Computational Modeling of the Cardiovascular System

Finite Element Method II

Finite Differences Method

CVRTI

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Overview

- Finite Element Method II
  - Element matrices
  - System matrix and vector
- Finite Differences Method
  - Partial Differential Equations
  - Discretization of Domains
  - Discretization of Operators
  - Discretization of Equations
- Homework III

Group work & pause

Group work

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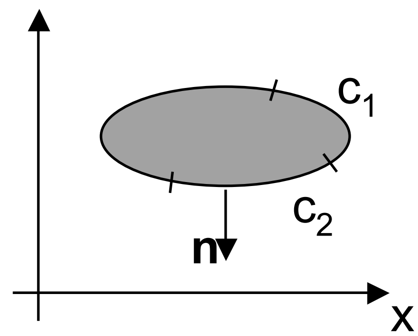
Boundary Conditions



Dirichlet: $u(s) = \varphi(s)$ at boundary c_1

Cauchy: $\frac{\partial u(s)}{\partial \mathbf{n}} + \alpha(s)u(s) = \gamma(s)$ at boundary c_2

Special case
Neumann: $\alpha(s) = \gamma(s) = 0$: $\frac{\partial u(s)}{\partial \mathbf{n}} = 0$

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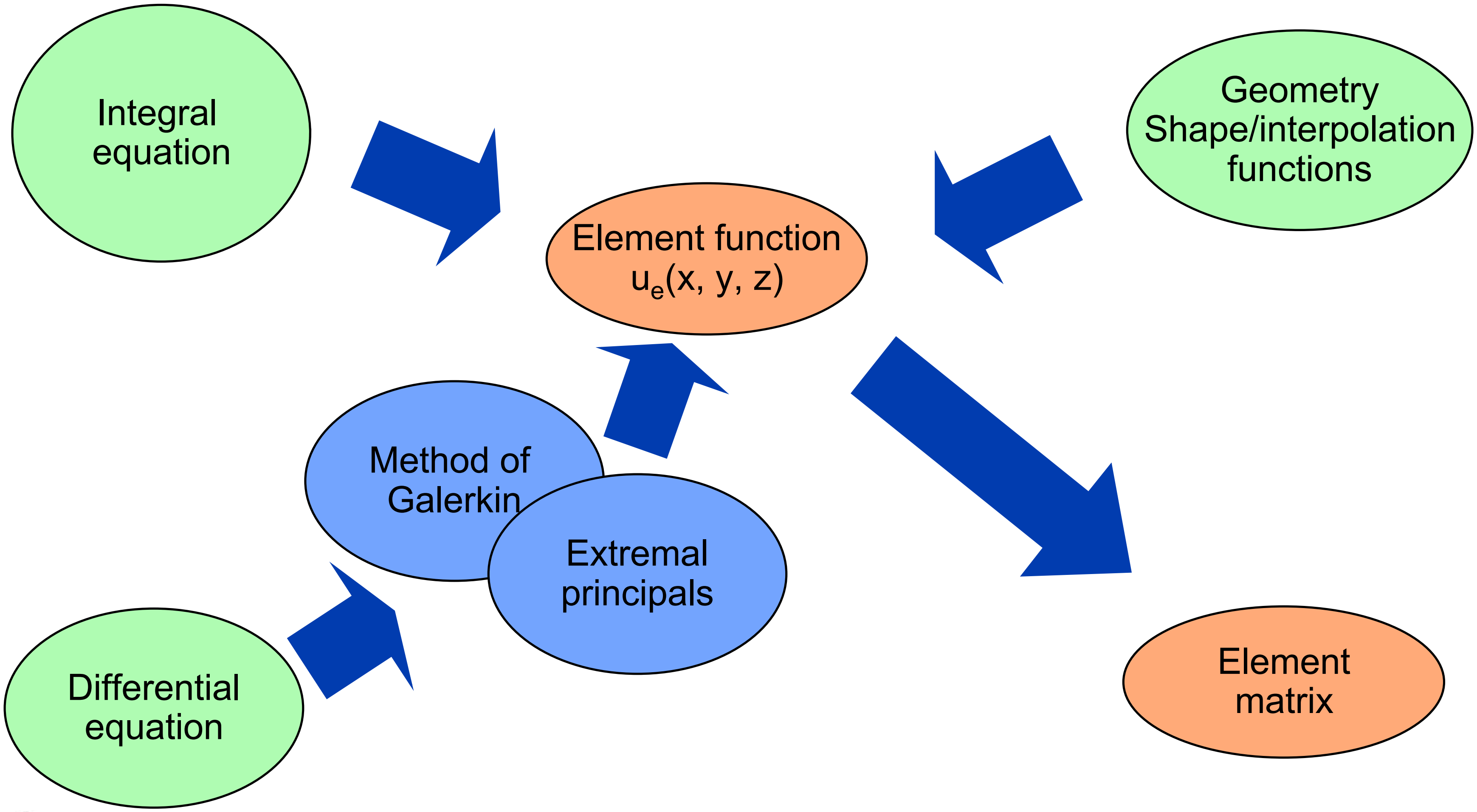
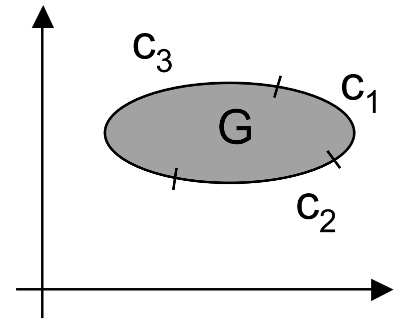
Finite Element Method: Element matrix



Extremal Principles for Classical Boundary Problem

Classical boundary problem:

$$\frac{\partial}{\partial \mathbf{x}}\left(\mathbf{k}_1(\mathbf{x},\mathbf{y})\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)+\frac{\partial}{\partial \mathbf{y}}\left(\mathbf{k}_2(\mathbf{x},\mathbf{y})\frac{\partial \mathbf{u}}{\partial \mathbf{y}}\right)+\varsigma(\mathbf{x},\mathbf{y})\,\mathbf{u}=\mathbf{f}(\mathbf{x},\mathbf{y})$$



$C = c_1 \cup c_2 \cup c_3$

$$\mathbf{k}_1,\mathbf{k}_2 \in \mathbf{C}^1(\overline{\mathbf{G}})$$

$$\varsigma,\mathbf{f} \in \mathbf{C}^0(\overline{\mathbf{G}})$$

$$\mathbf{u} \in \mathbf{C}^2(\mathbf{G}) \cap \mathbf{C}^1(\overline{\mathbf{G}})$$

$$\overline{\mathbf{G}} = \mathbf{G} \cup \mathbf{C}$$

Continuity

with Dirichlet and Cauchy boundary conditions for C_1 and C_2, resp.

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Solving of Classical Boundary Problem

Make

$$I = \iint_G \frac{1}{2}\left(k_1(x,y)\left(\frac{\partial u}{\partial x}\right)^2 + k_2(x,y)\left(\frac{\partial u}{\partial y}\right)^2\right) - \frac{1}{2}\varsigma(x,y)\,u^2 + f(x,y)\,u \quad dx\,dy$$

$$+\oint_C \frac{1}{2}\alpha(s)\,u^2 - \gamma(s)\,u \quad ds$$

stationary!

$$I(u) = \min!$$

Proof via variational calculus
(Schwarz „Methode der finiten Elemente“, page 23)

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Galerkin-Ritz Method

Determine solution function u for differential equation(s) on basis of linear independent problem adapted functions ϕ and boundary conditions:

$$u(x) = \phi_0 + \sum_{k=1}^{m} c_k \phi_k$$

ϕ_0: Problem adapted function, fulfills inhomogeneous boundary condition } $\phi_0(x)=c$

ϕ_k: Problem adapted function, fulfills homogeneous boundary condition and vanishes at location of inhomogeneous condition } $\phi_k(x)=0$

c_k: Unknown coefficients

Indirect method: Not

$$f(u,x) + q(u,x) = 0$$

u:	Problem adapted function	q:	Source term
f:	Differential equation	x:	Variable

is solved!

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Galerkin-Ritz Method: Weighted Residuals

Transform: Solve system of equations resulting from:

$$\int Rw \, dx = 0$$

Residuum: $R(u,x) = f(u,x) + q(u,x)$

Weighting function: $w(x)$

Galerkin: Use problem adapted functions as weighting functions:

$$w(x) \leftarrow \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_m \end{pmatrix}$$

Advantage: Order of derivatives is reduced in comparison to original differential equation system

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Example: Flow of Fluid in 2D

Flow: stationary

Fluid: viscous, incompressible, …

Partial differential equations:

$$\frac{\partial p}{\partial x} - \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = 0$$

Poisson-type equation

$$\frac{\partial p}{\partial y} - \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = 0$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

Continuity equation

u,v: Velocity in x- and y-direction, resp. [m/s]

μ: Viscosity [Ns/m^2]

p: Pressure [N/m^2]

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Example: Transforms

Problem adapted functions:

$$u(x,y) = \varphi_0(x,y) + \sum_{k=1}^{m} u_k \varphi_k(x,y) \qquad v(x,y) = \psi_0(x,y) + \sum_{k=1}^{m} v_k \psi_k(x,y)$$

$$p(x,y) = \chi_0(x,y) + \sum_{k=1}^{q} p_k \chi_k(x,y)$$

Substitution in original equations:

$$\iint_G \left[\frac{\partial \chi_0}{\partial x} + \sum_{k=1}^{q} p_k \frac{\partial \chi_k}{\partial x} - \mu\left(\Delta\phi_0 + \sum_{k=1}^{m} u_k \Delta\phi_k \right) \right] \phi_j \, dx\,dy \qquad j = 1,\ldots,m$$

$$\iint_G \left[\frac{\partial \chi_0}{\partial y} + \sum_{k=1}^{q} p_k \frac{\partial \chi_k}{\partial y} - \mu\left(\Delta\psi_0 + \sum_{k=1}^{m} v_k \Delta\psi_k \right) \right] \psi_j \, dx\,dy \qquad j = 1,\ldots,m$$

$$\iint_G \left[\frac{\partial \phi_0}{\partial x} + \sum_{k=1}^{m} u_k \frac{\partial \phi_k}{\partial x} + \frac{\partial \psi_0}{\partial y} + \sum_{k=1}^{m} u_k \frac{\partial \psi_k}{\partial y} \right] \chi_j \, dx\,dy \qquad j = 1,\ldots,q$$

Example: Transforms

(Schwarz ‚Methode der finiten Elemente‘, page 54-):

$$\sum_{k=1}^{m} u_k \iint_G \mu \nabla \phi_k \cdot \nabla \phi_j \, dx\, dy + \sum_{k=1}^{q} p_k \iint_G \frac{\partial \chi_k}{\partial x} \phi_j \, dx\, dy + R_j = 0$$

$$\sum_{k=1}^{m} v_k \iint_G \mu \nabla \psi_k \cdot \nabla \psi_j \, dx\, dy + \sum_{k=1}^{q} p_k \iint_G \frac{\partial \chi_k}{\partial y} \psi_j \, dx\, dy + S_j = 0$$

$$\sum_{k=1}^{m} u_k \iint_G \frac{\partial \phi_k}{\partial x} \chi_j \, dx\, dy + \sum_{k=1}^{m} v_k \iint_G \frac{\partial \psi_k}{\partial y} \chi_j \, dx\, dy + T_j = 0$$

R_j, S_j, T_j: Other terms

Transform in system of linear equations

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Assembly of System Matrix and Vector

Element matrix S_e und vector b_e determine element integral I_e for field variable vector u_e

$$I_e = \int_E f\left(u(\vec{x})\right) dV \quad \Rightarrow \quad I_e = \vec{u}_e^{\,T} S_e \vec{u}_e + \vec{b}_e^{\,T} \vec{u}_e + c_e$$

u: Solution function

$\vec{x}$: Coordinate vector

c_e: Constant

System matrix S_s und vector b_s determine system integral I_s for field variable vector u_s

$$S = \bigcup_i E_i: \quad I_s = \int_S f\left(u(\vec{x})\right) dV = \sum_i I_{e_i} \quad \Rightarrow \quad I_s = \vec{u}_s^{\,T} S_s \vec{u}_s + \vec{b}_s^{\,T} \vec{u}_s + c_s$$

