

# Practical Course: Modeling, Simulation, Optimization

Week 1

**Daniël Veldman**

Chair in Dynamics, Control, and Numerics, Friedrich-Alexander-University Erlangen-Nürnberg

## Contents

- 1.A** Organization
- 1.B** 1-D Conservation laws
- 1.C** 1-D Finite differences
- 1.D** Convergence analysis for 1-D finite differences



## 1.A Organization



## Practical course: modeling, simulation, optimization

Lecturer:

- ▶ Dr. Daniël Veldman (e-mail: [daniel.veldman@math.fau.de](mailto:daniel.veldman@math.fau.de))
- ▶ Prof.dr. Enrique Zuazua (e-mail: [enrique.zuazua@fau.de](mailto:enrique.zuazua@fau.de))

### Main objective

Gain *practical* experience in modeling, simulation, and optimization for physical systems governed by partial differential equations.

Main topics:

- ▶ Modelling, analysis, simulation and/or optimization of problems in engineering or the natural sciences
- ▶ Numerical algorithms for partial differential equation models (finite differences, finite elements, etc)
- ▶ Continuous optimization and optimal control

## Structure

The course consists of two parts:

Part I: Lectures and hand-in exercises.

- Acquire basic knowledge on modeling, simulation, and optimization.

Lecture 1: Finite differences for the 1-D Poisson equation.

Lecture 2: Time discretization.

Lecture 3: 1-D Finite elements.

Lecture 4: 2-D Finite elements.

Lecture 5: Static optimization.

Lecture 6: Dynamic optimal control.

Part II: Work on final project.

- Apply the techniques from part I to a problem of your choice.

Lecture 7: Select a topic and work on modeling part.

Lecture 8: Work on modeling part.

Lecture 9: Work on simulation part.

Lecture 10: Work on simulation part.

Lecture 11: Work on simulation/optimization part.

Lecture 12: Work on simulation/optimization part.

Lecture 13: Work on simulation/optimization part.

## Grading

The course consists of two parts:

Part I: Lectures and hand-in exercises.

- ▶ For each lecture there is a corresponding MATLAB exercise.
- ▶ You hand in your solutions (notes + MATLAB code) individually (by e-mail).
- ▶ **The deadline is before the next lecture!**
- ▶ For each exercise you can get a maximum of 10 points.
- ▶ Points for Part I are computed as

$$P_1 = \frac{1}{3} \left( \max \left\{ \frac{E_1 + E_2}{2}, E_2 \right\} + \max \left\{ \frac{E_3 + E_4}{2}, E_4 \right\} + \max \left\{ \frac{E_5 + E_6}{2}, E_6 \right\} \right).$$

Part II: Work on final project.

- ▶ You are allowed to do the final project in groups of 2.
- ▶ You write a report of 10-15 pages together.
- ▶ You hand in the report and MATLAB code (by e-mail) by **July 31st**.
- ▶ You can again get a maximum of 10 points for the report.

The final grade is computed based on the weighted sum:

$$P = 0.2P_1 + 0.8P_2.$$

$P = 10$  will lead to a 1,0.  $P = 6$  will lead to a grade around 4,0.

## Obtaining MATLAB

You need to use MATLAB to complete the hand-in exercises  
and to do the simulations for the final report.

You can use MATLAB in two ways:

- ▶ On your laptop
  - ▷ The FAU has a campus license for MATLAB.
  - ▷ Every student can install MATLAB for free on their own laptop/PC.
  - ▷ <https://de.mathworks.com/academia/tah-portal/fau-31563700.html>
- ▶ On the computers in the PC-Pools of the Department of Mathematics.
  - ▷ You need an RRZE-account to log in.
  - ▷ To get access to the PC-Pools outside the lecture hours,  
contact Mr. Bayer (Room 01.330) or Mrs. Zintchenko (Room 01.342)
  - ▷ <https://en.www.math.fau.de/departement/rechnerbetreuung/rechnerbetreuung-pc-pools/>

## 1.B 1-D Conservation laws



## Continuum mechanics

Do not model individual molecules but instead consider averaged quantities.



Figure: The coordinate system for a 1-D continuum with an example distribution of molecules [Roberts, 1994]

Examples:

- ▶ mass density  $\rho(\mathbf{x})$  [kg/m<sup>3</sup>] instead of positions of individual molecules
- ▶ temperature  $T(\mathbf{x})$  [K] instead of kinetic energy of individual particles.

Note: The continuum assumption is only justified when the *representative physical length scale*  $L$  [m] is much larger than the *mean free path length of molecules*  $\lambda$  [m].



