Computational comparison of the discretization and iteration errors

Tomáš Vejchodský (vejchod@math.cas.cz)

Institute of Mathematics, Academy of Sciences
Žitná 25, 115 67 Prague 1
Czech Republic

Iteration error

- $-\Delta u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega$
- $u_h \in V_h : \quad \underbrace{\int_\Omega \nabla u_h \cdot \nabla v_h \,\mathrm{d}x}_{a(u_h, v_h)} = \underbrace{\int_\Omega f v_h \,\mathrm{d}x}_{F(v_h)} \quad \forall v_h \in V_h$
- $u_h = \sum_{i=1}^{N_{DOF}} y_i \varphi_i \qquad Ay = b \qquad A_{ij} = a(\varphi_j, \varphi_i), \quad b_i = F(\varphi_i)$
- $u_h^* = \sum_{i=1}^{N_{DOF}} y_i^* \varphi_i \qquad Ay^* = b^*$
- $\|u - u_h^*\|_a^2 = \|u - u_h\|_a^2 + 2a(u - u_h, u_h - u_h^*) + \|u_h - u_h^*\|_a^2$

  discretization error: $\|u - u_h\|_a \approx O(h)$

  iteration error: $\|u_h - u_h^*\|_a \approx O(?)$ $\qquad \|u\|_a^2 = a(u, u)$

Iteration error

- $-\Delta u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega$
- $u_h \in V_h : \quad \underbrace{\int_\Omega \nabla u_h \cdot \nabla v_h \, \mathrm{d}x}_{a(u_h, v_h)} = \underbrace{\int_\Omega f v_h \, \mathrm{d}x}_{F(v_h)} \quad \forall v_h \in V_h$
- $u_h = \sum_{i=1}^{N_{DOF}} y_i \varphi_i \qquad Ay = b \qquad A_{ij} = a(\varphi_j, \varphi_i)$, $b_i = F(\varphi_i)$
- $u_h^* = \sum_{i=1}^{N_{DOF}} y_i^* \varphi_i \qquad Ay^* = b^*$
- $\|u - u_h^*\|_a^2 = \|u - u_h\|_a^2 + \|u_h - u_h^*\|_a^2$

  discretization error: $\|u - u_h\|_a \approx O(h)$

  iteration error: $\|u_h - u_h^*\|_a \approx O(?)$ $\qquad \|u\|_a^2 = a(u, u)$

Upper bound for the iteration error

Lemma

If $Ay = b, \quad Ay^* = b^*$, *and* $\varkappa(A) = \|A\| \left\|A^{-1}\right\|$ *then*

$$\frac{\|y - y^*\|}{\|y\|} \le \varkappa(A) \frac{\|b - Ay^*\|}{\|b\|}.$$

Proof.

$$\frac{\dfrac{\|y - y^*\|}{\|y\|}}{\dfrac{\|b - Ay^*\|}{\|b\|}} = \frac{\dfrac{\left\|A^{-1}(b - b^*)\right\|}{\|y\|}}{\dfrac{\|b - b^*\|}{\|Ay\|}} = \frac{\left\|A^{-1}(b - b^*)\right\|}{\|b - b^*\|} \frac{\|Ay\|}{\|y\|}$$

$$\le \left\|A^{-1}\right\| \|A\| \equiv \varkappa(A)$$

□

Choice of norm

$$\frac{\|u_h - u_h^*\|_a}{\|u_h\|_a} = \frac{\|y - y^*\|_A}{\|y\|_A} \leq \varkappa_A(A)\frac{\|b - Ay^*\|_A}{\|b\|_A} \qquad \|y\|_A^2 = y^T A y$$

$$\frac{\|u_h - u_h^*\|_{L^2(\Omega)}}{\|u_h\|_{L^2(\Omega)}} = \frac{\|y - y^*\|_M}{\|y\|_M} \leq \varkappa_M(A)\frac{\|b - Ay^*\|_M}{\|b\|_M} \qquad \|y\|_M^2 = y^T M y$$