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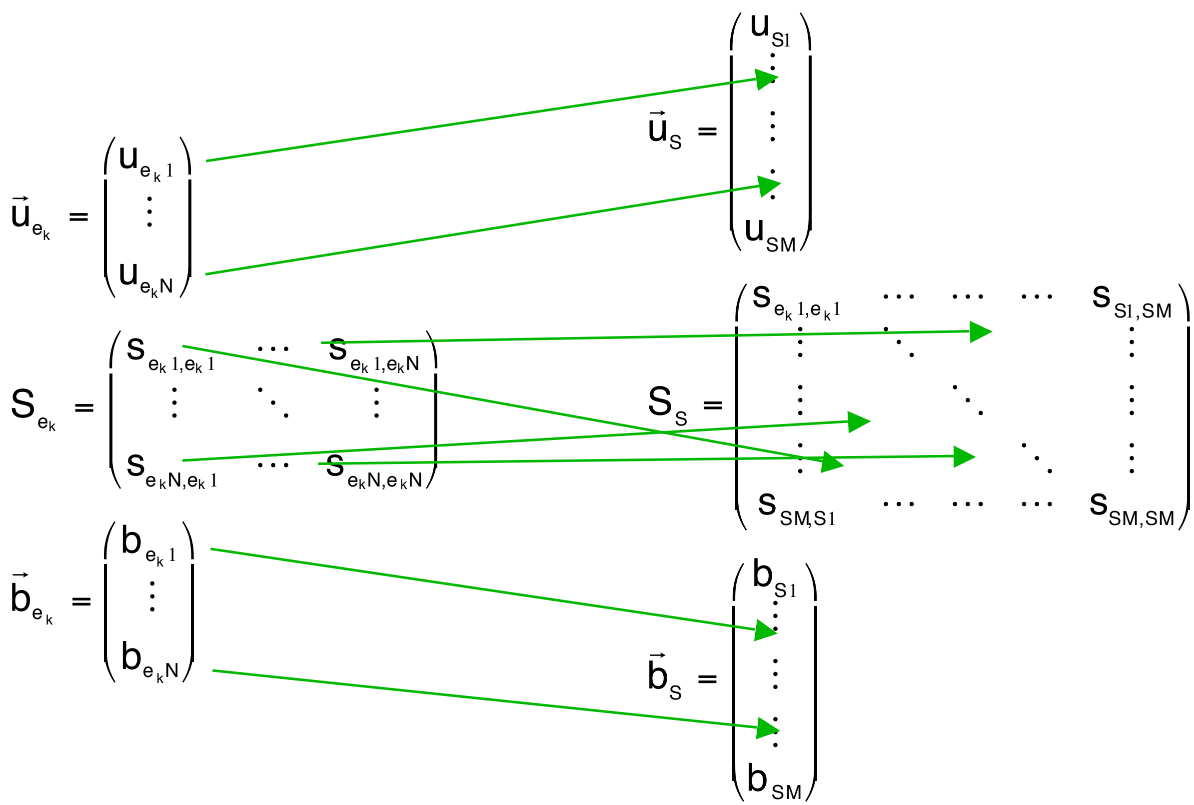
Field Variable Vector, System Matrix and Vector

Sorting

Adding



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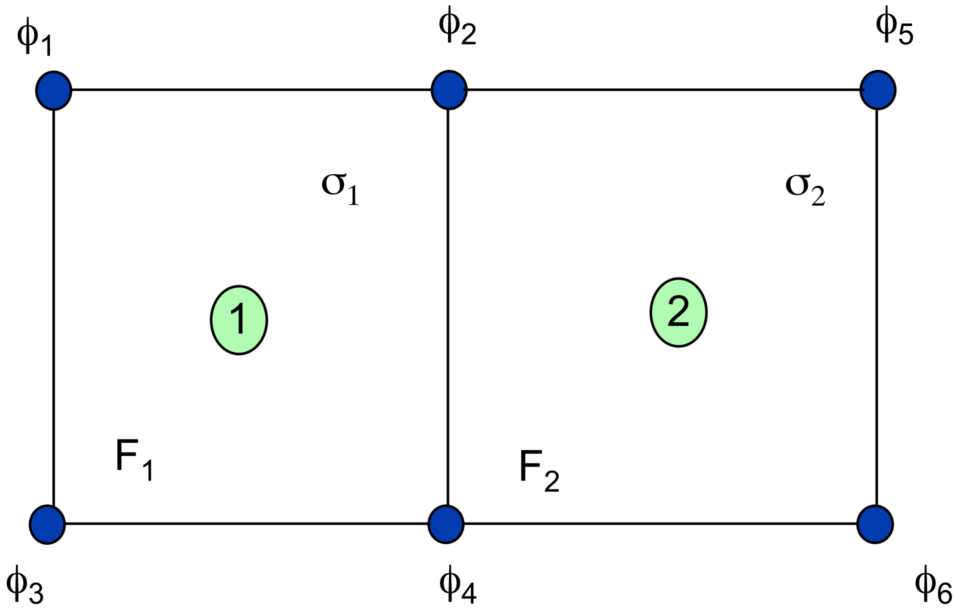
Example: Assembly of System Matrix

Power integral: $I = \iint_G \sigma E^2 \, dx \, dy$ $\qquad G = F_1 \cup F_2$

Elements: Quads, bilinear interpolation function

Assigned conductivities: σ_1, σ_2

Coupling for node variables: ϕ_2, ϕ_4



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Example: Element Integrals to Element Matrices

Element 1

$$\sigma_1 \iint_{F_1} E^2\,dx\,dy = \sigma_1 \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{pmatrix}^T \begin{pmatrix} \frac{2}{3} & -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{3}\\ -\frac{1}{6} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{6}\\ -\frac{1}{6} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{6}\\ -\frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} & \frac{2}{3}\end{pmatrix} \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{pmatrix}$$

$$\begin{pmatrix}\frac{\partial I_1}{\partial \phi_1}\\ \frac{\partial I_1}{\partial \phi_2}\\ \frac{\partial I_1}{\partial \phi_3}\\ \frac{\partial I_1}{\partial \phi_4}\end{pmatrix} = 2\sigma_1 \begin{pmatrix} \frac{2}{3} & -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{3}\\ -\frac{1}{6} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{6}\\ -\frac{1}{6} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{6}\\ -\frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} & \frac{2}{3}\end{pmatrix} \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{pmatrix}$$

Element 2

$$\sigma_2 \iint_{F_2} E^2\,dx\,dy = \sigma_2 \begin{pmatrix}\phi_2\\ \phi_5\\ \phi_4\\ \phi_6\end{pmatrix}^T \begin{pmatrix} \frac{2}{3} & -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{3}\\ -\frac{1}{6} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{6}\\ -\frac{1}{6} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{6}\\ -\frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} & \frac{2}{3}\end{pmatrix} \begin{pmatrix}\phi_2\\ \phi_5\\ \phi_4\\ \phi_6\end{pmatrix}$$

$$\begin{pmatrix}\frac{\partial I_2}{\partial \phi_2}\\ \frac{\partial I_2}{\partial \phi_5}\\ \frac{\partial I_2}{\partial \phi_4}\\ \frac{\partial I_2}{\partial \phi_6}\end{pmatrix} = 2\sigma_2 \begin{pmatrix} \frac{2}{3} & -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{3}\\ -\frac{1}{6} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{6}\\ -\frac{1}{6} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{6}\\ -\frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} & \frac{2}{3}\end{pmatrix} \begin{pmatrix}\phi_2\\ \phi_5\\ \phi_4\\ \phi_6\end{pmatrix}$$

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Example: Sorting and Addition

$$\left.\begin{matrix} \sigma_1 \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{pmatrix}^T \begin{pmatrix} \frac{4}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{2}{3} \\ -\frac{1}{3} & \frac{4}{3} & -\frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\ -\frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{pmatrix} \\ \sigma_2 \begin{pmatrix}\phi_2\\ \phi_5\\ \phi_4\\ \phi_6\end{pmatrix}^T \begin{pmatrix} \frac{4}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{2}{3} \\ -\frac{1}{3} & \frac{4}{3} & -\frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\ -\frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix}\phi_2\\ \phi_5\\ \phi_4\\ \phi_6\end{pmatrix} \end{matrix}\right\} \quad \sigma \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\\ \phi_5\\ \phi_6\end{pmatrix}^T \begin{pmatrix} \frac{4}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{2}{3} & 0 & 0 \\ -\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & -\frac{2}{3} \\ -\frac{1}{3} & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} & 0 & 0 \\ -\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{1}{3} \\ 0 & -\frac{1}{3} & 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\ 0 & -\frac{2}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\\ \phi_5\\ \phi_6\end{pmatrix}$$

$$\sigma_1 = \sigma_2 = \sigma$$

Example: Derivative of Quadratic System

$$
\begin{pmatrix} \frac{\partial}{\partial \phi_1} \\ \frac{\partial}{\partial \phi_2} \\ \frac{\partial}{\partial \phi_3} \\ \frac{\partial}{\partial \phi_4} \\ \frac{\partial}{\partial \phi_5} \\ \frac{\partial}{\partial \phi_6} \end{pmatrix}
\left(\sigma \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix}^T
\begin{pmatrix}
\frac{4}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{2}{3} & 0 & 0 \\
-\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & -\frac{2}{3} \\
-\frac{1}{3} & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} & 0 & 0 \\
-\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{1}{3} \\
0 & -\frac{1}{3} & 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\
0 & -\frac{2}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3}
\end{pmatrix}
\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} \right)
= 2\sigma
\begin{pmatrix}
\frac{4}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{2}{3} & 0 & 0 \\
-\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & -\frac{2}{3} \\
-\frac{1}{3} & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} & 0 & 0 \\
-\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{1}{3} \\
0 & -\frac{1}{3} & 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\
0 & -\frac{2}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3}
\end{pmatrix}
\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix}
$$

$$A_s \vec{x}_s$$

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Boundary Conditions: Overview

Boundary conditions ➡ 1. Extension of system
2. Modification of system

Extension method: Extend the system matrix and vector with rows and coefficients, resp., representing the boundary conditions

Example: Homogeneous Dirichlet boundary condition: $\phi_i = 0$

$$\begin{pmatrix} & & & A_S & & & \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_{i-1} \\ \phi_i \\ \phi_{i+1} \\ \vdots \\ \phi_n \end{pmatrix} = \vec{0}$$

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Boundary Conditions: Extension of System

Example: Inhomogeneous Dirichlet boundary condition: $\phi_i = c$

$$\begin{pmatrix} & & & A_S & & & \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_{i-1} \\ \phi_i \\ \phi_{i+1} \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ \vdots \\ b_n \\ c \end{pmatrix}$$

Example: Neumann boundary condition: $\phi_i = \phi_{i+1}$

$$\begin{pmatrix} & & & A_S & & & & \\ 0 & \cdots & 0 & 1 & -1 & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_{i-1} \\ \phi_i \\ \phi_{i+1} \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ \vdots \\ b_n \\ 0 \end{pmatrix}$$

Boundary Conditions: Modification of System

Homogeneous Dirichlet boundary condition: $x_s^j = 0$

- Set j-th element of b to 0: b_j:=0
- Set elements in j-th column und j-th row of A to 0
- Set j-th,j-th. element of A to 1: A_{jj}:=1

Inhomogeneous Dirichlet boundary condition $x_s^j = c, \quad c \neq 0$

- Subtract c-fold of A's j-th column vector from b
- Set j-th element of b to c: b_j:=c
- Set elements in j-th column und j-th row of A to 0
- Set j-th,j-th. element of A to 1: A_{jj}:=1

Advantage: Dimension of system matrix and vector is conserved!

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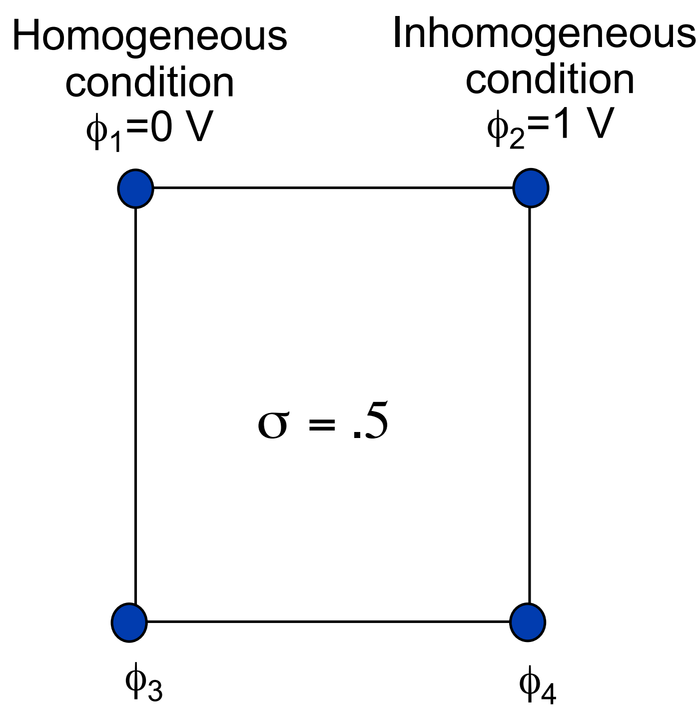
Example: Boundary Conditions I



$$I = \sigma \iint_{F_1} E^2 \, dxdy = \sigma \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix}^T \begin{pmatrix} \frac{2}{3} & -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{3} \\ -\frac{1}{6} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{6} \\ -\frac{1}{6} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{6} \\ -\frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} & \frac{2}{3} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix}$$

$$\begin{pmatrix} \frac{\partial I}{\partial \phi_1} \\ \frac{\partial I}{\partial \phi_2} \\ \frac{\partial I}{\partial \phi_3} \\ \frac{\partial I}{\partial \phi_4} \end{pmatrix} = 2\sigma \begin{pmatrix} \frac{4}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{2}{3} \\ -\frac{1}{3} & \frac{4}{3} & -\frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\ -\frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} = 0$$

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Example: Boundary Conditions II

ϕ_1=0 V

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{4}{3} & -\frac{2}{3} & -\frac{1}{3} \\ 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\ 0 & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} = 0$$

Solution

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} = \mathbf{0}$$

ϕ_1=0 V, ϕ_2=1 V

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{4}{3} & -\frac{1}{3} \\ 0 & 0 & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ -\frac{2}{3} \\ -\frac{1}{3} \end{pmatrix}$$

