Simulation and Scientific Computing

(Simulation und Wissenschaftliches Rechnen - SiWiR)

Winter Term 2014/15

Florian Schornbaum
Chair for System Simulation

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

Assignment 2: OpenMP-Parallel Red-Black Gauss-Seidel Method

November 3, 2014 – November 25, 2014

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Finite Differences: Differential Quotients

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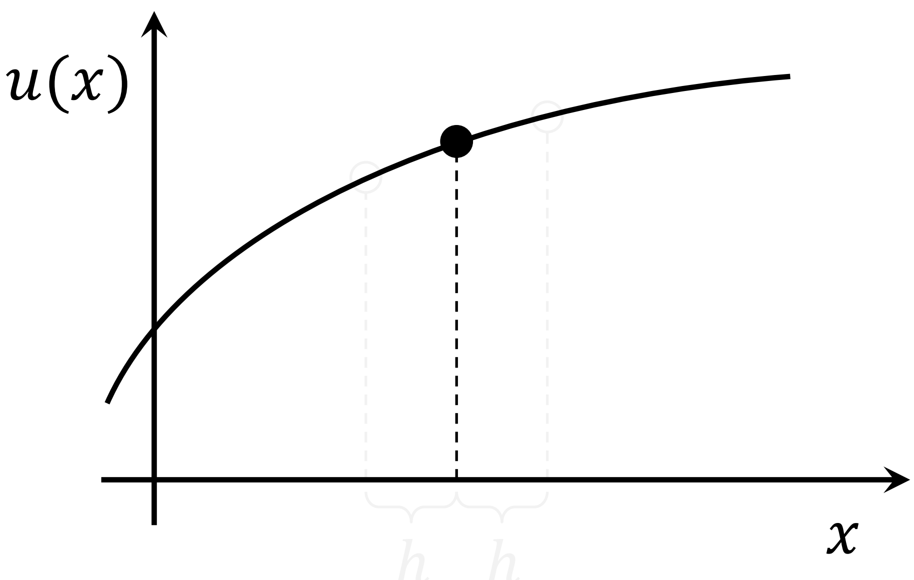
Differential Quotients

- Differential quotient for first derivative $u'(x) = \frac{\partial u(x)}{\partial x}$:
  - forward difference: $\frac{u(x+h)-u(x)}{h}$
  - backward difference: $\frac{u(x)-u(x-h)}{h}$
  - central difference: $\frac{u(x+h)-u(x-h)}{2h}$



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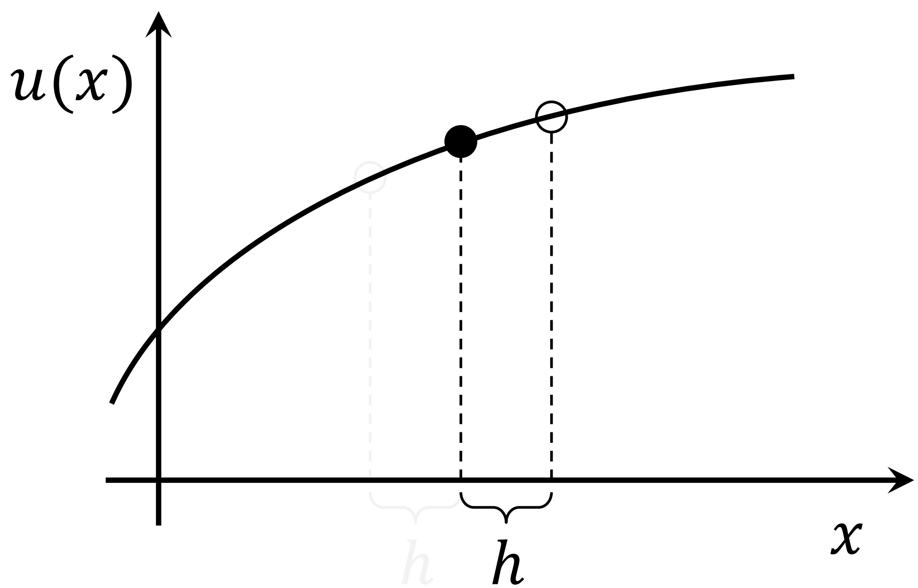