## Conservation of mass

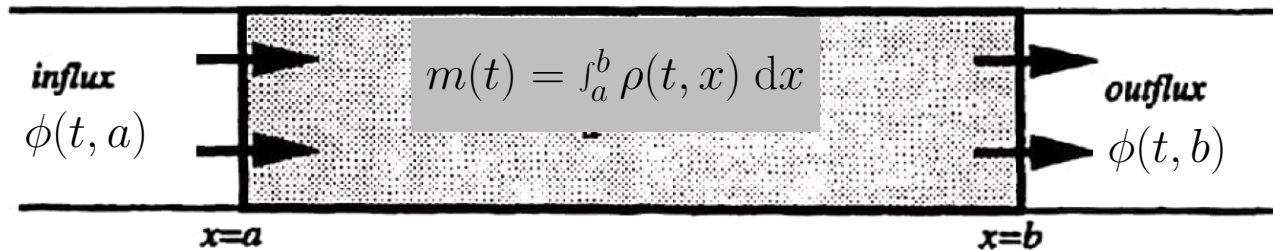


Figure: A slice of a 1-D continuum to investigate the conservation of mass (from [Roberts, 1994] but edited)

The mass  $m(t)$  [kg] in  $[a, b]$  changes only because of the mass fluxes  $\phi(\cdot, a)$  and  $\phi(\cdot, b)$  [kg/s]:

$$\frac{\partial m}{\partial t} = \phi(t, a) - \phi(t, b).$$

## Conservation of mass

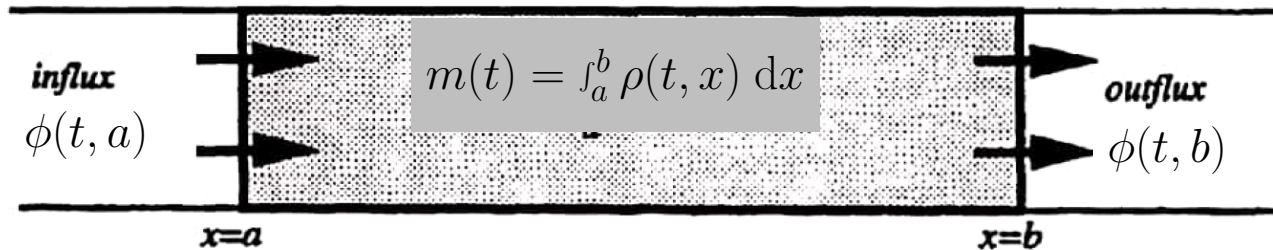


Figure: A slice of a 1-D continuum to investigate the conservation of mass (from [Roberts, 1994] but edited)

The mass  $m(t)$  [kg] in  $[a, b]$  changes only because of the mass fluxes  $\phi(\cdot, a)$  and  $\phi(\cdot, b)$  [kg/s]:

$$\frac{\partial m}{\partial t} = \phi(t, a) - \phi(t, b).$$

Using the fundamental theorem of calculus, we find

$$\int_a^b \frac{\partial \rho}{\partial t}(t, x) \, dx = - \int_a^b \frac{\partial \phi}{\partial x}(t, x) \, dx.$$

## Conservation of mass

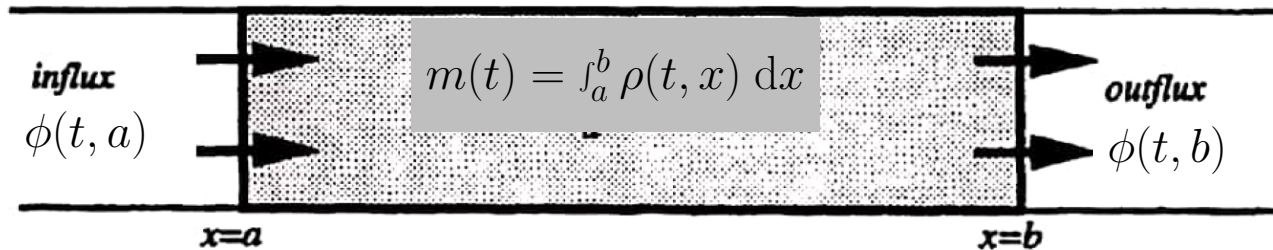


Figure: A slice of a 1-D continuum to investigate the conservation of mass (from [Roberts, 1994] but edited)

The mass  $m(t)$  [kg] in  $[a, b]$  changes only because of the mass fluxes  $\phi(\cdot, a)$  and  $\phi(\cdot, b)$  [kg/s]:

$$\frac{\partial m}{\partial t} = \phi(t, a) - \phi(t, b).$$

Using the fundamental theorem of calculus, we find

$$\int_a^b \frac{\partial \rho}{\partial t}(t, x) \, dx = - \int_a^b \frac{\partial \phi}{\partial x}(t, x) \, dx.$$

Because this holds for any interval  $[a, b]$  in the domain  $\Omega = [0, L]$ :

### Conservation of mass in 1-D

$$\frac{\partial \rho}{\partial t}(t, x) = - \frac{\partial \phi}{\partial x}(t, x).$$

## Completing the model

$$\frac{\partial \rho}{\partial t}(t, x) = -\frac{\partial \phi}{\partial x}(t, x).$$

To complete the model, we need a *constitutive relation* that relates the mass flux  $\phi(t, x)$  [kg/s] to the mass density  $\rho(t, x)$  [kg/m].