$$\frac{\|u_h - u_h^*\|_{L^\infty(\Omega)}}{\|u_h\|_{L^\infty(\Omega)}} = \frac{\|y - y^*\|_\infty}{\|y\|_\infty} \leq \varkappa_\infty(A)\frac{\|b - Ay^*\|_\infty}{\|b\|_\infty} \qquad \|y\|_\infty = \max_i |y_i|$$

$$? = \frac{\|y - y^*\|_{\ell^2}}{\|y\|_{\ell^2}} \leq \varkappa_{\ell^2}(A)\frac{\|b - Ay^*\|_{\ell^2}}{\|b\|_{\ell^2}} \qquad \|y\|_{\ell^2}^2 = y^T y$$

$$\|u_h\|_a = \|y\|_A \qquad \|u_h\|_{L^2(\Omega)} = \|y\|_M \qquad \|u_h\|_{L^\infty(\Omega)} = \|y\|_\infty \qquad ? = \|y\|_{\ell^2}$$

Condition number in M-norm

Lemma

$$A,\ M\ s.p.d \quad \Rightarrow \quad \varkappa_M(A) = \left\|A^{-1}\right\|_M \|A\|_M \le \varkappa_{\ell^2}(M)\varkappa_{\ell^2}(A)$$

Proof.

- M s.p.d. $\Rightarrow$ $$\left\|M^{-1}\right\| = \sup_{0\neq y\in\mathbb{R}^N} \frac{y^T M^{-1} y}{y^T y} = \sup_{\substack{0\neq z\in\mathbb{R}^N \\ z=M^{-1/2}y}} \frac{z^T z}{z^T M z}$$
- $$\|A\|_M^2 = \sup_{0\neq z\in\mathbb{R}^N} \frac{\|Az\|_M^2}{\|z\|_M^2} = \sup_{0\neq z\in\mathbb{R}^N} \frac{z^T AMAz}{z^T Mz}$$ $$= \sup_{0\neq z\in\mathbb{R}^N} \frac{z^T AMAz}{z^T A^2 z}\frac{z^T A^2 z}{z^T z}\frac{z^T z}{z^T Mz} \le \|M\| \left\|A^2\right\| \left\|M^{-1}\right\|$$
- $$\left\|A^{-1}\right\|_M^2 \le \|M\| \left\|A^{-2}\right\| \left\|M^{-1}\right\|$$
- $$\varkappa_M^2(A) \le \varkappa^2(M)\varkappa(A^2) = \varkappa^2(M)\varkappa^2(A) \qquad \|\cdot\| = \|\cdot\|_{\ell^2}$$

□

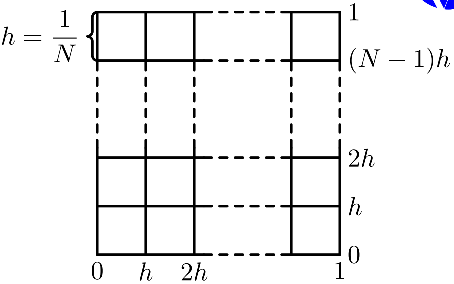
Numerical example – continuous problem

$$-\Delta u = f \quad \text{in } \Omega = (0,1)^2$$
$$u = 0 \quad \text{on } \partial\Omega$$

- $-\Delta \tilde{v}_{k\ell} = \tilde{\lambda}_{k\ell} \tilde{v}_{k\ell}$
- $\tilde{v}_{k\ell} = 2 \sin(k\pi x_1) \sin(\ell \pi x_2)$ $\qquad \int_\Omega v_{k\ell} v_{mn} = \delta_{(k\ell)(mn)}$

  $\tilde{\lambda}_{k\ell} = \pi^2 (k^2 + \ell^2)$ $\qquad k, \ell = 1, 2, \dots$
- $f = \sum_{k,\ell} c_{k\ell} \tilde{\lambda}_{k\ell} \tilde{v}_{k\ell} \quad \Rightarrow \quad u = \sum_{k,\ell} c_{k\ell} \tilde{v}_{k\ell}$