Solution

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \\ \mathbf{\frac{3}{5}} \\ \mathbf{\frac{2}{5}} \end{pmatrix}$$

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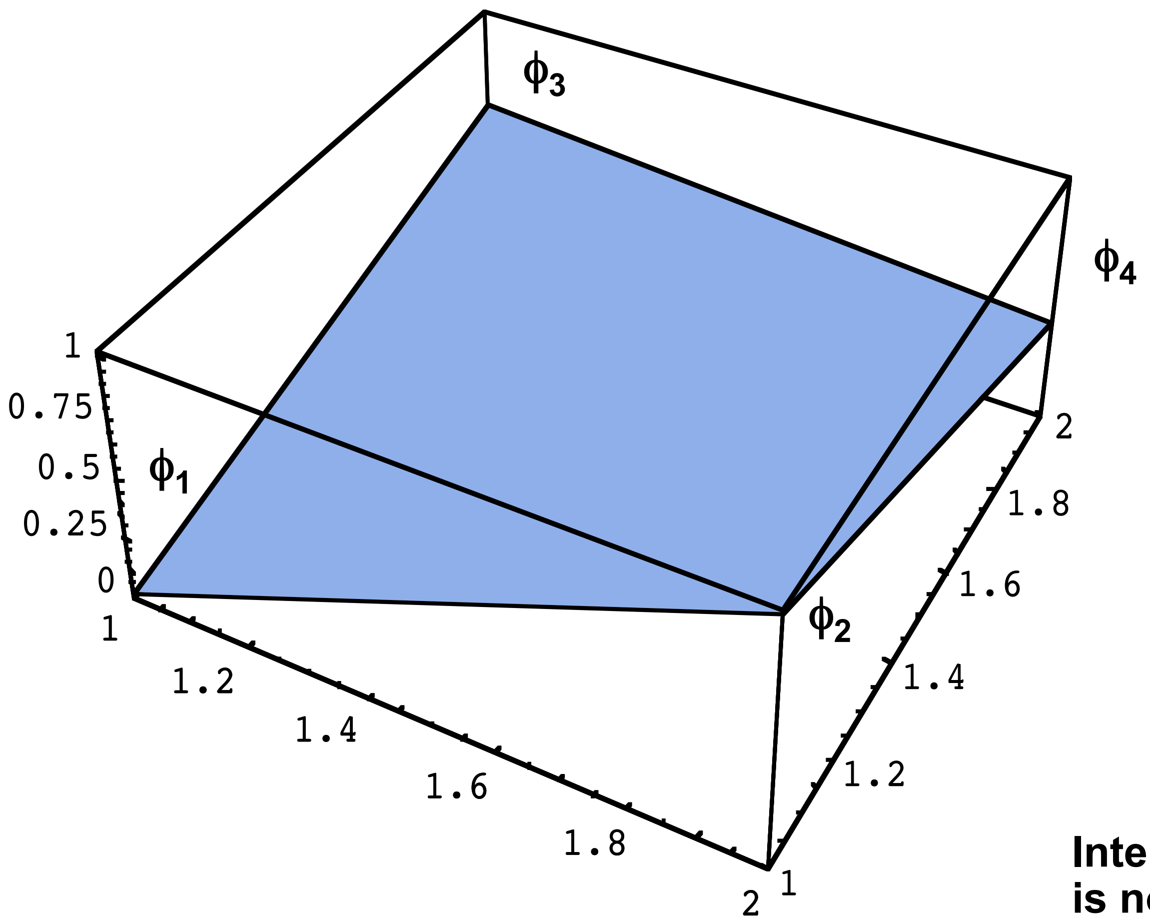
Exemplary Field Distribution



Interpolation function is not physically correct!

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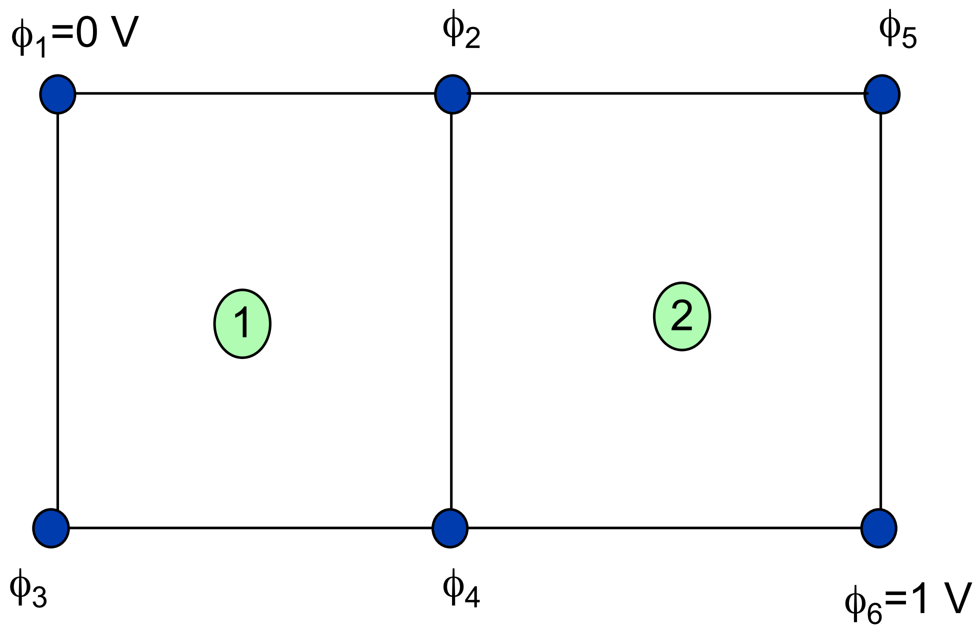
Example: Boundary Conditions

Homogeneous boundary condition



$\sigma = .5$

Inhomogeneous boundary condition

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Example: Homogeneous Boundary Condition

ϕ_1=0 V

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{8}{3} & -\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & -\frac{2}{3} \\ 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{2}{3} & -\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & -\frac{1}{3} \\ 0 & -\frac{1}{3} & 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} \\ 0 & -\frac{2}{3} & 0 & -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} = 0$$

Solution

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} = \mathbf{0}$$

Example: Add Inhomogeneous Boundary Condition

$\phi_1 = 0$ V, $\phi_6 = 1$ V

Solution

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{8}{3} & -\frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & -\frac{2}{3} & \frac{4}{3} & -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{2}{3} & -\frac{1}{3} & \frac{8}{3} & -\frac{2}{3} & 0 \\ 0 & -\frac{1}{3} & 0 & -\frac{2}{3} & \frac{4}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{2}{3} \\ 0 \\ -\frac{1}{3} \\ -\frac{1}{3} \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{7}{13} \\ \frac{5}{13} \\ \frac{6}{13} \\ \frac{8}{13} \\ 1 \end{pmatrix}$$

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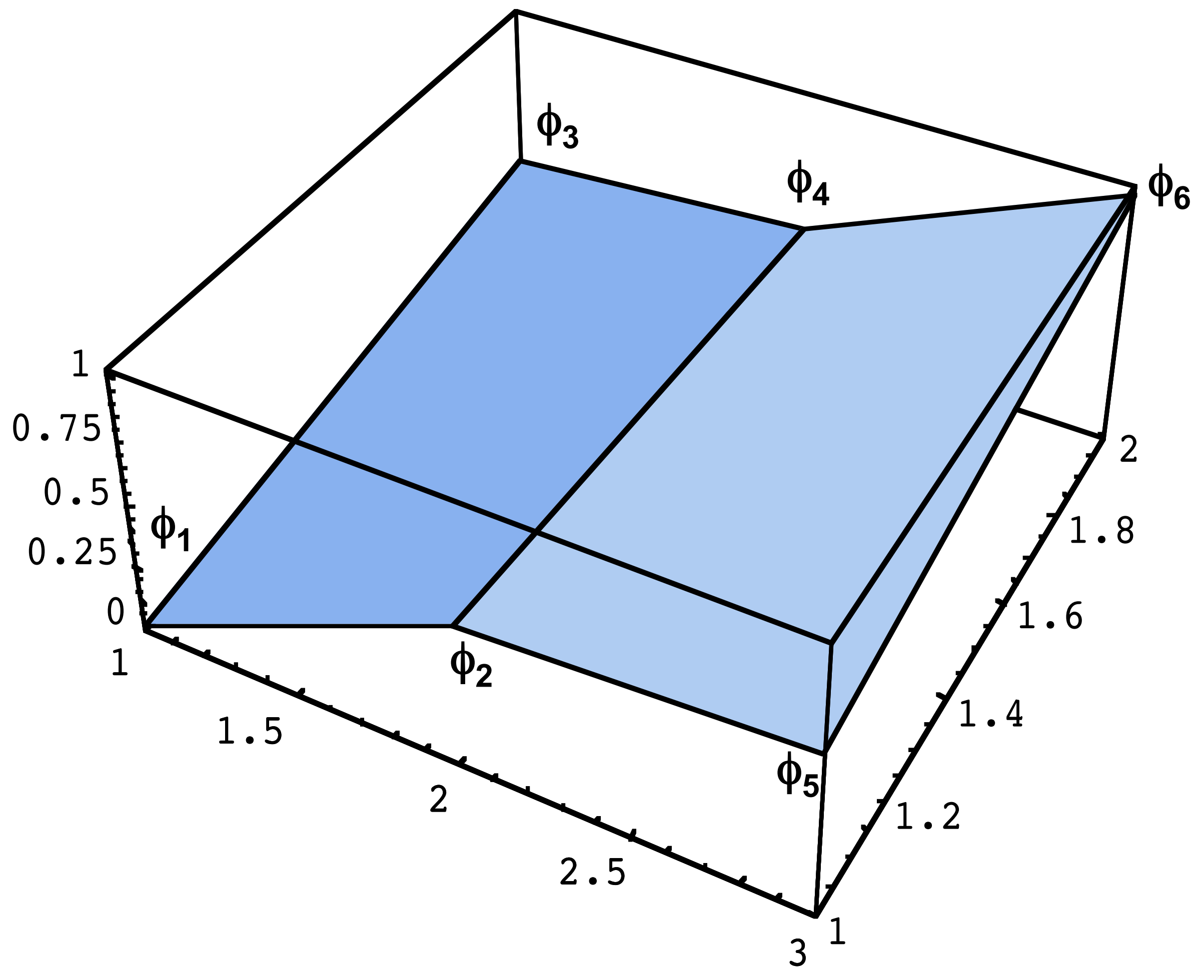
Exemplary Field Distribution



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Properties of System Matrix

- Commonly, large matrix dimension
  representing large number of degrees of freedom

- Sparse

- Sorting can lead to band shape
  $a_{i,k} = 0$ for all i,k with $|i-k|>m$
  m: Band width

- Symmetric for symmetric element matrices
  $a_{i,k} = a_{k,i}$ for all i,k

- Positive definite for positive definite element matrices

$$\underset{x \neq 0}{\forall} \; x^T A x > 0$$

⇒ Allows reduction of
- memory capacity
- computational demands

CVRTI

Efficient Storage of Symmetric Band Matrices

$$\begin{pmatrix} a & b & c & & \\ b & d & e & f & \\ c & e & g & h & i \\ & f & h & j & k \\ & & i & k & l \end{pmatrix} \Rightarrow \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \\ j & k & 0 \\ l & 0 & 0 \end{pmatrix}$$

Band width: 5

Sorting of Node Variables

Adjacencies of node variables determines band width of system matrix!