Two commonly used constitutive relations:

### Fick's law

$$\phi(t, x) = -\kappa(t, x) \frac{\partial \rho}{\partial x}(t, x).$$

The coefficient  $\kappa(t, x)$  [m<sup>2</sup>/s] is called the diffusivity.  
'Mass flows from locations with high concentrations to locations with low concentrations'

### Advective transport

$$\phi(t, x) = v(t, x) \rho(t, x).$$

The velocity field  $v(t, x)$  [m/s] is given.  
'Mass flows along the velocity field  $v(t, x)$ '

## Energy conservation

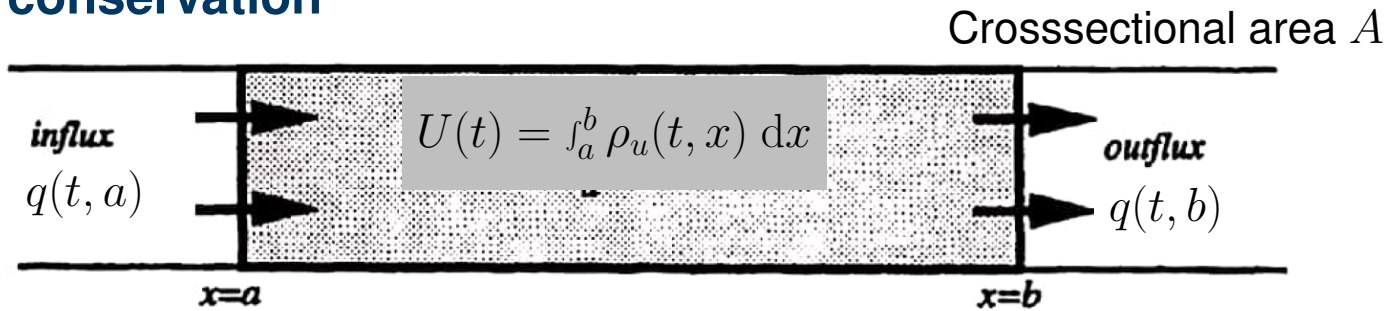


Figure: A slice of a 1-D continuum to investigate heat conduction (from [Roberts, 1994] but edited)

The internal energy  $U(t)$  [J] in  $[a, b]$  only changes because of the heat fluxes  $q(\cdot, a)$  and  $q(\cdot, b)$  [W/m<sup>2</sup>] and the heat  $\int_a^b Q(x) dx$  [W] generated inside  $[a, b]$ :

$$\frac{\partial U}{\partial t} = Aq(t, a) - Aq(t, b) + \int_a^b Q(t, x) dx.$$

## Energy conservation

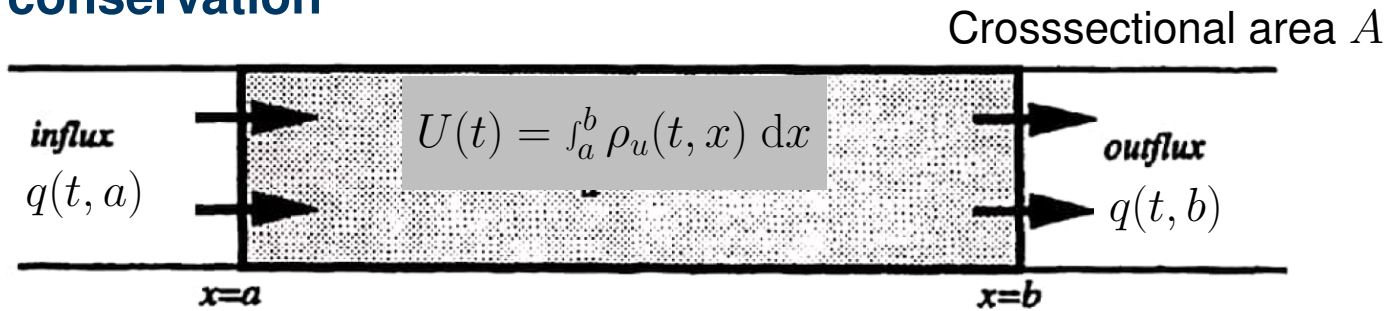


Figure: A slice of a 1-D continuum to investigate heat conduction (from [Roberts, 1994] but edited)