Numerical example – discretization



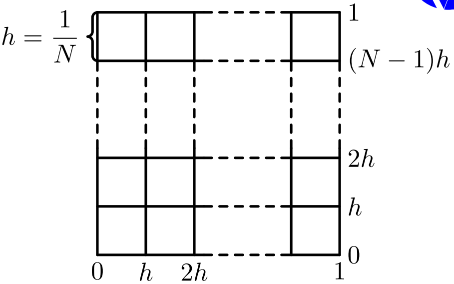
- $A = \frac{1}{3} \times \begin{array}{ccc} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{array}$
- $Aw^{k\ell} = \lambda_{k\ell} w^{k\ell}$ $\qquad k, \ell = 1, 2, \ldots, N-1$
- $w_{ij}^{k\ell} = h\,\tilde{v}(ih, jh) = 2h \sin(k\pi ih)\sin(\ell\pi jh)$ $\qquad i, j = 1, 2, \ldots, N-1$

$$\lambda_{k\ell} = \frac{2}{3}\Big(4 - \cos(k\pi h) - \cos(\ell\pi h) - 2\cos(k\pi h)\cos(\ell\pi h)\Big)$$

$$w^{k\ell} \cdot w^{mn} = \delta_{(k\ell)(mn)}$$

- $\varkappa(A) = \dfrac{2 + \cos^2(\pi h)}{2 - \cos(\pi h) - \cos^2(\pi h)} \approx O(h^{-2})$

Numerical example – discretization



- $M = \dfrac{h^2}{36} \times \begin{array}{ccc} 1 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 1 \end{array}$
- $M w^{k\ell} = \mu_{k\ell} w^{k\ell}$ $\qquad k, \ell = 1, 2, \ldots, N-1$
- $w_{ij}^{k\ell} =$ dtto. $\qquad i, j = 1, 2, \ldots, N-1$
- $\mu_{k\ell} = \dfrac{h^2}{9}\Big(4 + 2\cos(k\pi h) + 2\cos(\ell\pi h) + \cos(k\pi h)\cos(\ell\pi h)\Big)$
- $\varkappa(M) = \dfrac{4 + 4\cos(\pi h) + \cos^2(\pi h)}{4 - 4\cos(\pi h) + \cos^2(\pi h)} \xrightarrow{h \to 0} 9$

Numerical example – discretization

- $$\int_\Omega \tilde\lambda_{k\ell}\, \tilde v_{k\ell}(x_1,x_2)\varphi_{ij}(x_1,x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 = d_{k\ell} w_{ij}^{k\ell}$$
- $$d_{k\ell} = \frac{k^2+\ell^2}{k^2\ell^2\pi^2 h^3} 4\left(1-\cos(k\pi h)\right)\left(1-\cos(\ell\pi h)\right)$$
- $$f = \sum_{k,\ell} c_{k\ell}\tilde\lambda_{k\ell}\tilde v_{k\ell} \quad\Rightarrow\quad u = \sum_{k,\ell} c_{k\ell}\tilde v_{k\ell}$$
$$b = \sum_{k,\ell} c_{k\ell} d_{k\ell} w^{k\ell} \quad\Rightarrow\quad y = \sum_{k,\ell} \frac{c_{k\ell} d_{k\ell}}{\lambda_{k\ell}} w^{k\ell}$$
$$\Rightarrow\quad u_h = \sum_{i=1}^{N-1}\sum_{j=1}^{N-1} y_{ij}\varphi_{ij}$$