Node variables i und j (i ≠ j) are adjacent, if $a^{i,j} \neq 0$
Degree of node variable = number of adjacent node variables

Cuthill-McKee Algorithm

Choose a node x with minimal degree and add it to the result set R

$$R := \left(\left\{x\right\}\right)$$

For i=1,2,.. and while IRI < *n*

Construct the adjacency set A_i of R_i excluding nodes ∈ R

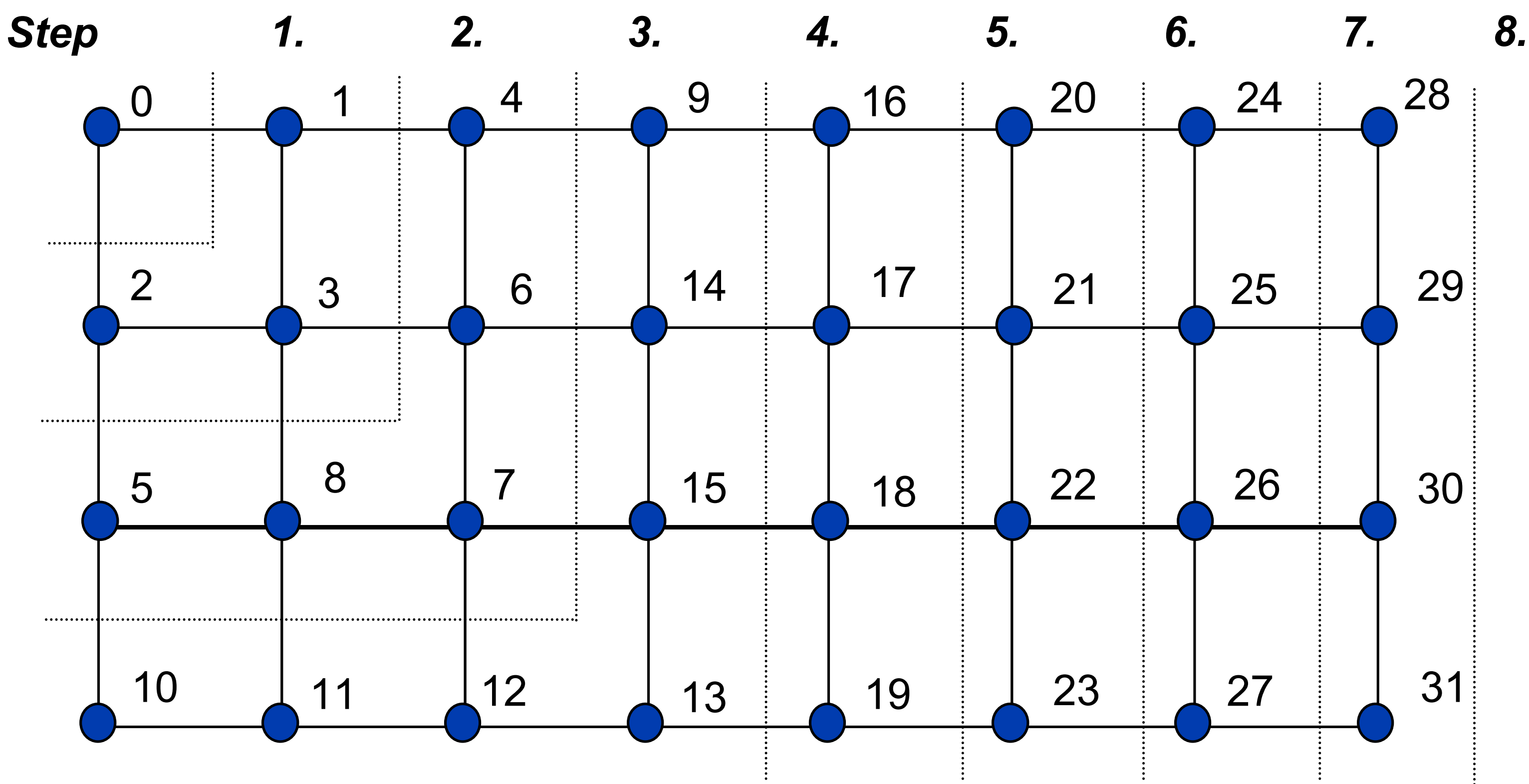
$$A_i := Adj\left(R_i\right) \setminus R$$

Sort A_i with ascending degree order
Append A_i to the result set R

$$R := R \cup A_i$$

CVRTI

Exemplary Application of Cuthill-McKee Algorithm



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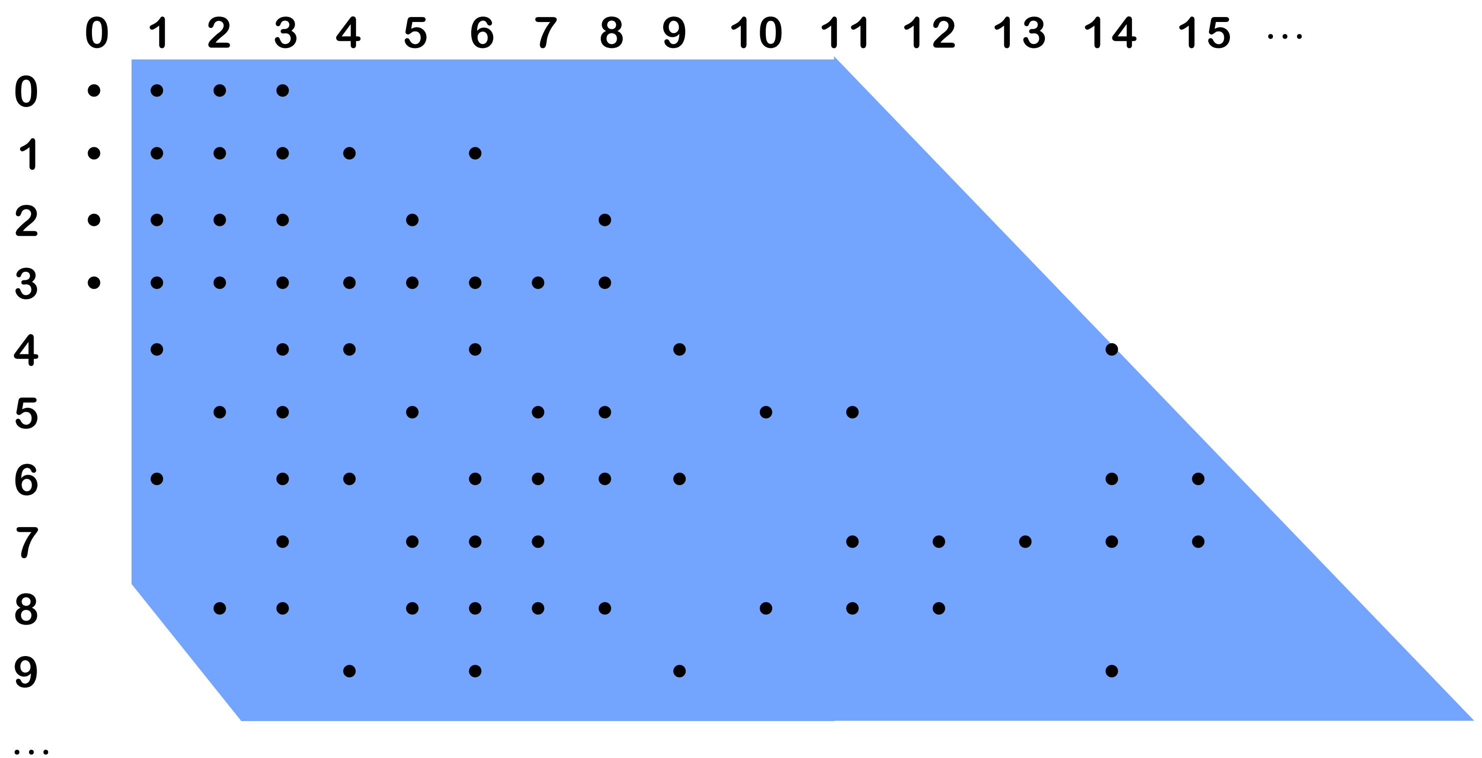
Example: System Matrix



• Elements of system matrix with values ≠ 0

CVRTI

Group Work

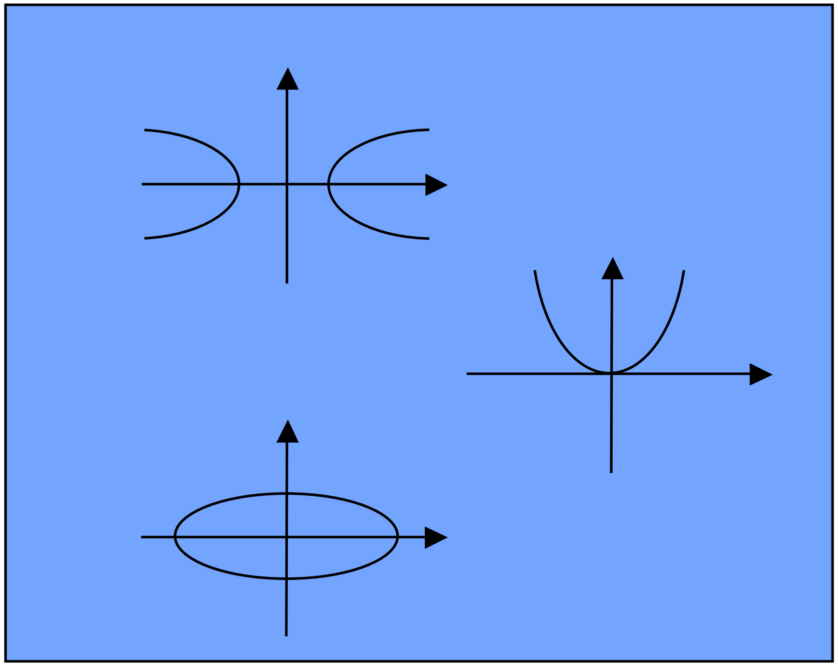
Which boundary conditions would you apply in a mechanical simulation of a human heart in situ?

Classification of Partial Differential Equations

$u(x,y)$ fulfills the linear partial differential equation:

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = H$$

in domain $G \subset \Re^2$



$AC - B^2 < 0$: hyperbolic

$AC - B^2 = 0$: parabolic

$AC - B^2 > 0$: elliptic

CVRTI

Elliptic Partial Differential Equations

2D Poisson equation: $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)$$

2D Laplace equation: $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

2D Helmholtz equation: $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k^2 u = 0$$

$\rho(x,y)$: Source term

k: Constant

→ **Boundary problem**
static/(quasi-)stationary solution

CVRTI

Elliptic Partial Differential Equations

Generalized Poisson Equation for Electrical Fields

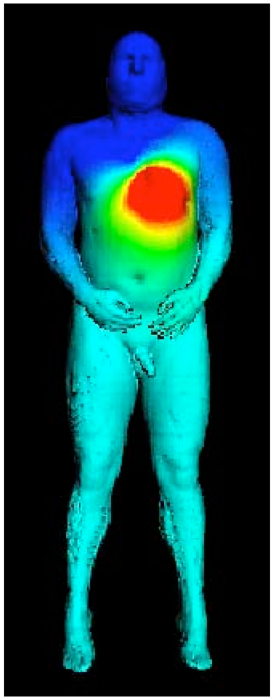
$$\nabla \cdot \left(\vec{\vec{\sigma}}\ \nabla \Phi \right) + f = 0$$

Φ: Electrical potential [V]

$\vec{\vec{\sigma}}$: Conductivity tensor [S/m]

f: Current source density [A/m^3]

Scalar/ complex quantities



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Elliptic Partial Differential Equations: Navier

Elastic deformation with infinitesimal displacements

$$\mu \Delta \vec{u} + (\mu + \lambda) \nabla \left(\nabla^T \vec{u} \right) + \vec{X} = 0$$

$\vec{u}$: Displacement [m]

μ, λ: Lame coefficients $[\frac{kg}{m\,s^2}]$

$\vec{X}$: Force density $[\frac{kg}{m^2 s^2}]$

$$\Delta = \nabla^2$$

CVRTI

Partial Differential Equations: Navier-Stokes

Fluid mechanics

$$-\nabla p + \eta \Delta \vec{v} - \vec{X} = 0$$

p:	Pressure	$[\frac{kg}{m\,s^2}]$
η:	Viscosity	$[\frac{kg}{m\,s}]$
$\vec{v}$:	Velocity vector	$[\frac{m}{s}]$
$\vec{X}$:	Force density	$[\frac{kg}{m^2 s^2}]$

CVRTI

Hyperbolic and Parabolic Differential Equations

1D wave equation - hyperbolic:

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

v: Velocity of wave propagation

1D diffusion equation - parabolic:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial u}{\partial x}\right)$$