The internal energy  $U(t)$  [J] in  $[a, b]$  only changes because of the heat fluxes  $q(\cdot, a)$  and  $q(\cdot, b)$  [W/m<sup>2</sup>] and the heat  $\int_a^b Q(x) \, dx$  [W] generated inside  $[a, b]$ :

$$\frac{\partial U}{\partial t} = Aq(t, a) - Aq(t, b) + \int_a^b Q(t, x) \, dx.$$

Using the fundamental theorem of calculus, we find

$$\int_a^b \frac{\partial \rho_u}{\partial t}(t, x) \, dx = \int_a^b \left( -A \frac{\partial q}{\partial x}(t, x) + Q(t, x) \right) \, dx.$$

Because this holds for any interval  $[a, b]$  in the domain  $\Omega = [0, L]$ :

### Energy conservation in 1-D

$$\frac{\partial \rho_u}{\partial t}(t, x) = -A \frac{\partial q}{\partial x}(t, x) + Q(t, x).$$

## Completing the model

$$\frac{\partial \rho_u}{\partial t}(t, x) = -A \frac{\partial q}{\partial x}(t, x) + Q(t, x).$$

We again need constitutive relations to complete the model.

### Fourier's law of heat conduction

$$q(t, x) = -k \frac{\partial T}{\partial x}(t, x).$$

The coefficient  $k$  [W/m/K] is the thermal conductivity and  $T(t, x)$  [K] is the temperature. 'Heat flows from locations with high temperatures to locations with low temperatures'

### Internal energy

$$\rho_u(t, x) = cAT(t, x).$$

The coefficient  $c$  [J/K/m<sup>3</sup>] heat capacity per unit length.

## 1.C 1-D Finite differences





## Finite differences

Suppose we want to approximate the solution  $u(x)$  of the boundary value problem

$$\begin{aligned}\frac{d^2u}{dx^2}(x) + f(x) &= 0, & x \in (0, L), \\ u(0) &= 0, & \frac{du}{dx}(L) = 0.\end{aligned}$$

## Finite differences

Suppose we want to approximate the solution  $u(x)$  of the boundary value problem

$$\begin{aligned} \frac{d^2 u}{dx^2}(x) + f(x) &= 0, & x \in (0, L), \\ u(0) &= 0, & \frac{du}{dx}(L) = 0. \end{aligned}$$

Introduce an  $M$ -point grid in the interval  $[0, L]$  with a grid spacing  $\Delta x = L/(M - 1)$



Also introduce  $f_m = f(x_m)$  and the approximation  $u_m \approx u(x_m)$ .

## Finite difference approximation (2nd derivative)

We want to write a system of equations in terms of  $f_m (= f(x_m))$  and  $u_m (\approx u(x_m))$ .

Observe that (for  $u \in C^4([0, L])$ )

$$\begin{aligned} u(x + \Delta x) &= u(x) + \Delta x \frac{du}{dx}(x) + \frac{(\Delta x)^2}{2} \frac{d^2u}{dx^2}(x) + \frac{(\Delta x)^3}{6} \frac{d^3u}{dx^3}(x) + O((\Delta x)^4), \\ u(x - \Delta x) &= u(x) - \Delta x \frac{du}{dx}(x) + \frac{(\Delta x)^2}{2} \frac{d^2u}{dx^2}(x) - \frac{(\Delta x)^3}{6} \frac{d^3u}{dx^3}(x) + O((\Delta x)^4). \end{aligned}$$

Adding these two equations:

$$u(x + \Delta x) + u(x - \Delta x) = 2u(x) + (\Delta x)^2 \frac{d^2u}{dx^2}(x) + O((\Delta x)^4).$$

Rearranging and dividing by  $(\Delta x)^2$  yields

$$\frac{d^2u}{dx^2}(x) = \frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{(\Delta x)^2} + O((\Delta x)^2).$$

### Finite difference approximation (for the 2nd derivative)

$$\frac{d^2u}{dx^2}(x_m) \approx \frac{u_{m+1} - 2u_m + u_{m-1}}{(\Delta x)^2}.$$

## Finite difference approximation (1st derivative)

We want to write a system of equations in terms of  $f_m (= f(x_m))$  and  $u_m (\approx u(x_m))$ .

