_0(t) \\ Q_1(t) \\ \vdots \\ Q_{N-1}(t) \end{pmatrix} \quad \text{and} \quad \mathbf{S}(t) = \begin{pmatrix} S_0(t) \\ S_1(t) \\ \vdots \\ S_{N-1}(t) \end{pmatrix} \quad \text{and}$$

$\mathbf{A} \in \mathbb{R}^{N\times N}$ is tri-diagonal matrix with elements given by coefficients in front of Q_j's:

$$\mathbf{A} = \frac{1}{h^2}\begin{pmatrix} -k_{\frac{1}{2}} & k_{\frac{1}{2}} & 0 & \dots & \dots & \dots & 0 \\ k_{\frac{3}{2}} & -(k_{\frac{3}{2}} + k_{\frac{1}{2}}) & k_{\frac{1}{2}} & 0 & \dots & \dots & 0 \\ 0 & k_{\frac{5}{2}} & -(k_{\frac{5}{2}} + k_{\frac{3}{2}}) & k_{\frac{3}{2}} & 0 & \dots & 0 \\ & & \ddots & \ddots & \ddots & & 0 \\ 0 & \dots & \dots & \dots & 0 & k_{N-\frac{3}{2}} & -k_{N-\frac{3}{2}} \end{pmatrix}.$$

Finite Volume Discretization - Heat equation in 1d

5. Assemble linear system of ordinary differential equations for $Q_j(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Q} = \mathbf{A}\mathbf{Q} + \mathbf{S}.$$

Time integration *(simple)*.

Forward Euler:

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t\, \mathbf{A}\mathbf{Q}^n + \triangle t\, \mathbf{S}.$$

Backward Euler:

$$\begin{aligned} \mathbf{Q}^{n+1} &= \mathbf{Q}^n + \triangle t\, \mathbf{A}\mathbf{Q}^{n+1} + \triangle t\, \mathbf{S} \\ \Rightarrow \qquad (\mathrm{Id} - \triangle t\mathbf{A})\mathbf{Q}^{n+1} &= \mathbf{Q}^n + \triangle t\, \mathbf{S} \\ \Rightarrow \qquad \mathbf{Q}^{n+1} &= (\mathrm{Id} - \triangle t\mathbf{A})^{-1}\left(\mathbf{Q}^n + \triangle t\, \mathbf{S}\right). \end{aligned}$$

Finite Volume Discretization - Heat equation in $1d$

5. Assemble linear system of ordinary differential equations for $Q_j(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Q} = \mathbf{A}\mathbf{Q} + \mathbf{S}.$$

Backward Euler: $\mathbf{Q}^{n+1} = (\mathrm{Id} - \triangle t\mathbf{A})^{-1}\,(\mathbf{Q}^n + \triangle t\,\mathbf{S})$.

Note:

- If $\mathbf{A}$ is constant only need to compute inverse once.
- Should not really compute the inverse (expensive) but rather use **LU** decomposition (see Homework) to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$:

$$\mathbf{A} = \mathbf{L}\mathbf{U} \quad \overset{\mathbf{y}:=\mathbf{U}\mathbf{x}}{\Rightarrow} \quad \mathbf{L}\mathbf{y} = \mathbf{b} \quad \Rightarrow \quad \mathbf{y} = \mathbf{L}^{-1}\mathbf{b} \quad \text{Forward substitution cheap}$$

$$\mathbf{U}\mathbf{x} = \mathbf{y} \quad \Rightarrow \quad \mathbf{x} = \mathbf{U}^{-1}\mathbf{y} \quad \text{Backward substitution cheap}$$

- For source $S(x)$ we can approximate the load $\mathbf{S}_j = \int_{C_j} S(x)\,dx$ by

$$\mathbf{S}_j = S(x_j) + \mathcal{O}(h^2).$$