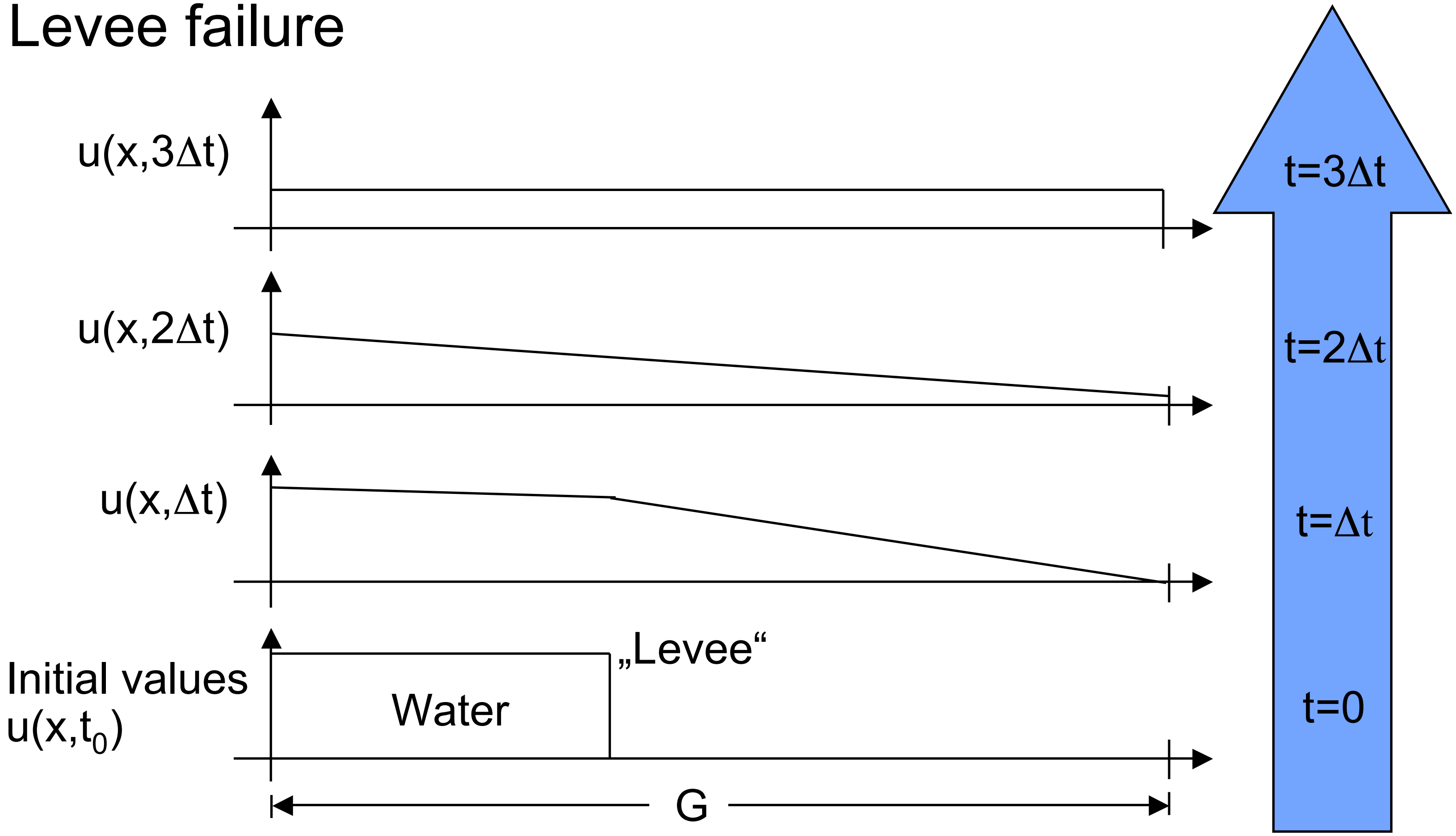
D: Diffusion coefficient

→ **Initial value problem**

CVRTI

Exemplary Initial Value Problem: Diffusion Equation

Levee failure



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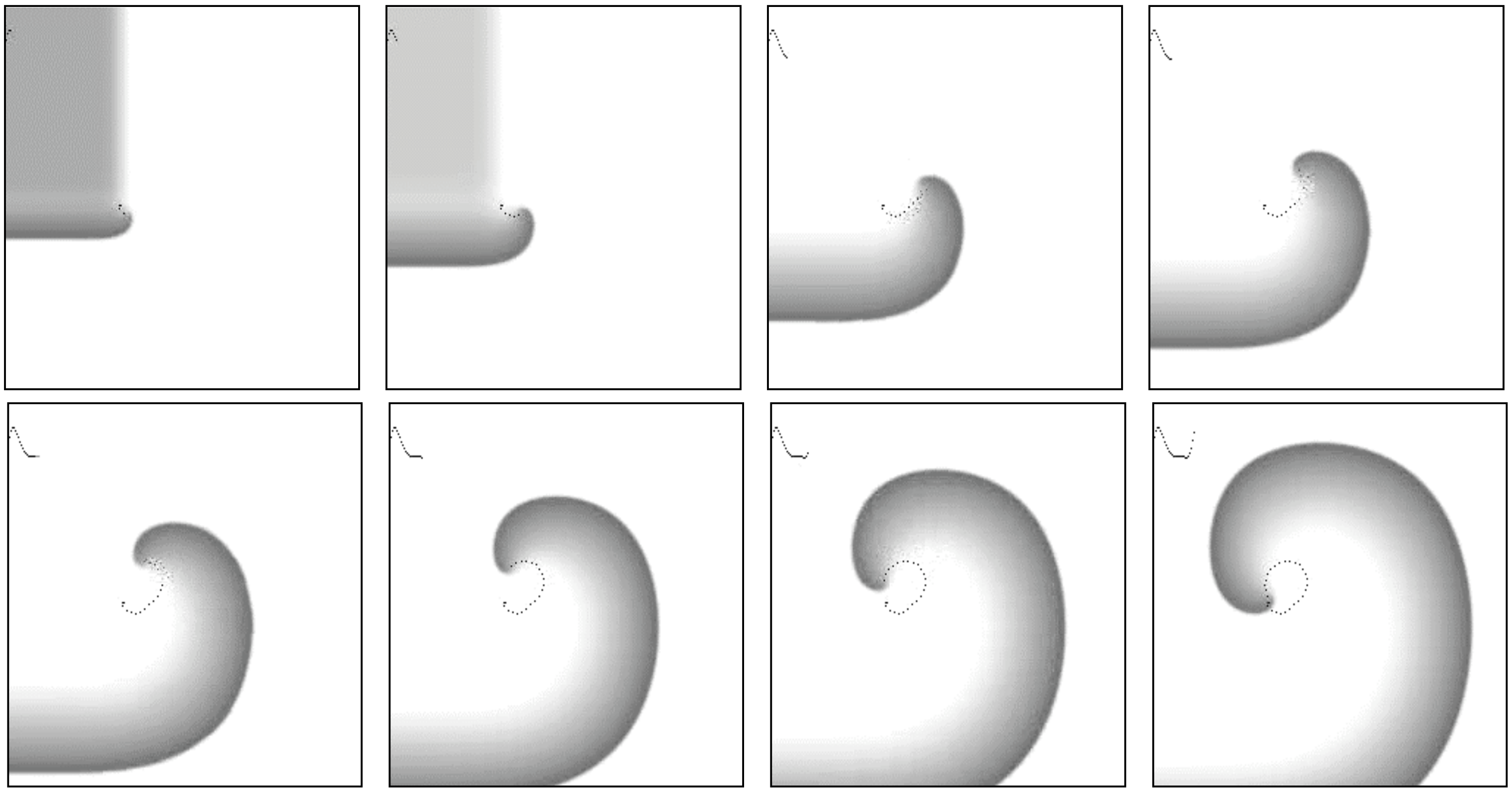
Exemplary Initial Value Problem: Diffusion Equation

Cardiac arrhythmia (2D)



http://www.musc.edu/~starmerf

CVRTI

Exemplary Initial Value Problem: Diffusion Equation

Heat Conduction

$$\frac{\lambda}{\rho c}\Delta T - \frac{\partial T}{\partial t} = 0$$

T: Temperature [°C]

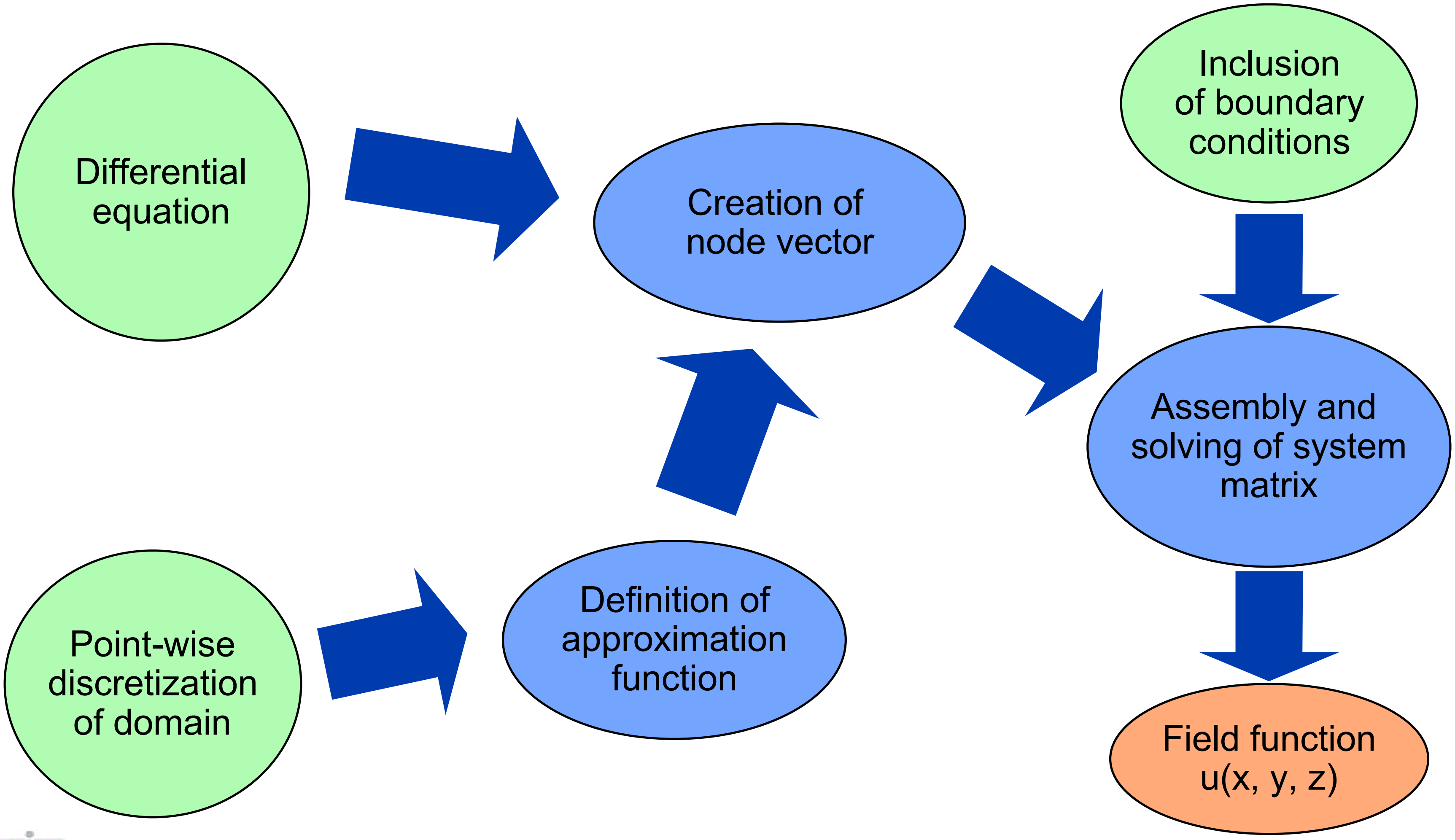
λ: Thermal conductivity [W/m/K]

ρ: Density [kg/m^3]

c: Specific thermal conductivity [J/ K kg]

CVRTI

Finite Differences Method: Overview



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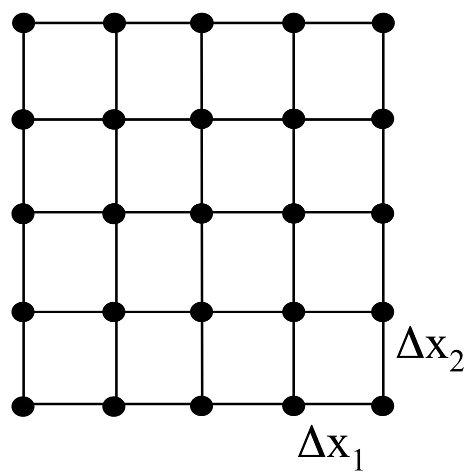
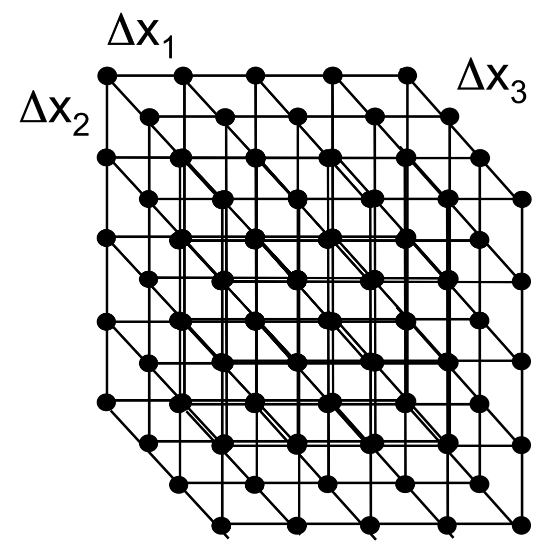
Exemplary Spatial Discretizations

2 D



3 D



- Node, eg. with node variables Φ [V], **E** [V/m], **A** [Vs/m], **H** [A/m]

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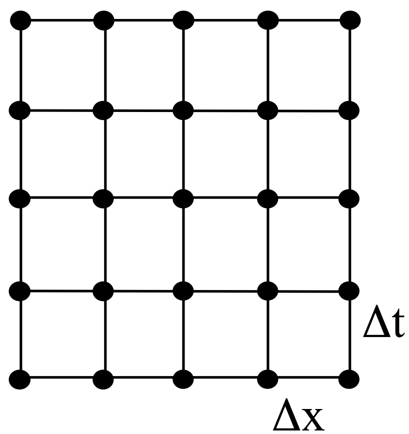
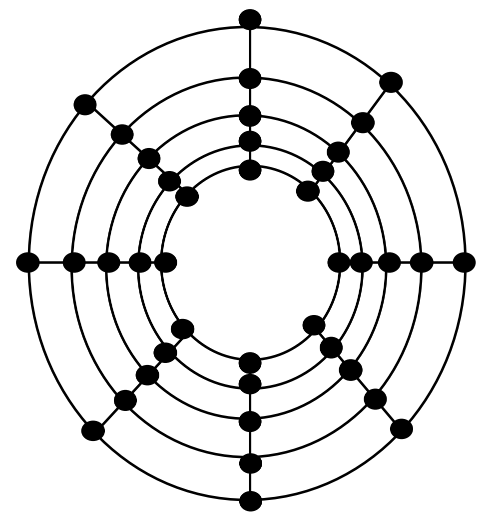
Exemplary Discretizations