Observe that (for  $u \in C^4([0, L])$ )

$$\begin{aligned} u(x + \Delta x) &= u(x) + \Delta x \frac{du}{dx}(x) + \frac{(\Delta x)^2}{2} \frac{d^2u}{dx^2}(x) + \frac{(\Delta x)^3}{6} \frac{d^3u}{dx^3}(x) + O((\Delta x)^4), \\ u(x - \Delta x) &= u(x) - \Delta x \frac{du}{dx}(x) + \frac{(\Delta x)^2}{2} \frac{d^2u}{dx^2}(x) - \frac{(\Delta x)^3}{6} \frac{d^3u}{dx^3}(x) + O((\Delta x)^4). \end{aligned}$$

Subtracting these two equations:

$$u(x + \Delta x) - u(x - \Delta x) = 2\Delta x \frac{du}{dx}(x) + O((\Delta x)^3).$$

Rearranging and dividing by  $2\Delta x$  yields

$$\frac{du}{dx}(x) = \frac{u(x + \Delta x) - u(x - \Delta x)}{2\Delta x} + O((\Delta x)^2).$$

**(Centered) finite difference approximation (for the 1st derivative)**

$$\frac{du}{dx}(x_m) \approx \frac{u_{m+1} - u_{m-1}}{2\Delta x}.$$

## Intermezzo: left- and right-sided finite differences

For right-sided finite differences, observe that

$$u(x + \Delta x) = u(x) + \Delta x \frac{du}{dx}(x) + O((\Delta x)^2).$$

Rearranging yields

$$\frac{du}{dx}(x) = \frac{u(x + \Delta x) - u(x)}{\Delta x} + O(\Delta x).$$

### Right-sided finite differences

$$\frac{du}{dx}(x_n) \approx \frac{u_{m+1} - u_m}{\Delta x}.$$

For left-sided finite differences, we do a similar derivation starting from

$$u(x - \Delta x) = u(x) - \Delta x \frac{du}{dx}(x) + O((\Delta x)^2).$$

### Left-sided finite differences

$$\frac{du}{dx}(x_m) \approx \frac{u_m - u_{m-1}}{\Delta x}.$$

Note: the error in left- and right-sided finite differences is  $O(\Delta x)$ , not  $O((\Delta x)^2)$ !

## Boundary conditions

$$\begin{aligned}\frac{d^2 u}{dx^2}(x) + f(x) &= 0, & x \in (0, L), \\ u(0) &= 0, & \frac{du}{dx}(L) = 0.\end{aligned}$$

$$\frac{u_{m+1} - 2u_m + u_{m-1}}{\Delta x^2} + f_m = 0.$$

## Boundary conditions

$$\begin{aligned} \frac{d^2 u}{dx^2}(x) + f(x) &= 0, & x \in (0, L), & \quad \frac{u_{m+1} - 2u_m + u_{m-1}}{\Delta x^2} + f_m = 0. \\ u(0) &= 0, & \frac{du}{dx}(L) &= 0. \end{aligned}$$

Introduce two fictitious ('ghost') points  $x_0$  and  $x_{M+1}$ .



Two additional equations for the boundary conditions:

- ▶ The boundary condition  $u(0) = 0$  becomes  $u_1 = 0$ .
- ▶ For the boundary condition  $\frac{du}{dx}(L) = 0$ , we use that

$$\begin{aligned} \frac{du}{dx}(L) &= \frac{u(x_{M+1}) - u(x_{M-1})}{2\Delta x} + O(\Delta x^2), & \frac{u_{M+1} - u_{M-1}}{2\Delta x} &= 0. \end{aligned}$$

## Matrix formulation (implicit formulation for the BCs)

We now have a set of  $M + 2$  linear equations:

$$\frac{u_{m+1} - 2u_m + u_{m-1}}{\Delta x^2} + f_m = 0, \quad (m = 1, 2, \dots, M),$$
$$u_1 = 0, \quad \frac{u_{M+1} - u_{M-1}}{\Delta x} = 0.$$



## Matrix formulation (implicit formulation for the BCs)

We now have a set of  $M + 2$  linear equations:

$$\frac{u_{m+1} - 2u_m + u_{m-1}}{\Delta x^2} + f_m = 0, \quad (m = 1, 2, \dots, M),$$

$$u_1 = 0, \quad \frac{u_{M+1} - u_{M-1}}{\Delta x} = 0.$$

Write these equations in matrix form

$$\frac{1}{\Delta x^2} \begin{bmatrix} 0 & \Delta x^2 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & & 0 & 0 & 0 & 0 \\ \vdots & \vdots & & & \ddots & & \vdots & \vdots & \\ 0 & 0 & 0 & 0 & & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & \frac{-\Delta x}{2} & 0 & \frac{\Delta x}{2} \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{M-2} \\ u_{M-1} \\ u_M \\ u_{M+1} \end{bmatrix} + \begin{bmatrix} 0 \\ f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{M-2} \\ f_{M-1} \\ f_M \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

## Matrix formulation (towards an explicit formulation for the BCs)

$$\frac{1}{\Delta x^2} \begin{bmatrix} 0 & \Delta x^2 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & & 0 & 0 & 0 & 0 \\ \vdots & \vdots & & & \ddots & & \vdots & \vdots & \\ 0 & 0 & 0 & 0 & & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & \frac{-\Delta x}{2} & 0 & \frac{\Delta x}{2} \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{M-2} \\ u_{M-1} \\ u_M \\ u_{M+1} \end{bmatrix} + \begin{bmatrix} 0 \\ f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{M-2} \\ f_{M-1} \\ f_M \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Step 1:

- ▶ The first equation states that  $u_1 = 0$  (first row)  $\Rightarrow$  we can eliminate  $u_1$ .
  - ▶ The last line states that  $u_{M+1} = u_{M-1}$  (last row)  $\Rightarrow$  we can eliminate  $u_{M+1}$ .
- $\Rightarrow$  Delete the first and last row.  
 $\Rightarrow$  Delete the second and last column.