$c_{11} = 10 \quad c_{23} = 2 \quad c_{33} = 1$

Energy norms

- $\|u\|_a^2 = \sum_{k,\ell} c_{k\ell}^2 \tilde{\lambda}_{k\ell}$ $\qquad \|u\|_a \approx O(1)$
- $\|u_h\|_a^2 = \|y\|_A^2 = \sum_{k,\ell} c_{k\ell}^2 d_{k\ell}^2 / \lambda_{k\ell}$ $\qquad \|u_h\|_a \approx O(1)$
- $\|u - u_h\|_a^2 = \|u\|_a^2 - \|u_h\|_a^2$ $\qquad \|u - u_h\|_a \approx O(h)$
- $\|f\|_a^2 = \sum_{k,\ell} c_{k\ell}^2 \tilde{\lambda}_{k\ell}^3$ $\qquad \|f\|_a \approx O(1)$
- $\|b\|_A^2 = \sum_{k,\ell} c_{k\ell}^2 d_{k\ell}^2 \lambda_{k\ell}$ $\qquad \|b\|_A \approx O(h^2)$

$$d_{k\ell} \approx O(h) \quad \lambda_{k\ell} \approx O(h^2)$$

L^2 norms

- $\|u\|^2_{L^2(\Omega)} = \sum_{k,\ell} c^2_{k\ell}$ $\qquad \|u\|_{L^2(\Omega)} \approx O(1)$
- $\|u_h\|^2_{L^2(\Omega)} = \|y\|^2_M = \sum_{k,\ell} \frac{c^2_{k\ell} d^2_{k\ell} \mu_{k\ell}}{\lambda^2_{k\ell}}$ $\qquad \|u_h\|_{L^2(\Omega)} \approx O(1)$
- $\int_\Omega u u_h \,\mathrm{d}x_1 \,\mathrm{d}x_2 = \sum_{k,\ell} \frac{c^2_{k\ell} d^2_{k\ell}}{\lambda_{k\ell} \tilde{\lambda}_{k\ell}}$ $\qquad \approx O(1)$
- $\|u - u_h\|^2_{L^2(\Omega)} = \|u\|^2_{L^2(\Omega)} - 2\int_\Omega u u_h \,\mathrm{d}x_1 \,\mathrm{d}x_2 + \|u_h\|^2_{L^2(\Omega)}$
  $\qquad \|u - u_h\|_{L^2(\Omega)} \approx O(h^2)$

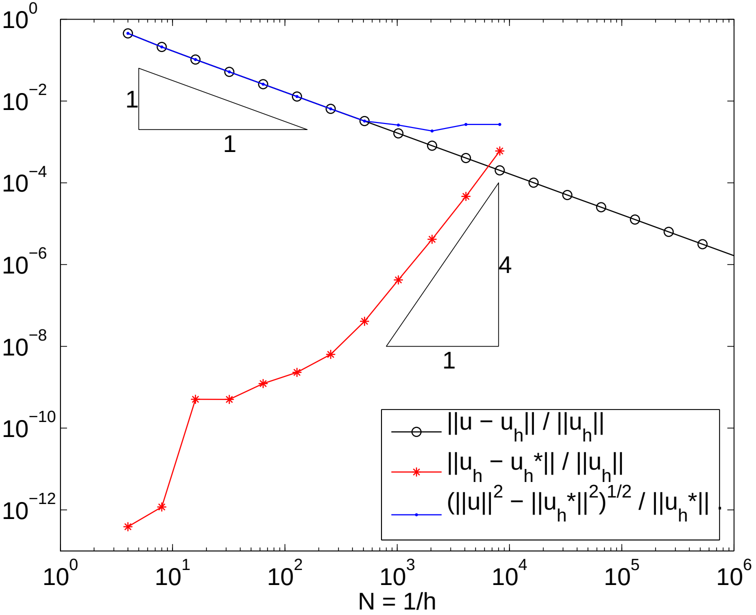
- $\|f\|^2_{L^2(\Omega)} = \sum_{k,\ell} c^2_{k\ell} \tilde{\lambda}^2_{k\ell}$ $\qquad \|f\|_{L^2(\Omega)} \approx O(1)$
- $\|b\|^2_M = b^T M b = \sum_{k,\ell} c^2_{k\ell} d^2_{k\ell} \mu_{k\ell}$ $\qquad \|b\|_M \approx O(h^2)$
- $\|b\|^2_{\ell^2} = b^T b = \sum_{k,\ell} c^2_{k\ell} d^2_{k\ell}$ $\qquad \|b\|_{\ell^2} \approx O(h)$