1 D+t



2 D



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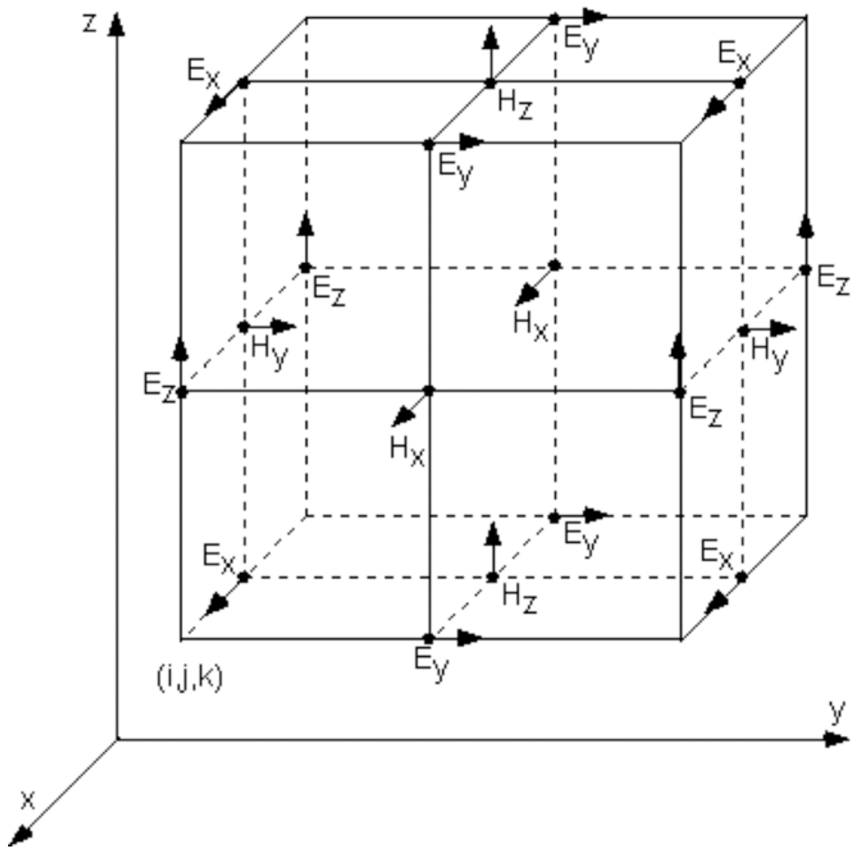
Exemplary Spatial Discretizations: Dual Grid

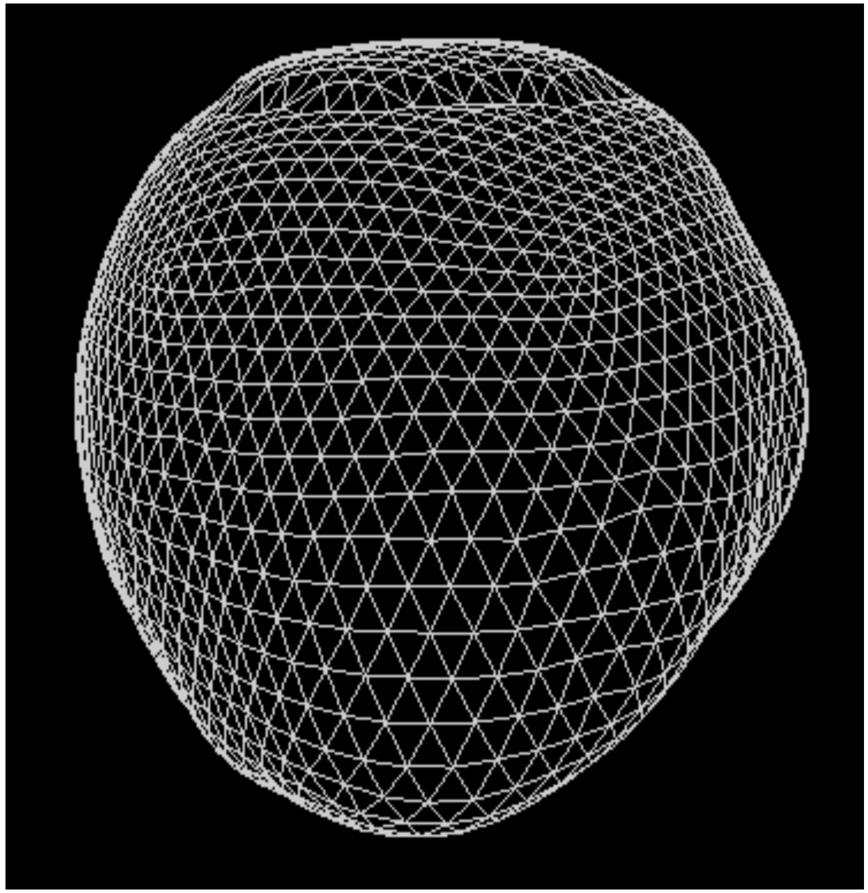


E: Electrical field
E=$(E_x, E_y, E_z)^T$

H: Magnetic field
H=$(H_x, H_y, H_z)^T$

CVRTI

Exemplary Spatial Discretizations: Irregular Mesh



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Principle

Partial differential equation

- elliptical
- parabolic
- hyperbolic
- ...

Operators

- 1. Derivative spatial/temporal
- 2. Derivative spatial/temporal/mixed
- Grad / Div / Rot
- ...

Example

$$\alpha \frac{\partial u}{\partial t} + \beta \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(\gamma \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial u}{\partial y}\right)$$

Approximation with differences

$$\frac{\partial u}{\partial t} \approx \frac{u_k - u_{k-1}}{\Delta t}$$

$$\frac{\partial^2 u}{\partial t^2} \approx \frac{u_{k+1} - 2u_k + u_{k-1}}{2\Delta t}$$

...

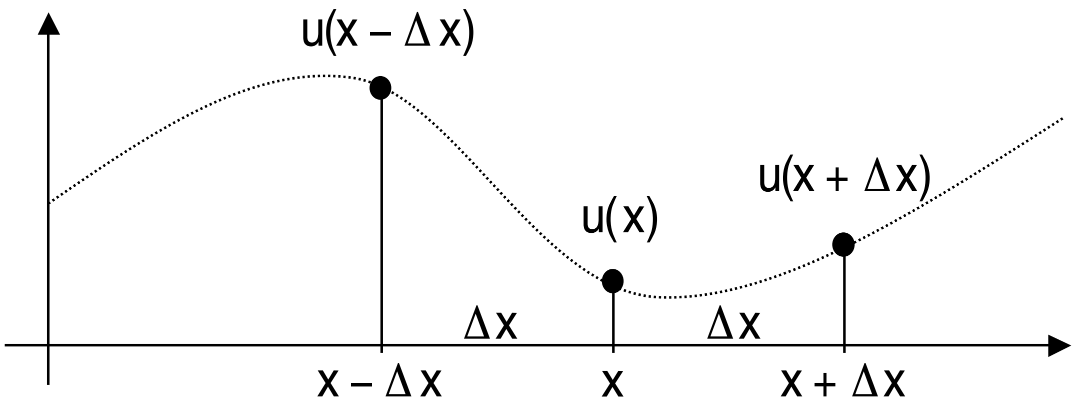
Compare with Euler-Method

Discretization of 1D-Operators: 1st Spatial Derivative

Forward
$$u_x(x) = \lim_{\Delta x \to 0} \frac{u(x+\Delta x) - u(x)}{\Delta x} \quad \rightarrow \quad u_x(k) = \frac{u(k+1) - u(k)}{\Delta x}$$

Backward
$$u_x(x) = \lim_{\Delta x \to 0} \frac{u(x) - u(x-\Delta x)}{\Delta x} \quad \rightarrow \quad u_x(k) = \frac{u(k) - u(k-1)}{\Delta x}$$

Central
$$u_x(x) = \lim_{\Delta x \to 0} \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} \quad \rightarrow \quad u_x(k) = \frac{u(k+1) - u(k-1)}{2\Delta x}$$



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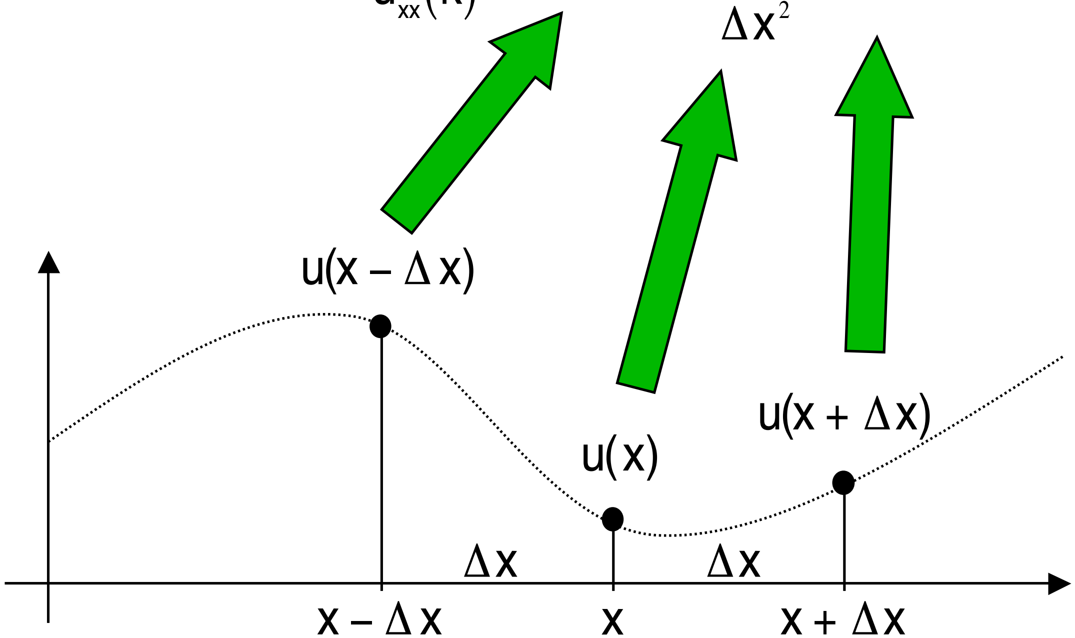
Discretization of 1D-Operators: 2nd Spatial Derivative

$$u_{xx}(k) = \frac{u_x\left(k + \frac{1}{2}\right) - u_x\left(k - \frac{1}{2}\right)}{\Delta x} \text{ mit } u_x(k) = \frac{u\left(k + \frac{1}{2}\right) - u\left(k - \frac{1}{2}\right)}{\Delta x}$$

$$\rightarrow \quad u_{xx}(k) = \frac{u(k+1) - 2u(k) + u(k-1)}{\Delta x^2}$$



CVRTI

Error of Finite Differences Approximation

Taylor series approximation

$$u(k \pm \Delta x) = u(k) \pm \frac{\partial u}{\partial x}(k)\frac{\Delta x}{1!} + \frac{\partial^2 u}{\partial x^2}(k)\frac{\Delta x^2}{2!} \pm \frac{\partial^3 u}{\partial x^3}(k)\frac{\Delta x^3}{3!} + \ldots$$

Forward difference

$$\frac{u(k + \Delta x) - u(k)}{\Delta x} = \frac{\partial u}{\partial x}(k) + \frac{\partial^2 u}{\partial x^2}(k)\frac{\Delta x}{2!} + \ldots = \frac{\partial u}{\partial x}(k) + E$$

$$\text{Error: } E = E(u, \Delta x) = \frac{\partial^2 u}{\partial x^2}(k)\frac{\Delta x}{2!} + \ldots$$

Central difference

$$\frac{u(k + \Delta x) - u(k - \Delta x)}{2\Delta x} = \frac{1}{2}\left(\frac{\partial u}{\partial x}(k) + \frac{\partial^3 u}{\partial x^3}(k)\frac{\Delta x^2}{3!} + \ldots\right) = \frac{1}{2}\left(\frac{\partial u}{\partial x}(k) + E\right)$$

$$\text{Error: } E = E(u, \Delta x) = \frac{1}{2}\left(\frac{\partial^3 u}{\partial x^3}(k)\frac{\Delta x^2}{3!} + \ldots\right)$$

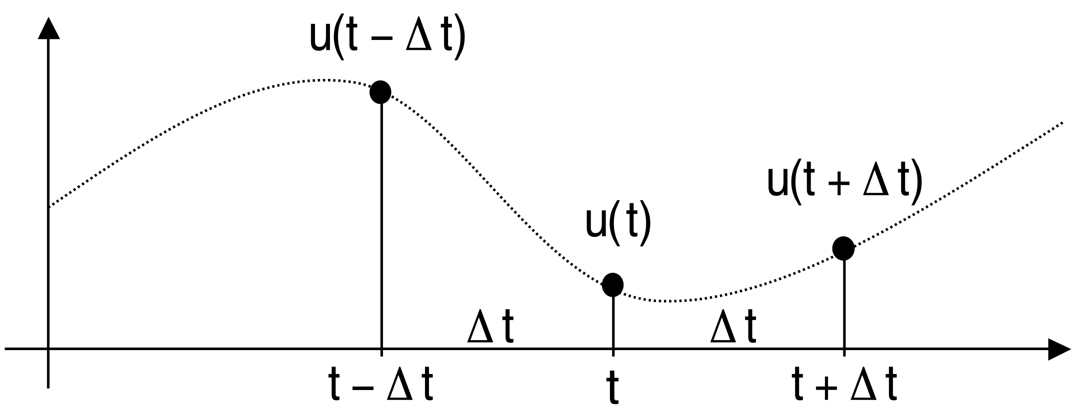
CVRTI

Discretization of 1D-Operators: 1st Temporal Derivative

Forward $$u_t(x,t) = \lim_{\Delta t \to 0} \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} \quad \to \quad u_t(k,n) = \frac{u(k,n+1) - u(k,n)}{\Delta t}$$