Step 2:

- ▶ We are not interested in the value  $u_0$ , because  $x_0$  is a fictitious (ghost) node.
  - ▶  $u_0$  only appears in the first equation.
- $\Rightarrow$  Delete the first row and column.

## Matrix formulation (explicit formulation for the BCs)

(Following the steps from the previous slide)

$$\frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 0 & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & \dots & 0 & 2 & -2 \end{bmatrix} \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ u_{M-2} \\ u_{M-1} \\ u_M \end{bmatrix} + \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{M-2} \\ f_{M-1} \\ f_M \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

## Matrix formulation (explicit formulation for the BCs)

(Following the steps from the previous slide)

$$\frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 0 & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & \dots & 0 & 2 & -2 \end{bmatrix} \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ u_{M-2} \\ u_{M-1} \\ u_M \end{bmatrix} + \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{M-2} \\ f_{M-1} \\ f_M \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Both the explicit and implicit formulation lead to a linear system of the form

$$\mathbf{A}\mathbf{u} + \mathbf{f} = 0.$$

This system can be solved to determine  $\mathbf{u}$ .

The implicit formulation for the BCs contains  $M + 2$  unknowns.

The explicit formulation for the BCs contains  $M$  unknowns.

In the implicit formulation,  $\mathbf{u}$  contains the fictious ('ghost') values  $u_0$  and  $u_{M+1}$ .

In the explicit formulation,  $\mathbf{u}$  does not contain  $u_0$  and  $u_{M+1}$ .

## 1.D Convergence analysis for 1-D finite differences



## What about convergence?

Two ingredients:

1) A continuous (ODE, PDE) problem  
with a continuous solution  $u(x)$ .

$$F(u) = 0.$$

In our example,  $F(u) = \frac{d^2u}{dx^2} + f$ .

2) A numerical (FD) scheme  
with a discrete solution  $\mathbf{u}$ .

$$\mathbf{F}_{\Delta x}(\mathbf{u}) = 0.$$

In our example,  $\mathbf{F}_{\Delta x}(\mathbf{u}) = \mathbf{A}\mathbf{u} + \mathbf{f}$ .

## What about convergence?

Two ingredients:

1) A continuous (ODE, PDE) problem with a continuous solution  $u(x)$ .

$$F(u) = 0.$$

In our example,  $F(u) = \frac{d^2u}{dx^2} + f$ .

2) A numerical (FD) scheme with a discrete solution  $\mathbf{u}$ .

$$\mathbf{F}_{\Delta x}(\mathbf{u}) = 0.$$

In our example,  $\mathbf{F}_{\Delta x}(\mathbf{u}) = \mathbf{A}\mathbf{u} + \mathbf{f}$ .

Let  $u(\mathbf{x})$  denote the continuous solution evaluated in the grid points.

What can we say about the error  $\mathbf{e} = \mathbf{u} - u(\mathbf{x})$  when  $\Delta x \rightarrow 0$ ?

## What about convergence?

Two ingredients:

1) A continuous (ODE, PDE) problem with a continuous solution  $u(x)$ .

$$F(u) = 0.$$

In our example,  $F(u) = \frac{d^2u}{dx^2} + f$ .

2) A numerical (FD) scheme with a discrete solution  $\mathbf{u}$ .

$$\mathbf{F}_{\Delta x}(\mathbf{u}) = 0.$$

In our example,  $\mathbf{F}_{\Delta x}(\mathbf{u}) = \mathbf{A}\mathbf{u} + \mathbf{f}$ .

Let  $u(\mathbf{x})$  denote the continuous solution evaluated in the grid points.

What can we say about the error  $\mathbf{e} = \mathbf{u} - u(\mathbf{x})$  when  $\Delta x \rightarrow 0$ ?

### Definition (Convergent numerical scheme)

The numerical scheme is convergent if the error  $\|\mathbf{e}\| \rightarrow 0$  when  $\Delta x \rightarrow 0$ .

Note: the problem is subtle because the number of elements in  $\mathbf{e}$  grows when  $\Delta x \rightarrow 0$ . Convergence in one norm does not (always) imply convergence in another norm!



## Two criteria for a convergent scheme

Two ingredients:

1) A continuous (ODE, PDE) problem  
with a continuous solution  $u(x)$ .