Conjugate gradient algorithm

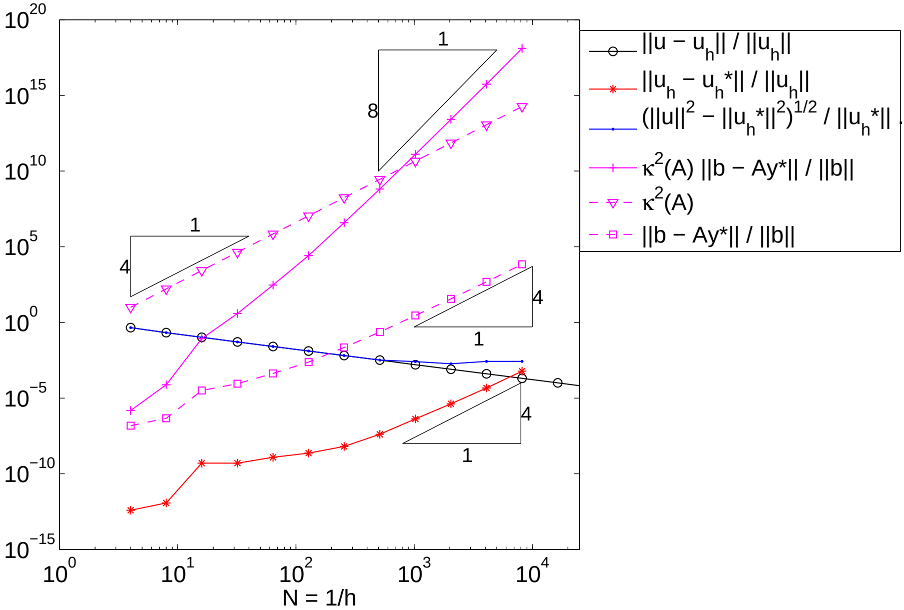
$p_0 = r_0 = b - Ay_0$
for $k = 0, 1, 2, \dots$ do

- if $\dfrac{r_k^T r_k}{b^T b} \leq TOL^2$ then STOP — $TOL = 10^{-4}$
- $\alpha_k = \dfrac{r_k^T r_k}{p_k^T A p_k}$ (step length)
- $y_{k+1} = y_k + \alpha_k p_k$ (approximate solution)
- $r_{k+1} = r_k - \alpha_k A p_k$ (residual)
- $\beta_k = \dfrac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$ (residual improvement)
- $p_{k+1} = r_{k+1} - \beta_k p_k$ (search direction)

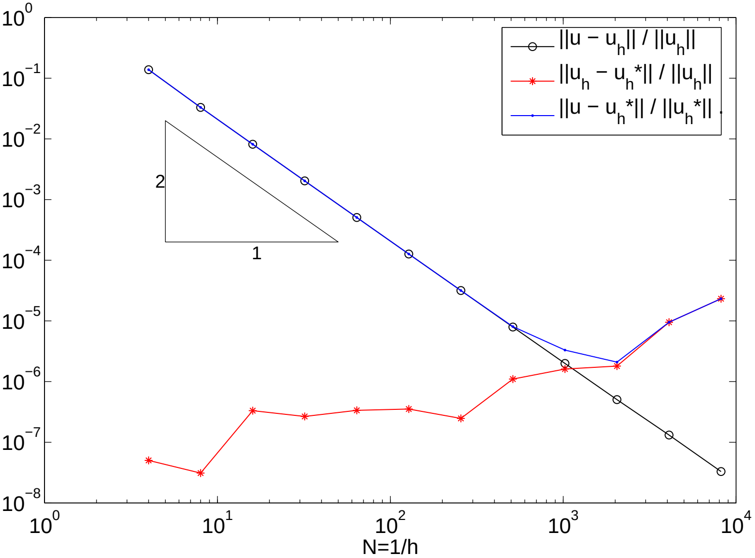
Relative errors – energy norm – $\|\cdot\|_a$