Backward $$u_t(x,t) = \lim_{\Delta t \to 0} \frac{u(x,t) - u(x,t-\Delta t)}{\Delta t} \quad \to \quad u_t(k,n) = \frac{u(k,n) - u(k,n-1)}{\Delta t}$$

Central $$u_t(x,t) = \lim_{\Delta t \to 0} \frac{u(x,t+\Delta t) - u(x,t-\Delta t)}{2\Delta t} \quad \to \quad u_t(k,n) = \frac{u(k,n+1) - u(k,n-1)}{2\Delta t}$$



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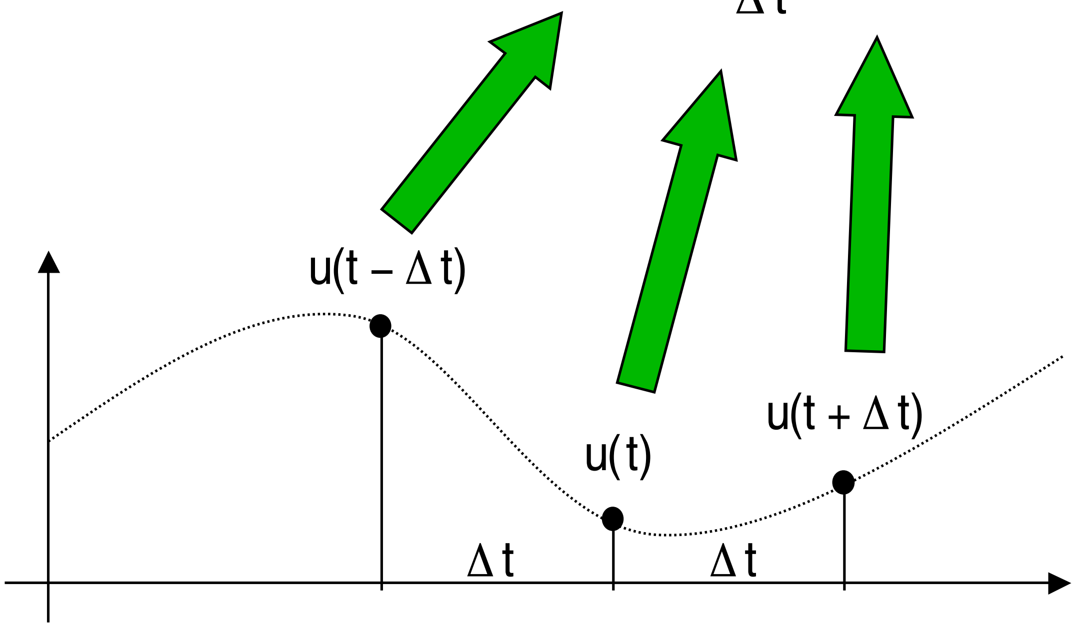
Discretization of 1D-Operators: 2nd Temporal Derivative

$$u_{tt}(k,n) = \frac{u_t\left(k,n+\tfrac{1}{2}\right) - u_t\left(k,n-\tfrac{1}{2}\right)}{\Delta t} \text{ mit } u_t(k,n) = \frac{u\left(k,n+\tfrac{1}{2}\right) - u\left(k,n-\tfrac{1}{2}\right)}{\Delta t}$$

$$\rightarrow \quad u_{tt}(k,n) = \frac{u(k,n+1) - 2u(k,n) + u(k,n-1)}{\Delta t^2}$$



CVRTI

Discretization of 2D-Operators: 1st/2nd Spatial Derivative

$$u_x(x,y) = \lim_{\Delta x \to 0} \frac{u(x+\Delta x, y) - u(x-\Delta x, y)}{2\Delta x} \quad \rightarrow \quad u_x(k,j) = \frac{u(k+1,j) - u(k-1,j)}{2\Delta x}$$

$$u_y(x,y) = \lim_{\Delta x \to 0} \frac{u(x, y+\Delta y) - u(x, y-\Delta y)}{2\Delta y} \quad \rightarrow \quad u_y(k,j) = \frac{u(k,j+1) - u(k,j-1)}{2\Delta y}$$

$$u_{xx}(x,y) = \lim_{\Delta x \to 0} \frac{u_x\left(x + \frac{\Delta x}{2}, y\right) - u_x\left(x - \frac{\Delta x}{2}, y\right)}{\Delta x} \quad \rightarrow \quad u_{xx}(k,j) = \frac{u(k+1,j) - 2u(k,j) + u(k-1,j)}{\Delta x^2}$$

$$u_{yy}(x,y) = \lim_{\Delta y \to 0} \frac{u_y\left(x, y + \frac{\Delta y}{2}\right) - u_y\left(x, y - \frac{\Delta y}{2}\right)}{\Delta y} \quad \rightarrow \quad u_{yy}(k,j) = \frac{u(k,j+1) - 2u(k,j) + u(k,j-1)}{\Delta y^2}$$

$$u_{xy}(x,y) = \lim_{\Delta y \to 0} \frac{u_x\left(x, y + \frac{\Delta y}{2}\right) - u_x\left(x, y - \frac{\Delta y}{2}\right)}{\Delta y} \quad \rightarrow \quad u_{xy}(k,j) = \frac{u(k+1,j+1) - u(k-1,j+1) - u(k+1,j-1) + u(k-1,j-1)}{4\Delta x \Delta y}$$

Usage e.g. with 2D Poisson equation
Proceeding similar to discretization of mixed function u(x,t)

CVRTI

Discretization of 3D-Operators: div / grad of Scalar Functions

$$\nabla u(\vec{x}) = \begin{pmatrix} \dfrac{\partial u}{\partial x_1} \\ \dfrac{\partial u}{\partial x_2} \\ \dfrac{\partial u}{\partial x_3} \end{pmatrix} \rightarrow \nabla u(\vec{k}) = \begin{pmatrix} \dfrac{u(k_1+1,k_2,k_3) - u(k_1-1,k_2,k_3)}{2\Delta k_1} \\ \dfrac{u(k_1,k_2+1,k_3) - u(k_1,k_2-1,k_3)}{2\Delta k_2} \\ \dfrac{u(k_1,k_2,k_3+1) - u(k_1,k_2,k_3-1)}{2\Delta k_3} \end{pmatrix}$$

$$\nabla \cdot u(\vec{x}) = \frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} + \frac{\partial u}{\partial x_3}$$

$$\rightarrow \nabla \cdot u(\vec{k}) = \frac{u(k_1+1,k_2,k_3) - u(k_1-1,k_2,k_3)}{2\Delta k_1} + \frac{u(k_1,k_2+1,k_3) - u(k_1,k_2-1,k_3)}{2\Delta k_2} + \frac{u(k_1,k_2,k_3+1) - u(k_1,k_2,k_3-1)}{2\Delta k_3}$$

CVRTI

Discretization of 3D-Operators: rot of Vectorial Functions

$$\nabla \times \vec{A}(\vec{x}) = \begin{pmatrix} \dfrac{\partial A_3}{\partial x_2} - \dfrac{\partial A_2}{\partial x_3} \\ \dfrac{\partial A_1}{\partial x_3} - \dfrac{\partial A_3}{\partial x_1} \\ \dfrac{\partial A_2}{\partial x_1} - \dfrac{\partial A_1}{\partial x_2} \end{pmatrix}$$

$$\rightarrow \nabla \times \vec{A}\left(\vec{k}\right) = \begin{pmatrix} \dfrac{A_3(k_1,k_2+1,k_3) - A_3(k_1,k_2-1,k_3)}{2\Delta k_2} - \dfrac{A_2(k_1,k_2,k_3+1) - A_2(k_1,k_2,k_3-1)}{2\Delta k_3} \\ \dfrac{A_1(k_1,k_2,k_3+1) - A_1(k_1,k_2,k_3-1)}{2\Delta k_3} - \dfrac{A_3(k_1+1,k_2,k_3) - A_3(k_1-1,k_2,k_3)}{2\Delta k_1} \\ \dfrac{A_2(k+1_1,k_2,k_3) - A_2(k_1-1,k_2,k_3)}{2\Delta k_1} - \dfrac{A_1(k_1,k_2+1,k_3) - A_1(k_1,k_2-1,k_3)}{2\Delta k_2} \end{pmatrix}$$

CVRTI

Discretization of 1D Wave Equation with Central Differences

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

v: Velocity of wave propagation

$$u_{tt}(k,n) = v^2 u_{xx}(k,n)$$

$$\frac{u(k,n+1) - 2u(k,n) + u(k,n-1)}{\Delta t^2} = v^2 \frac{u(k+1,n) - 2u(k,n) + u(k-1,n)}{\Delta x^2}$$

$$\frac{u(k,n+1)}{\Delta t^2} = v^2 \frac{u(k+1,n) - 2u(k,n) + u(k-1,n)}{\Delta x^2} - \frac{u(k,n-1) - 2u(k,n)}{\Delta t^2}$$

$$u(k,n+1) = \Delta t^2 v^2 \frac{u(k+1,n) - 2u(k,n) + u(k-1,n)}{\Delta x^2} - u(k,n-1) + 2u(k,n)$$

k: Spatial coordinate/index

n: Temporal coordinate/index

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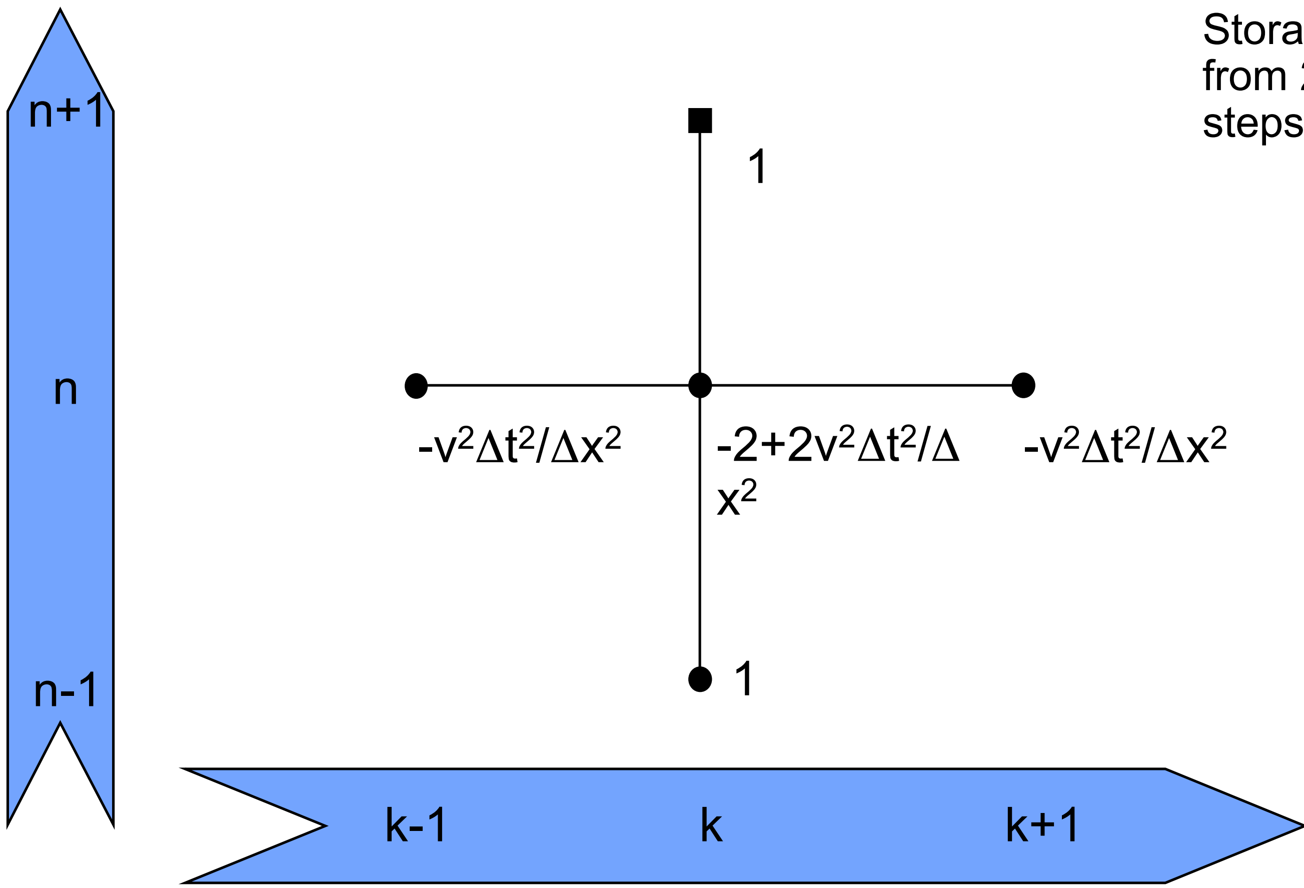
Schematic of 1D Wave Equation with Central Differences

Storage of node values from 2 previous time steps necessary!