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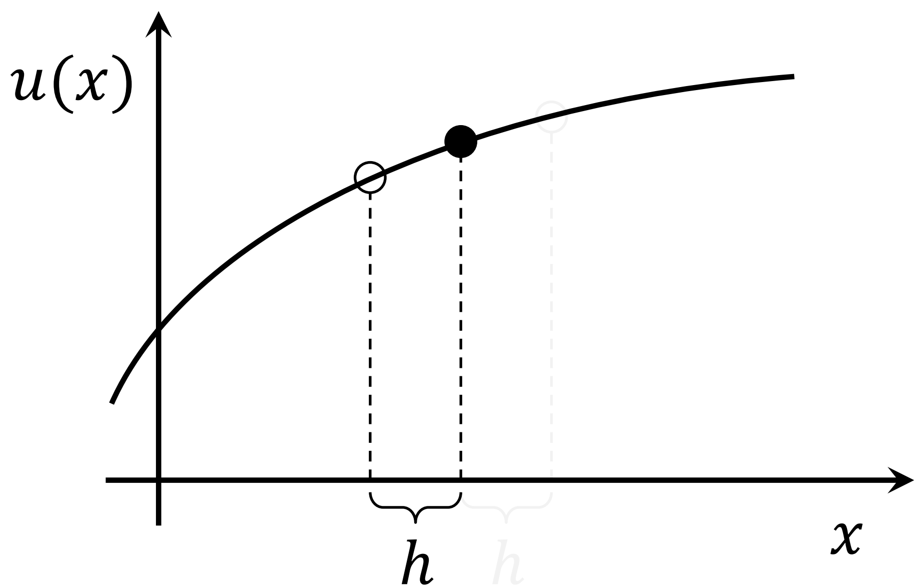

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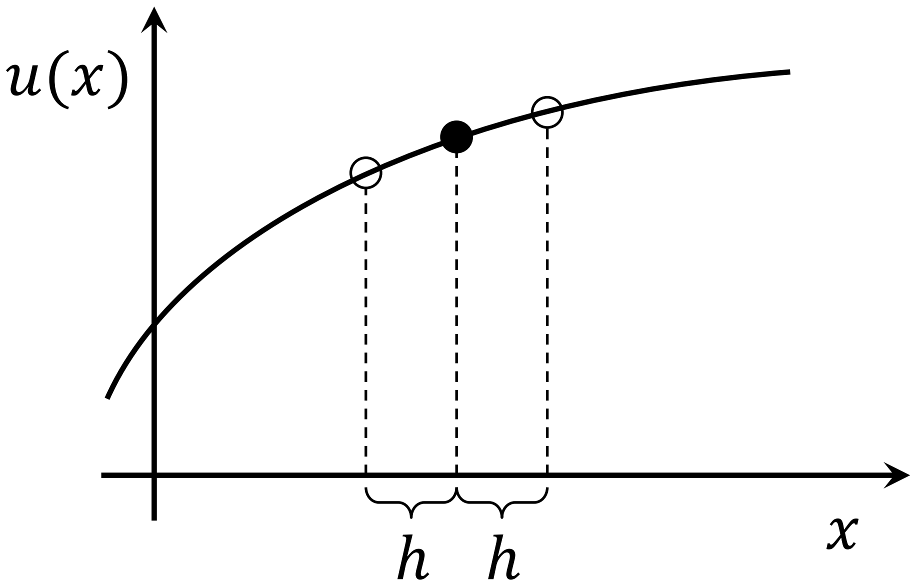


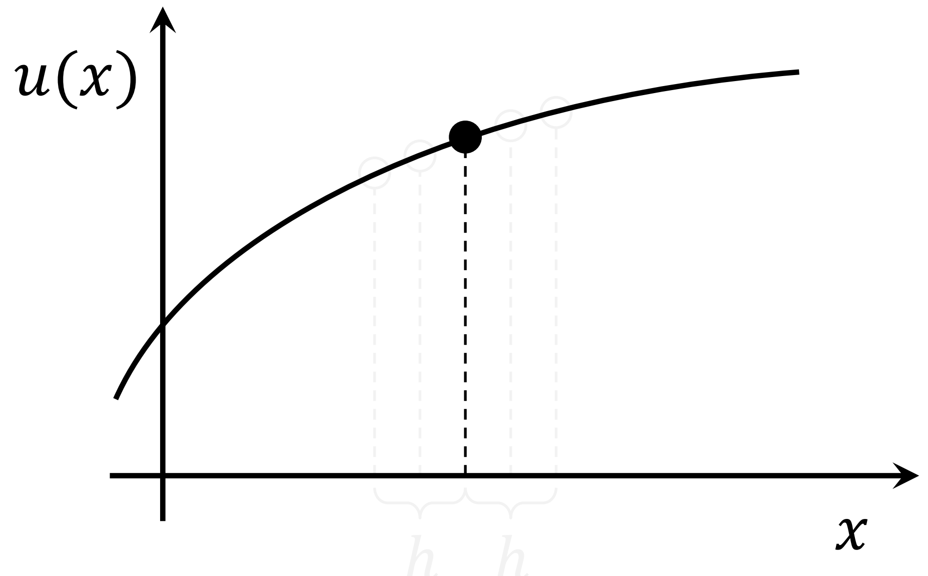
Differential Quotients

- Differential quotient for second derivative $u''(x) = \frac{\partial^2 u(x,y)}{\partial x^2}$:

$$\frac{\partial^2 u(x,y)}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial u(x)}{\partial x}\right) \approx \frac{\frac{u(x+h)-u(x)}{h} - \frac{u(x)-u(x-h)}{h}}{h}$$

$$= \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

three central differences with $^h/_2$!



Differential Quotients

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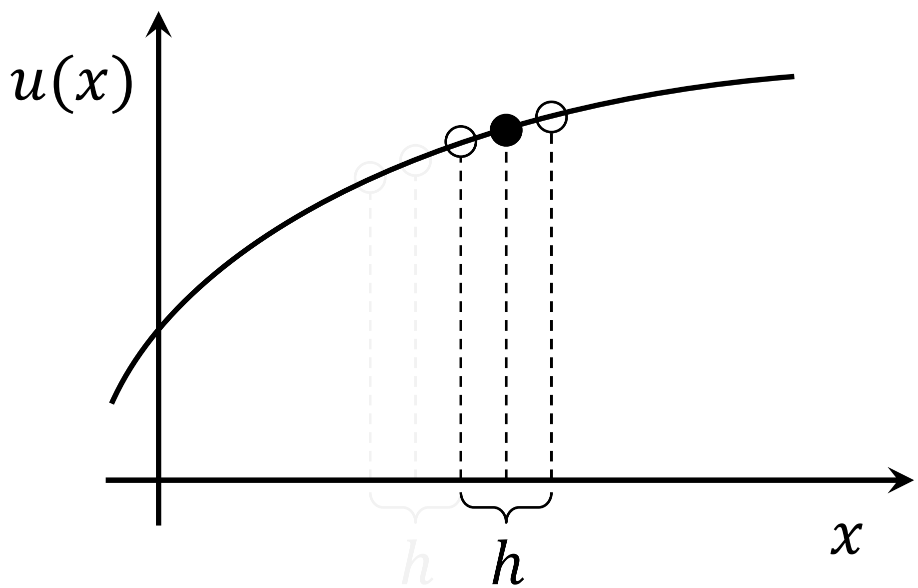

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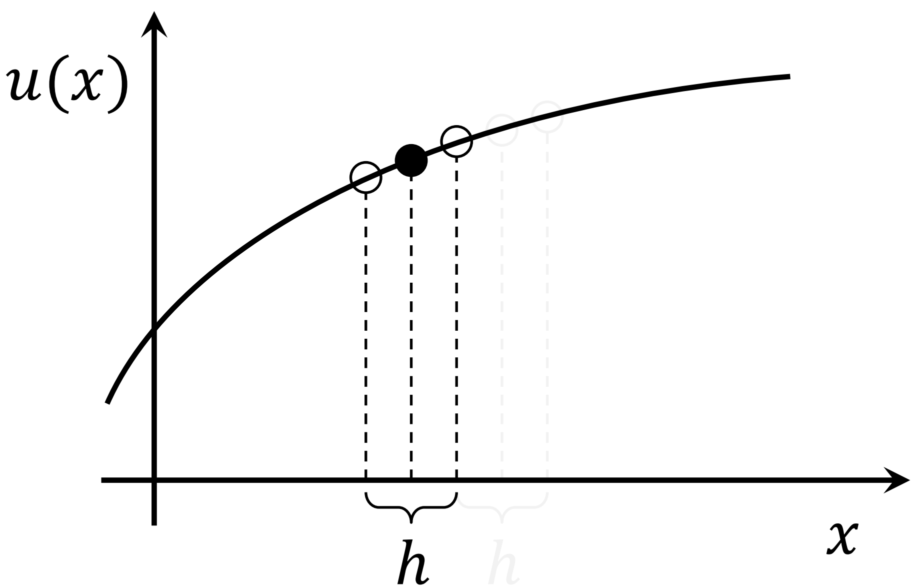