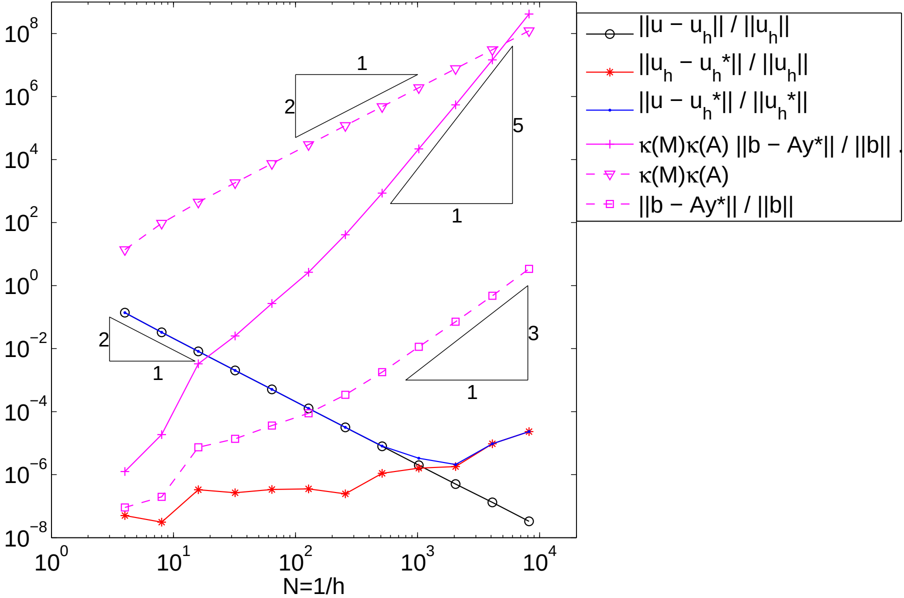
Relative err. and upper bound – energy norm – $\|\cdot\|_a$



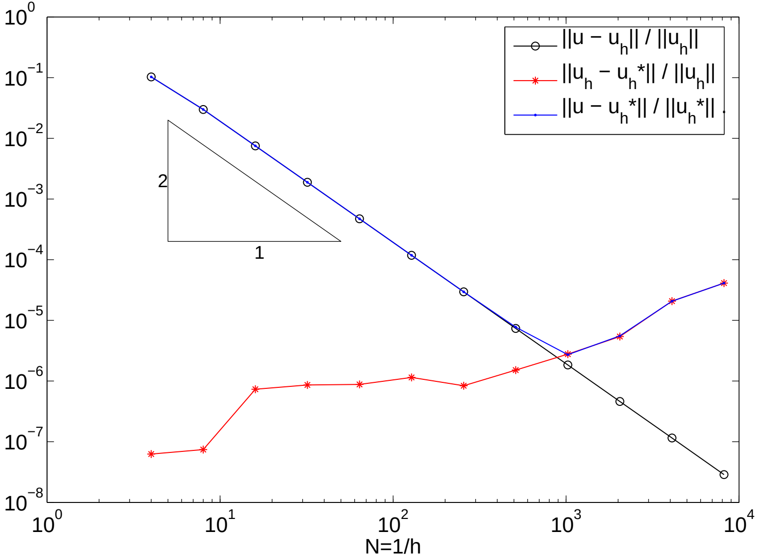
Relative errors – $L^2(\Omega)$ norm – $\|\cdot\|_{L^2(\Omega)}$