CVRTI

Discretization of 1D Diffusion Equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)$$

D: Diffusion coefficient

$$u_t(k,n) = D\, u_{xx}(k,n)$$

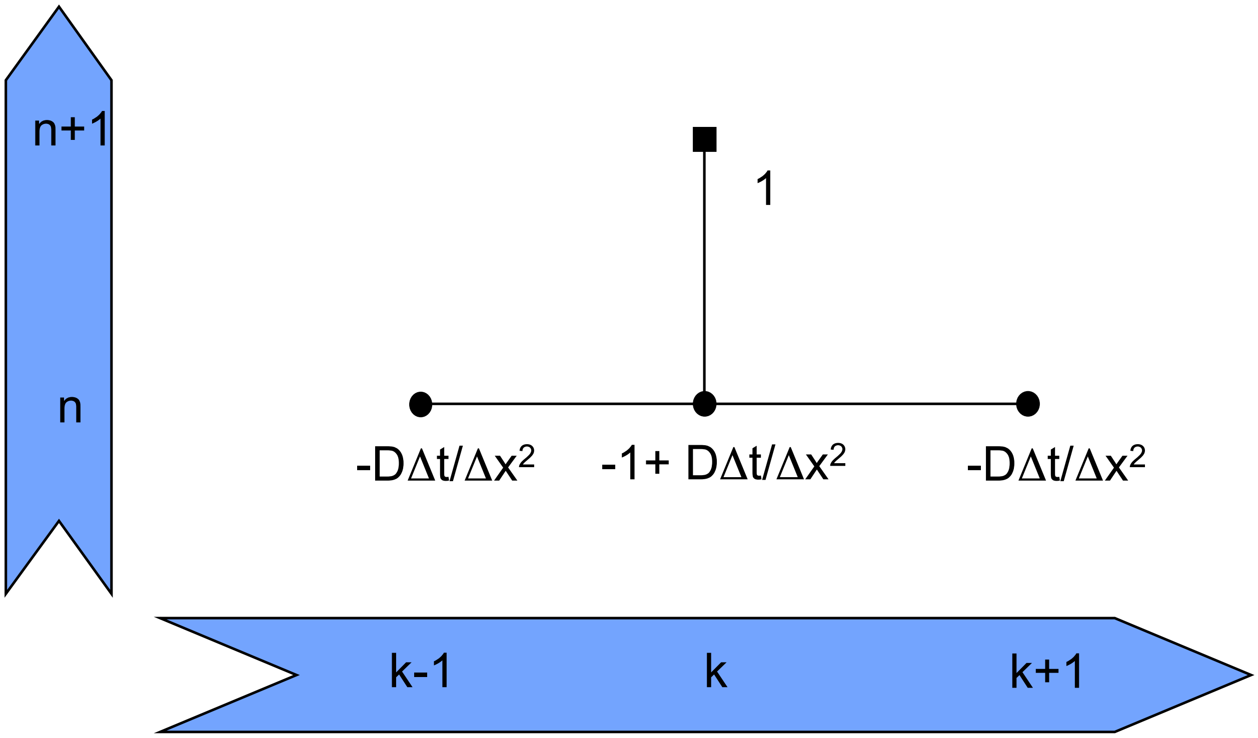
$$\frac{u(k,n) - u(k,n+1)}{\Delta t} = D\frac{u(k+1,n) - 2u(k,n) + u(k-1,n)}{\Delta x^2}$$

$$\frac{u(k,n+1)}{\Delta t} = D\frac{u(k+1,n) - 2u(k,n) + u(k-1,n)}{\Delta x^2} + \frac{u(k,n)}{\Delta t}$$

$$u(k,n+1) = \Delta t\, D\frac{u(k+1,n) - 2u(k,n) + u(k-1,n)}{\Delta x^2} + u(k,n)$$

CVRTI

Schematic of 1D Diffusion Equation



CVRTI

Discretization of 2D Poisson Equation

$$\rho(x,y) = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

$\rho(x,y)$: Source term

$$\rho(k,l) = u_{xx}(k,l) + u_{yy}(k,l)$$

$$\rho(k,l) = \frac{u(k+1,l) - 2u(k,l) + u(k-1,l)}{\Delta x^2} + \frac{u(k,l+1) - 2u(k,l) + u(k,l-1)}{\Delta y^2}$$

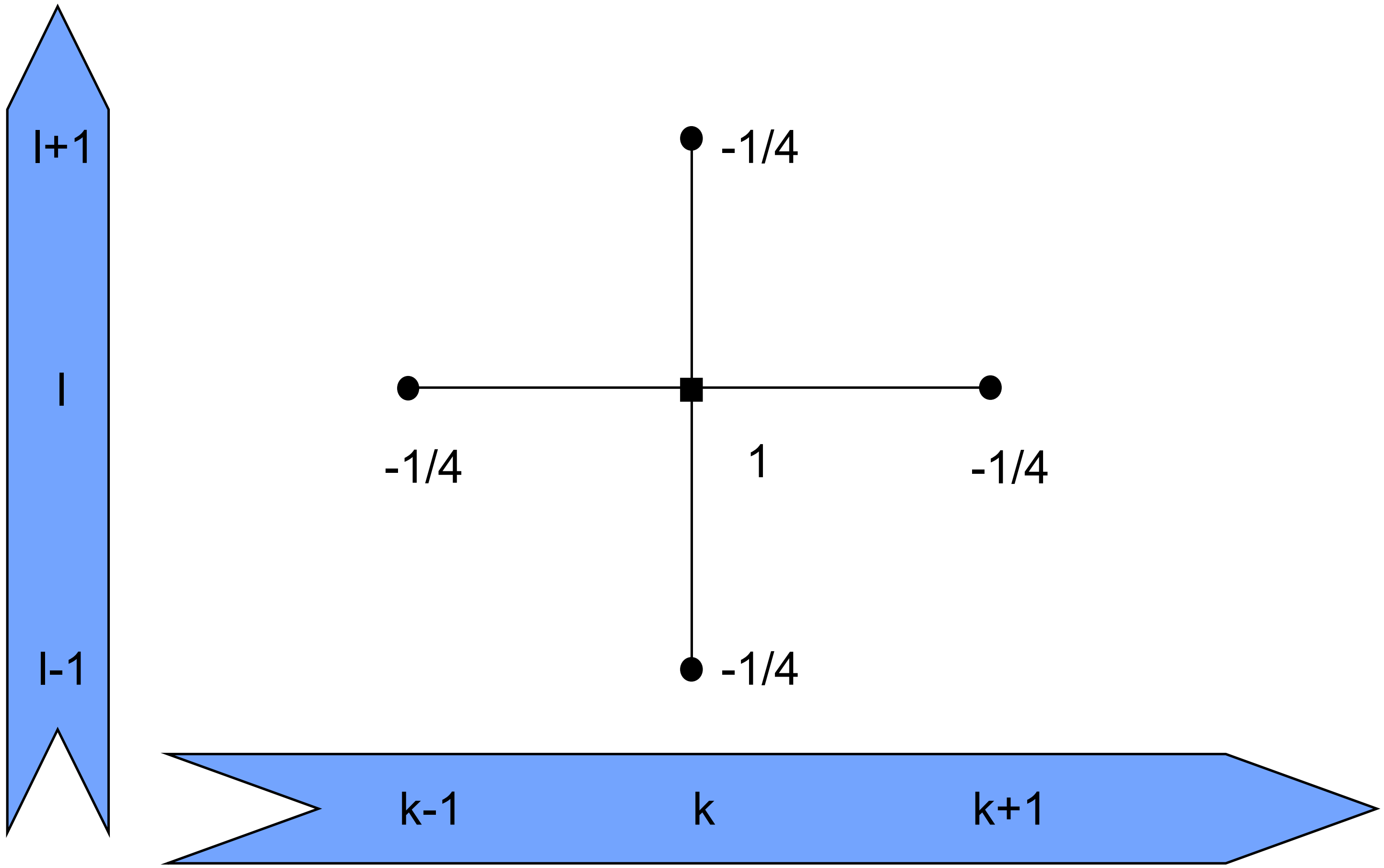
$$\frac{2u(k,l)}{\Delta x^2} + \frac{2u(k,l)}{\Delta y^2} = \frac{u(k+1,l) + u(k-1,l)}{\Delta x^2} + \frac{u(k,l+1) + u(k,l-1)}{\Delta y^2} - \rho(k,l)$$

$$\Delta x^2 = \Delta y^2 = \Delta^2$$

$$\rightarrow \quad u(k,l) = \frac{u(k+1,l) + u(k-1,l) + u(k,l+1) + u(k,l-1)}{4} - \frac{\Delta^2 \rho(k,l)}{4}$$

CVRTI

Schematic of 2D Poisson Equation



CVRTI

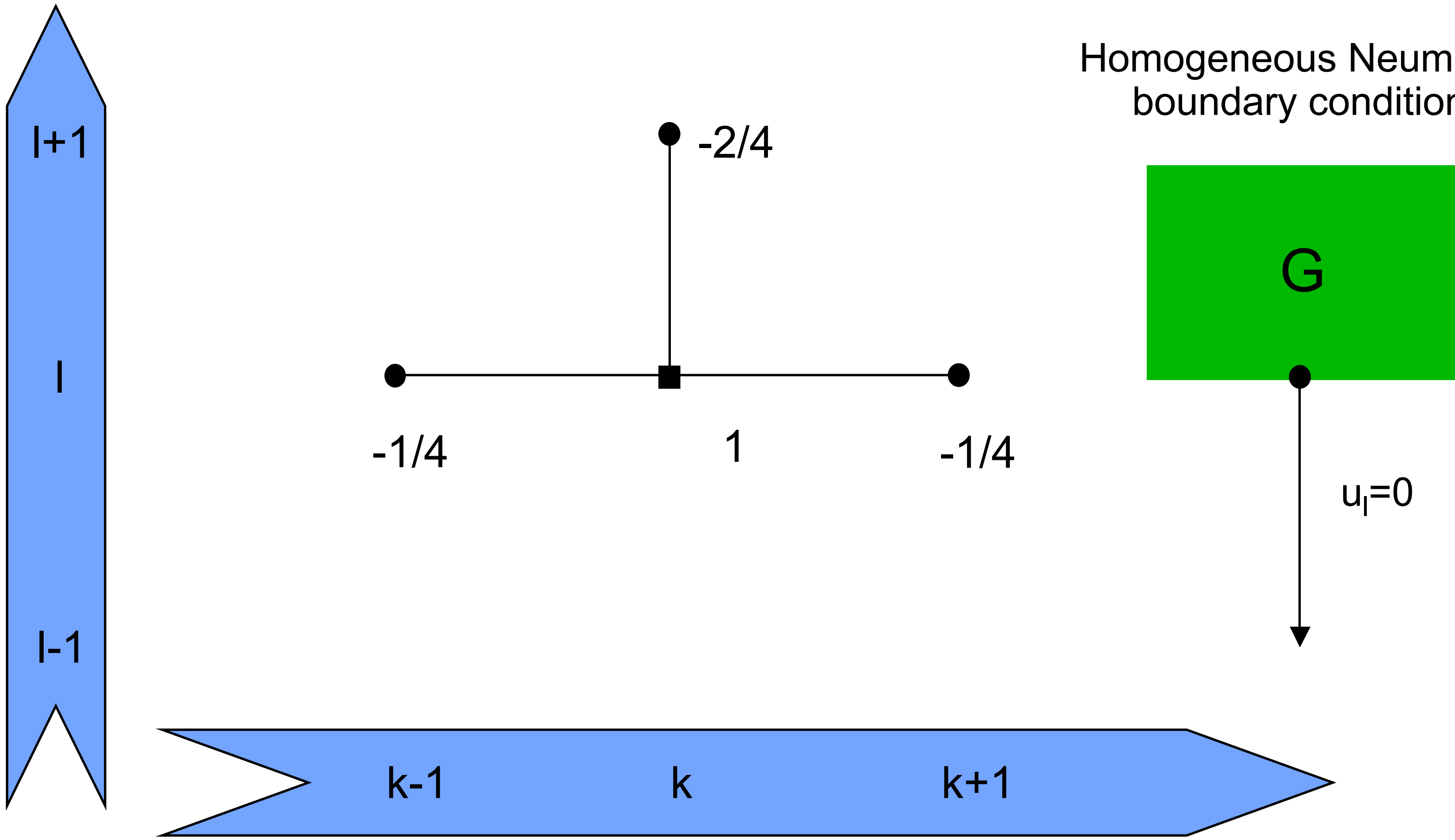
System Matrix For 2D Poisson Equation

$$\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & -.25 & & & \\ & & & -.25 & & & \\ & -.25 & -.25 & 1 & -.25 & -.25 & \\ & & & -.25 & & & \\ & & & -.25 & & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{k,l-1} \\ \phi_{k-1,l} \\ \phi_{k,l} \\ \phi_{k+1,l} \\ \phi_{k,l+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \vdots \\ \vdots \\ -\frac{\Delta^2 \rho(k,l)}{4} \\ \vdots \\ \vdots \\ \vdots \end{pmatrix}$$

- large dimension
- sparse
- banded
- symmetric
- positive semidefinite $\forall_{\vec{\phi}_s} \quad \vec{\phi}_s^T A_s \vec{\phi}_s \geq 0$

CVRTI

Schematic of 2D Poisson Equation with Boundary Condition



Group Work

How can the approximation error be controlled in
- finite differences and
- finite elements methods?

CVRTI