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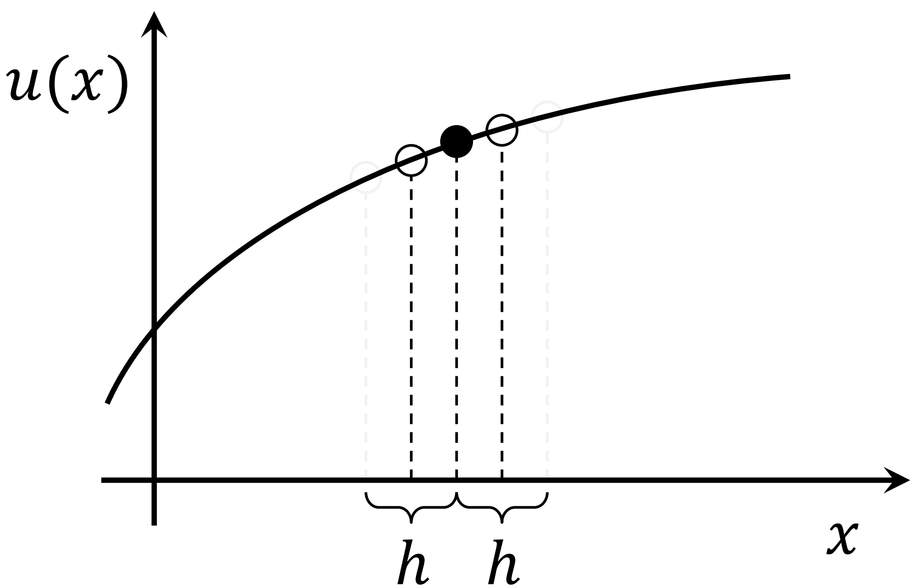

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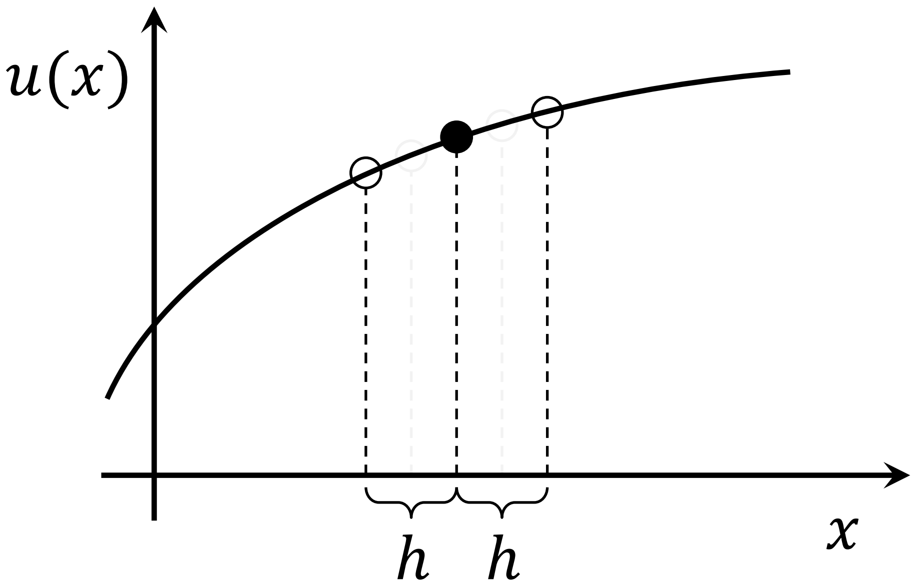

Finite Differences: Discretization

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Finite Differences - Discretization

- Example – Poisson's equation:

$$\Delta u(x,y) = f(x,y) \quad in\ \Omega$$
$$u(x,y) = g(x,y) \quad on\ \delta\Omega\ (Dirichlet\ boundaries)$$

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

- Discretization using **differential quotients** for $\Delta u(x,y)$:

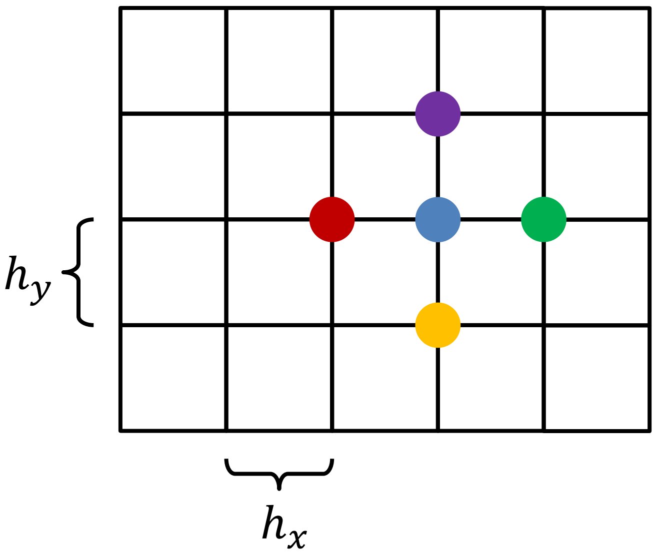
$$\frac{u(x-h_x,y) - 2u(x,y) + u(x+h_x,y)}{h_x^2} + \frac{u(x,y-h_y) - 2u(x,y) + u(x,y+h_y)}{h_y^2} = f(x,y)$$