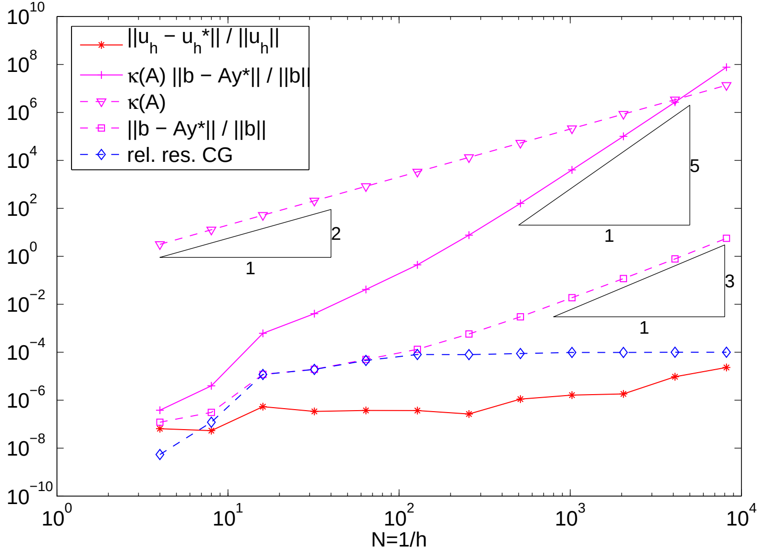
Relative err. and upper bound – $L^2(\Omega)$ norm – $\|\cdot\|_{L^2(\Omega)}$



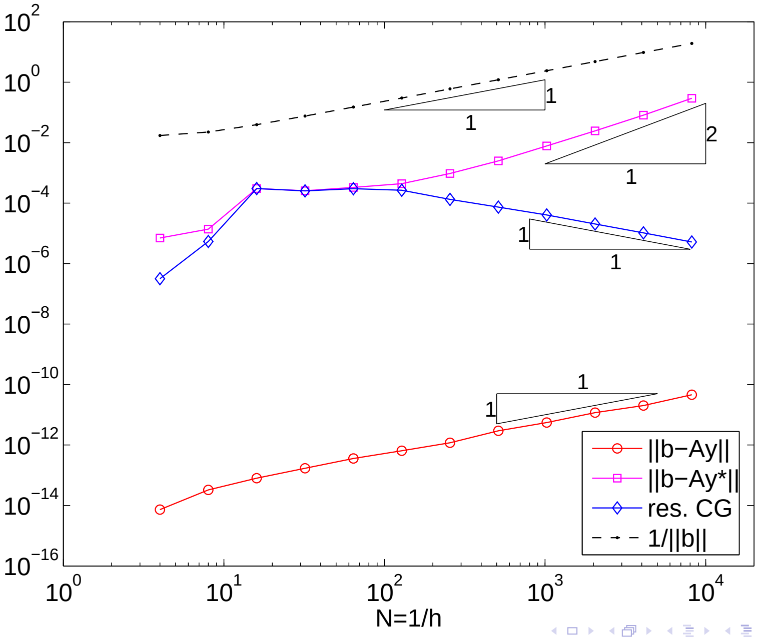
Relative errors – discrete ℓ^∞ norm – $\|\cdot\|_\infty$



Relative iteration error – Euclidean norm – $\|\cdot\|_{\ell^2}$



Absolute residuals – Euclidean norm – $\|\cdot\|_{\ell^2}$



Conclusions and open questions

- iteration error – single precission – relevant from 10^{6-8} DOFs
- $\frac{\|y - y^*\|}{\|y\|} \leq \varkappa(A) \frac{\|b - Ay^*\|}{\|b\|}$ overestimation by 10^{2-22}
- Correct norm?
- Better stopping criterion for CG?
- Theory?

Thank you for your attention

Tomáš Vejchodský (vejchod@math.cas.cz)

Institute of Mathematics, Academy of Sciences
Žitná 25, 115 67 Prague 1
Czech Republic