2) A numerical (FD) scheme  
with a discrete solution  $\mathbf{u}$ .

$$F(u) = 0.$$

$$\mathbf{F}_{\Delta x}(\mathbf{u}) = 0.$$

Let  $u(\mathbf{x})$  denote the continuous solution evaluated in the grid points.

## Two criteria for a convergent scheme

Two ingredients:

1) A continuous (ODE, PDE) problem  
with a continuous solution  $u(x)$ .

2) A numerical (FD) scheme  
with a discrete solution  $\mathbf{u}$ .

$$F(u) = 0.$$

$$\mathbf{F}_{\Delta x}(\mathbf{u}) = 0.$$

Let  $u(\mathbf{x})$  denote the continuous solution evaluated in the grid points.

### Theorem (Lax)

*The numerical scheme is convergent if it is both*

- ▶ *consistent and*
- ▶ *stable.*

### Definition (Consistent numerical scheme)

The numerical scheme is consistent iff  $\mathbf{F}_{\Delta x}(u(\mathbf{x})) = O(\Delta x^p)$  for some  $p > 0$ .

## Two criteria for a convergent scheme

Two ingredients:

1) A continuous (ODE, PDE) problem with a continuous solution  $u(x)$ .

2) A numerical (FD) scheme with a discrete solution  $\mathbf{u}$ .

$$F(u) = 0.$$

$$\mathbf{F}_{\Delta x}(\mathbf{u}) = 0.$$

Let  $u(\mathbf{x})$  denote the continuous solution evaluated in the grid points.

### Theorem (Lax)

*The numerical scheme is convergent if it is both*

- ▶ *consistent and*
- ▶ *stable.*

### Definition (Consistent numerical scheme)

The numerical scheme is consistent iff  $\mathbf{F}_{\Delta x}(u(\mathbf{x})) = O(\Delta x^p)$  for some  $p > 0$ .

Stability question: does  $\mathbf{F}_{\Delta x}(\mathbf{u}) - \mathbf{F}_{\Delta x}(u(\mathbf{x})) = O(\Delta x^p)$  imply  $\mathbf{u} - u(\mathbf{x}) = O(\Delta x^p)$ ?

### Definition (Stable numerical scheme (for a static problem))

The numerical scheme is stable if there exists a constant  $K$  independent of  $\Delta x$  s.t.

$$|\mathbf{u} - u(\mathbf{x})| \leq K |\mathbf{F}_{\Delta x}(\mathbf{u}) - \mathbf{F}_{\Delta x}(u(\mathbf{x}))|$$

## Consistency (the easy part)

By Taylor's theorem, we have

$$u(x_{m+1}) = u(x_m) + \Delta x \frac{du}{dx}(x_m) + \frac{\Delta x^2}{2} \frac{d^2u}{dx^2}(x_m) + \frac{\Delta x^3}{6} \frac{d^3u}{dx^3}(x_m) + \frac{\Delta x^4}{24} \frac{d^4u}{dx^4}(\xi_m^+),$$

$$u(x_{m-1}) = u(x_m) - \Delta x \frac{du}{dx}(x_m) + \frac{\Delta x^2}{2} \frac{d^2u}{dx^2}(x_m) - \frac{\Delta x^3}{6} \frac{d^3u}{dx^3}(x_m) + \frac{\Delta x^4}{24} \frac{d^4u}{dx^4}(\xi_m^-),$$

for certain  $\xi_m^+ \in [x_m, x_{m+1}]$  and  $\xi_m^- \in [x_{m-1}, x_m]$ .

## Consistency (the easy part)

By Taylor's theorem, we have

$$u(x_{m+1}) = u(x_m) + \Delta x \frac{du}{dx}(x_m) + \frac{\Delta x^2}{2} \frac{d^2u}{dx^2}(x_m) + \frac{\Delta x^3}{6} \frac{d^3u}{dx^3}(x_m) + \frac{\Delta x^4}{24} \frac{d^4u}{dx^4}(\xi_m^+),$$

$$u(x_{m-1}) = u(x_m) - \Delta x \frac{du}{dx}(x_m) + \frac{\Delta x^2}{2} \frac{d^2u}{dx^2}(x_m) - \frac{\Delta x^3}{6} \frac{d^3u}{dx^3}(x_m) + \frac{\Delta x^4}{24} \frac{d^4u}{dx^4}(\xi_m^-),$$

for certain  $\xi_m^+ \in [x_m, x_{m+1}]$  and  $\xi_m^- \in [x_{m-1}, x_m]$ .