Finite Differences - Discretization

- Discretization using differential quotients for $\Delta u(x, y)$:

$$\frac{1}{h_x^2}\left[u(x-h_x,y)+u(x+h_x,y)\right]+\frac{1}{h_y^2}\left[u\left(x,y-h_y\right)+u\left(x,y+h_y\right)\right] - \left(\frac{2}{h_x^2}+\frac{2}{h_y^2}\right)u(x,y)=f(x,y)$$

- We are solving Poisson's equation on a **discretized domain** Ω:



$u(x,y)\ /\ f(x,y)$

$u(x-h_x,y)$

$u(x+h_x,y)$

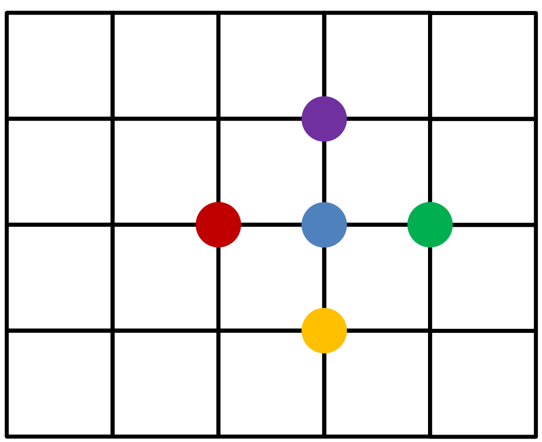
$u\left(x,y-h_y\right)$

$u\left(x,y+h_y\right)$

Finite Differences - Discretization

- For every point $u_{x,y}$ on the grid, we can formulate a linear equation:

$$\frac{1}{h_x^2}\left(u_{x-1,y}+u_{x+1,y}\right)+\frac{1}{h_y^2}\left(u_{x,y-1}+u_{x,y+1}\right)-\left(\frac{2}{h_x^2}+\frac{2}{h_y^2}\right)u_{x,y}=f_{x,y}$$



$u_{x,y}$ / $f_{x,y}$

$u_{x-1,y}$

$u_{x+1,y}$

$u_{x,y-1}$

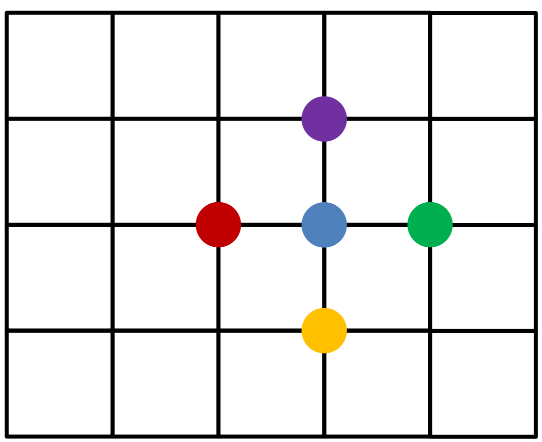
$u_{x,y+1}$

$$\underbrace{\begin{bmatrix} 0 & \frac{1}{h_y^2} & 0 \\ \frac{1}{h_x^2} & -\left(\frac{2}{h_x^2}+\frac{2}{h_y^2}\right) & \frac{1}{h_x^2} \\ 0 & \frac{1}{h_y^2} & 0 \end{bmatrix}}_{\text{stencil}}$$

Finite Differences - Discretization

- For every point $u_{x,y}$ on the grid, we can formulate a linear equation:

$$\frac{1}{h_x^2}\left(u_{x-1,y} + u_{x+1,y}\right) + \frac{1}{h_y^2}\left(u_{x,y-1} + u_{x,y+1}\right) - \left(\frac{2}{h_x^2} + \frac{2}{h_y^2}\right) u_{x,y} = f_{x,y}$$



$u_{x,y}$ / $f_{x,y}$

$u_{x-1,y}$

$u_{x+1,y}$

$u_{x,y-1}$

$u_{x,y+1}$

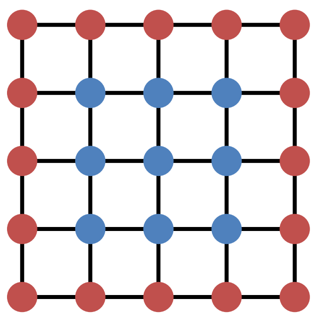
$$\left.\begin{bmatrix} 0 & \gamma & 0 \\ \beta & \alpha & \beta \\ 0 & \gamma & 0 \end{bmatrix}\right\} \text{stencil}$$

$$\alpha = -\left(\frac{2}{h_x^2} + \frac{2}{h_y^2}\right)$$

$$\beta = \frac{1}{h_x^2} \quad \gamma = \frac{1}{h_y^2}$$

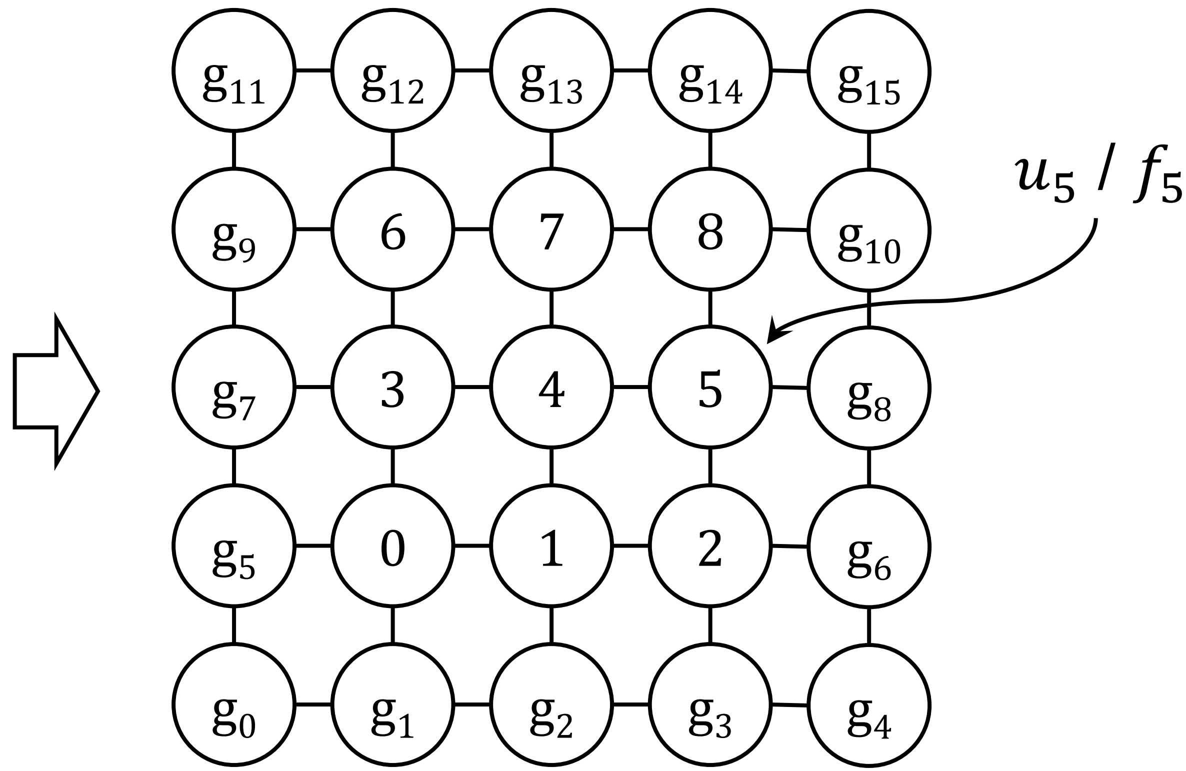
Finite Differences - Discretization

- Solving Poisson's equation $\Delta u(x, y) = f(x, y)$ with $u(x, y) = g(x, y)$ on the boundary $\delta\Omega$ on 5×5 grid with 9 unknowns:



domain Ω
boundary $\delta\Omega$

$\Rightarrow$ 9 unknown values ($u_0 \dots u_8$)



Finite Differences - Discretization

- Solving Poisson's equation $\Delta u(x,y) = f(x,y)$ with $u(x,y) = g(x,y)$ on the boundary $\delta\Omega$ on 5×5 grid with 9 unknowns:

$$\underbrace{\begin{bmatrix} \alpha & \beta & 0 & \gamma & 0 & 0 & 0 & 0 & 0 \\ \beta & \alpha & \beta & 0 & \gamma & 0 & 0 & 0 & 0 \\ 0 & \beta & \alpha & 0 & 0 & \gamma & 0 & 0 & 0 \\ \gamma & 0 & 0 & \alpha & \beta & 0 & \gamma & 0 & 0 \\ 0 & \gamma & 0 & \beta & \alpha & \beta & 0 & \gamma & 0 \\ 0 & 0 & \gamma & 0 & \beta & \alpha & 0 & 0 & \gamma \\ 0 & 0 & 0 & \gamma & 0 & 0 & \alpha & \beta & 0 \\ 0 & 0 & 0 & 0 & \gamma & 0 & \beta & \alpha & \beta \\ 0 & 0 & 0 & 0 & 0 & \gamma & 0 & \beta & \alpha \end{bmatrix}}_{A} \cdot \underbrace{\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{bmatrix}}_{u} = \underbrace{\begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \end{bmatrix}}_{f} - \underbrace{\begin{bmatrix} \beta g_5 + \gamma g_1 \\ \gamma g_2 \\ \beta g_6 + \gamma g_3 \\ \beta g_7 \\ 0 \\ \beta g_8 \\ \beta g_9 + \gamma g_{12} \\ \gamma g_{13} \\ \beta g_{10} + \gamma g_{14} \end{bmatrix}}_{\tilde{g}}$$

Finite Differences - Discretization

- Solving Poisson's equation $\Delta u(x,y) = f(x,y)$ with $u(x,y) = g(x,y)$ on the boundary $\delta\Omega$ on 5×5 grid with 9 unknowns:

$$
\begin{bmatrix}
\alpha & \beta & 0 & \gamma & 0 & 0 & 0 & 0 & 0 \\
\beta & \alpha & \beta & 0 & \gamma & 0 & 0 & 0 & 0 \\
0 & \beta & \alpha & 0 & 0 & \gamma & 0 & 0 & 0 \\
\gamma & 0 & 0 & \alpha & \beta & 0 & \gamma & 0 & 0 \\
0 & \gamma & 0 & \beta & \alpha & \beta & 0 & \gamma & 0 \\
0 & 0 & \gamma & 0 & \beta & \alpha & 0 & 0 & \gamma \\
0 & 0 & 0 & \gamma & 0 & 0 & \alpha & \beta & 0 \\
0 & 0 & 0 & 0 & \gamma & 0 & \beta & \alpha & \beta \\
0 & 0 & 0 & 0 & 0 & \gamma & 0 & \beta & \alpha
\end{bmatrix}
\cdot
\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{bmatrix}
=
\begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \end{bmatrix}
-
\begin{bmatrix} \beta g_5 + \gamma g_1 \\ \gamma g_2 \\ \beta g_6 + \gamma g_3 \\ \beta g_7 \\ 0 \\ \beta g_8 \\ \beta g_9 + \gamma g_{12} \\ \gamma g_{13} \\ \beta g_{10} + \gamma g_{14} \end{bmatrix}
$$

One "block" on the diagonal of the matrix for each row/line in the grid.

$$\Rightarrow \; Au = f + \tilde{g}$$

Finite Differences: Consistency

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Finite Differences - Consistency

- Taylor Expansion for $u(x+h)$:

$$\xi^+ \in \,]x, x+h[$$

$$\begin{aligned} u(x+h) &= u(x) + hu'(x) + \tfrac{h^2}{2}u''(\xi^+) && (1)\\ &= u(x) + hu'(x) + \tfrac{h^2}{2}u''(x) + \tfrac{h^3}{6}u^{(3)}(\xi^+) && (2)\\ &= u(x) + hu'(x) + \tfrac{h^2}{2}u''(x) + \tfrac{h^3}{6}u^{(3)}(x) + \tfrac{h^4}{24}u^{(4)}(\xi^+) && (3) \end{aligned}$$

- Taylor Expansion for $u(x-h)$:

$$\xi^- \in \,]x-h, x[$$

$$\begin{aligned} u(x-h) &= u(x) - hu'(x) + \tfrac{h^2}{2}u''(\xi^-) && (4)\\ &= u(x) - hu'(x) + \tfrac{h^2}{2}u''(x) - \tfrac{h^3}{6}u^{(3)}(\xi^-) && (5)\\ &= u(x) - hu'(x) + \tfrac{h^2}{2}u''(x) - \tfrac{h^3}{6}u^{(3)}(x) + \tfrac{h^4}{24}u^{(4)}(\xi^-) && (6) \end{aligned}$$

- For this to work, the function u must be C^2, C^3, or C^4 continuous in the neighborhood of x,respectively.