Adding these two equations shows that

$$u(x_{m+1}) + u(x_{m-1}) = 2u(x_m) + \Delta x^2 \frac{d^2u}{dx^2}(x_m) + \frac{\Delta x^4}{24} \left( \frac{d^4u}{dx^4}(\xi_m^+) + \frac{d^4u}{dx^4}(\xi_m^-) \right).$$

## Consistency (the easy part)

By Taylor's theorem, we have

$$u(x_{m+1}) = u(x_m) + \Delta x \frac{du}{dx}(x_m) + \frac{\Delta x^2}{2} \frac{d^2u}{dx^2}(x_m) + \frac{\Delta x^3}{6} \frac{d^3u}{dx^3}(x_m) + \frac{\Delta x^4}{24} \frac{d^4u}{dx^4}(\xi_m^+),$$

$$u(x_{m-1}) = u(x_m) - \Delta x \frac{du}{dx}(x_m) + \frac{\Delta x^2}{2} \frac{d^2u}{dx^2}(x_m) - \frac{\Delta x^3}{6} \frac{d^3u}{dx^3}(x_m) + \frac{\Delta x^4}{24} \frac{d^4u}{dx^4}(\xi_m^-),$$

for certain  $\xi_m^+ \in [x_m, x_{m+1}]$  and  $\xi_m^- \in [x_{m-1}, x_m]$ .

Adding these two equations shows that

$$u(x_{m+1}) + u(x_{m-1}) = 2u(x_m) + \Delta x^2 \frac{d^2u}{dx^2}(x_m) + \frac{\Delta x^4}{24} \left( \frac{d^4u}{dx^4}(\xi_m^+) + \frac{d^4u}{dx^4}(\xi_m^-) \right).$$

Rearranging shows that

$$\frac{u(x_{m+1}) - 2u(x_m) + u(x_{m-1}))}{\Delta x^2} - \frac{d^2u}{dx^2}(x_m) = O(\Delta x^2).$$

Note that  $\frac{d^2u}{dx^2}(x_m) + f(x_m) = 0$ .

Similarly, we can check that  $u(x)$  also satisfies the discretized BCs up to  $O(\Delta x^2)$ .

Therefore,

$$\mathbf{A}u(\mathbf{x}) + \mathbf{f} = O(\Delta x^2).$$

## Stability (the hard part)

By definition of  $\mathbf{u}$

$$\mathbf{A}\mathbf{u} + \mathbf{f} = 0.$$

From the previous slide

$$\mathbf{A}u(\mathbf{x}) + \mathbf{f} = O(\Delta x^2).$$

## Stability (the hard part)

By definition of  $\mathbf{u}$

$$\mathbf{A}\mathbf{u} + \mathbf{f} = 0.$$

Therefore also,

$$\mathbf{A}(\mathbf{u} - u(\mathbf{x})) = \mathbf{A}\mathbf{e} = O(\Delta x^2).$$

From the previous slide

$$\mathbf{A}u(\mathbf{x}) + \mathbf{f} = O(\Delta x^2).$$



## Stability (the hard part)

By definition of  $\mathbf{u}$

$$\mathbf{A}\mathbf{u} + \mathbf{f} = 0.$$

From the previous slide

$$\mathbf{A}u(\mathbf{x}) + \mathbf{f} = O(\Delta x^2).$$

Therefore also,

$$\mathbf{A}(\mathbf{u} - u(\mathbf{x})) = \mathbf{A}\mathbf{e} = O(\Delta x^2).$$

But we need to bound  $|\mathbf{e}|$ , not  $|\mathbf{A}\mathbf{e}|$ !

**Stability:** there exists a constant  $K$  independent of  $\Delta x$  such that  $|\mathbf{e}| \leq K|\mathbf{A}\mathbf{e}|$ .  
(in which norm  $|\cdot|$ ?)

## Stability (the hard part)

By definition of  $\mathbf{u}$

$$\mathbf{A}\mathbf{u} + \mathbf{f} = 0.$$

From the previous slide

$$\mathbf{A}u(\mathbf{x}) + \mathbf{f} = O(\Delta x^2).$$

Therefore also,

$$\mathbf{A}(\mathbf{u} - u(\mathbf{x})) = \mathbf{A}\mathbf{e} = O(\Delta x^2).$$

But we need to bound  $|\mathbf{e}|$ , not  $|\mathbf{A}\mathbf{e}|$ !

**Stability:** there exists a constant  $K$  independent of  $\Delta x$  such that  $|\mathbf{e}| \leq K|\mathbf{A}\mathbf{e}|$ .  
(in which norm  $|\cdot|$ ?)

It can be shown that we can take the  $\ell^\infty$ -norm and  $K = \frac{1}{8}$ .  
The argument is based on the discrete maximum principle.

(see e.g. [L. Chen, Finite difference methods for Poisson equation])

We conclude there exists a constant  $C$  such that

$$|\mathbf{u} - u(\mathbf{x})|_\infty \leq C(\Delta x)^2,$$