Finite Differences - Consistency

- First derivative – forward difference [using (1)]:

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2}u''(\xi^+)$$
$$\Rightarrow \frac{u(x+h)-u(x)}{h} = u'(x) + \frac{h}{2}u''(\xi^+)$$
$$\Rightarrow \left|\frac{u(x+h)-u(x)}{h} - u'(x)\right| \le h \cdot C$$

$\Rightarrow$ first order consistent approximation of $u'(x)$

- First derivative – backward difference [using (4)]:

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2}u''(\xi^-)$$
$$\Rightarrow \frac{u(x)-u(x-h)}{h} = u'(x) - \frac{h}{2}u''(\xi^-)$$
$$\Rightarrow \left|\frac{u(x)-u(x-h)}{h} - u'(x)\right| \le h \cdot C$$

$\Rightarrow$ first order consistent approximation of $u'(x)$

Finite Differences - Consistency

- First derivative – central difference [using $(2) - (5)$]:

$$\begin{aligned} u(x+h) - u(x-h) & \\ &= u(x) + hu'(x) + \tfrac{h^2}{2}u''(x) + \tfrac{h^3}{6}u^{(3)}(\xi^+) \\ &- \left(u(x) - hu'(x) + \tfrac{h^2}{2}u''(x) - \tfrac{h^3}{6}u^{(3)}(\xi^-)\right) \\ &= 2hu'(x) + \tfrac{h^3}{6}\left(u^{(3)}(\xi^+) + u^{(3)}(\xi^-)\right) \end{aligned}$$

$$\Rightarrow \frac{u(x+h)-u(x-h)}{2h} = u'(x) + \frac{h^2}{3}\left(u^{(3)}(\xi^+) + u^{(3)}(\xi^-)\right)$$

$$\Rightarrow \left|\frac{u(x+h)-u(x-h)}{2h} - u'(x)\right| \le h^2 \cdot C$$

$\Rightarrow$ second order consistent approximation of $u'(x)$

Finite Differences - Consistency

- Second derivative [using $(3) + (6)$]:

$$
\begin{aligned}
u(x+h) + u(x-h) \\
&= u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u^{(3)}(x) + \frac{h^4}{24}u^{(4)}(\xi^+) \\
&+ \left(u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u^{(3)}(x) + \frac{h^4}{24}u^{(4)}(\xi^-)\right) \\
&= 2u(x) + h^2u''(x) + \frac{h^4}{24}\left(u^{(4)}(\xi^+) + u^{(4)}(\xi^-)\right)
\end{aligned}
$$

$$\Rightarrow \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = u''(x) + \frac{h^2}{24}\left(u^{(4)}(\xi^+) + u^{(4)}(\xi^-)\right)$$

$$\Rightarrow \left|\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} - u''(x)\right| \leq h^2 \cdot C$$

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Finite Differences: Convergence

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Finite Differences - Convergence

- Split matrix A into a diagonal, lower, and upper triangular matrix:

$$Au = f \quad \Rightarrow \quad A = D - L - U = \begin{bmatrix} \times & & \\ & \times & \\ & & \times \end{bmatrix} - \begin{bmatrix} & & \\ \times & & \\ \times & \times & \end{bmatrix} - \begin{bmatrix} & \times & \times \\ & & \times \\ & & \end{bmatrix}$$

- Jacobi iteration:

$$u^{k+1} = \underbrace{D^{-1}(L+U)}_{C_J \text{ (iteration matrix)}} u^k + D^{-1} f$$

- Gauss-Seidel iteration:

$$u^{k+1} = \underbrace{(D-L)^{-1} U}_{C_G \text{ (iteration matrix)}} u^k + (D-L)^{-1} f$$

Finite Differences - Convergence

- These iterative methods converge if and only if the spectral radius of the iteration C matrix satisfies $\rho(C) < 1$.

- If A is strictly diagonally dominant:

$$\rho(C) \leq \|C\|_\infty = \max_i \sum_j |c_{ij}| \leq \max_i \frac{1}{|a_{ii}|} \sum_{i \neq j} |a_{ij}|$$

- If Jacobi converges, Gauss-Seidel also converges: $\rho(C_G) < \rho(C_J)$

- $\|C\|_\infty$, an upper bound for the convergence factor:

$$e^k := \tilde{u} - u^k \quad (\tilde{u}\text{: exact solution})$$

$$\Rightarrow \quad \left\|e^{k+1}\right\|_\infty \leq \|C\|_\infty^{k+1} \left\|e^k\right\|_\infty$$

Finite Differences: Additional Resources

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Finite Differences

- Additional material on finite differences by Pascal Frey:

  http://www.ann.jussieu.fr/~frey/cours/UPMC/finite-differences.pdf

  $\Rightarrow$ get it and read it!

- Another well written article on solving linear systems by the same author which might also be worth reading:

  http://www.ann.jussieu.fr/~frey/cours/UPMC/linear%20systems.pdf

The End

Questions ?