Remarks on algebraic computations within numerical solution of partial differential equations

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Liesen, S, OUP, 2012, Motto:

A short while ago, I found a rather elegant solution.
The reason why I am strongly drawn to such
approximation mathematics problems is not
the practical applicability of the solution,
but rather the fact that a very “economical”
solution is possible only when it is very “adequate”.
To obtain a solution in very few steps
means nearly always that one has found a way
that does justice to the inner nature of the problem.

Cornelius Lanczos in a letter to Albert Einstein on March 9, 1947

Liesen, S, OUP, 2012, Motto:

Your remark on the importance of
adapted approximation methods makes very
good sense to me, and I am convinced
that this is a fruitful mathematical aspect,
and not just a utilitarian one.

Einstein’s reply to Lanczos on March 18, 1947

Albert Einstein Archives, The Hebrew University of Jerusalem, Israel
(the original is in German).

Adapted approximation methods?

Doing justice to the inner nature of the problem concerns the whole solution process

PROBLEM $\rightleftharpoons$ MODEL $\rightleftharpoons$ DISCRETIZATION $\rightleftharpoons$ COMPUTATION

Individual stages are accompanied by errors, in particular by approximation errors of the model, discretization errors, linearization errors, and truncation and/or rounding errors in numerical matrix computations.

We are going to present several related points with a focus on iterative algebraic computations.

Outline

1. Model and its discretization
2. Stability, consistency and convergence of numerical discretizations
3. Conditioning, a-priori and a-posteriori algebraic error estimates
4. How to measure errors?
5. Preconditioning as transformation of the discretization basis
6. Reaching an arbitrary accuracy?
7. Conclusions

1 Basic functional analysis setting

Let V be a real infinite dimensional Hilbert space with the inner product

$$(\cdot,\cdot)_V : V \times V \to R, \quad \text{the associated norm } \|\cdot\|_V \,,$$

$V^{\#}$ be the dual space of bounded (continuous) linear functionals on V with the duality pairing

$$\langle \cdot,\cdot \rangle : V^{\#} \times V \to R\,.$$

For each $f \in V^{\#}$ there exists a unique $\tau f \in V$ such that

$$\langle f, v \rangle = (\tau f, v)_V \quad \text{for all } v \in V\,.$$

In this way the inner product $(\cdot,\cdot)_V$ determines the Riesz map

$$\tau : \; V^{\#} \to V\,.$$

1 Model and its analysis

Let $a(\cdot, \cdot) : V \times V \to R$ be a bounded and V-elliptic bilinear form. For a fixed $u \in V$ we can see $\mathcal{A}u \equiv a(u, \cdot) \in V^{\#}$, i.e. ,

$$\langle \mathcal{A}u, v \rangle = a(u, v) \quad \text{for all } v \in V \, .$$

This defines the bounded and $(\alpha-)$coercive operator

$$\mathcal{A} : V \to V^{\#}, \qquad \inf_{u \in V, \, \|u\|_V = 1} \langle \mathcal{A}u, u \rangle = \alpha > 0, \; \|\mathcal{A}\| = C \, .$$

Using the Lax-Milgram theorem, the problem is well-posed: For any $b \in V^{\#}$ there exist a unique solution $x \in V$ of

$$a(x, v) = \langle b, v \rangle \quad \text{for all } v \in V \, .$$

and x depends continuously on the data b ,

$$\|x\|_V \; \leq \; \frac{1}{\alpha} \, \|b\|_{V^{\#}} \, .$$

1 Functional formulation and preconditioning

$$\langle \mathcal{A}x - b, v \rangle = 0 \quad \text{for all } v \in V$$

gives the (functional) equation in (the data space) $V^{\#}$,

$$\mathcal{A}x = b, \quad , \quad \mathcal{A} : V \to V^{\#}, \quad x \in V, \quad b \in V^{\#} .$$

Using the Riesz map,

$$(\tau \mathcal{A}x - \tau b, v)_V = 0 \quad \text{for all } v \in V .$$

Clearly, application of the Riesz map τ can be interpreted as transformation of the original problem $\mathcal{A}x = b$ in the data space $V^{\#}$ into the equation in the solution space V ,

$$\tau \mathcal{A}x = \tau b, \qquad \tau \mathcal{A} : V \to V, \quad x \in V, \quad \tau b \in V ,$$

which is commonly (and inaccurately) called preconditioning.

1 Galerkin discretization

Consider an N-dimensional discrete solution subspace $V_h \subset V$ with the duality pairing, the inner product and the Riesz map as above. Then the restriction to V_h gives an approximation $x_h \in V_h$ to $x \in V$,

$$a(x_h, v) = \langle b, v \rangle \qquad \text{for all} \quad v \in V_h \, .$$

As above, the bilinear form $a(\cdot, \cdot) : V_h \times V_h \to R$ defines the operator $\mathcal{A}_h : V_h \to V_h^{\#}$ such that

$$\langle \mathcal{A}_h x_h - b, v \rangle = 0 \qquad \text{for all} \quad v \in V_h \, .$$

With restricting b to V_h, i.e. $\langle b_h, v \rangle \equiv \langle b, v \rangle$ for all $v \in V_h$, we get the equation in the discrete data space $V_h^{\#}$,

$$\mathcal{A}_h x_h = b_h, \qquad x_h \in V_h, \quad b_h \in V_h^{\#}, \quad \mathcal{A}_h : V_h \to V_h^{\#} \, .$$

1 Operator preconditioning references

Arnold, Falk, and Winther (1997, 1997); Steinbach and Wendland (1998); Mc Lean and Tran (1997); Christiansen and Nédélec (2000, 2000); Powell and Silvester (2003); Elman, Silvester, and Wathen (2005); Axelsson and Karátson (2009); Mardal and Winther (2011); Kirby (2011); Zulehner (2011); Preconditioning Conference 2013, Oxford; ...

Inner product $\longrightarrow$ Riesz map $\longrightarrow$ Preconditioning $\longrightarrow$ Spectral bounds

However, there is a point to consider. What is the appropriate inner product ? A standard way is to focus on the mesh (model) parameters independence of the condition number-based convergence bounds.

Operator preconditioning $\longrightarrow$ PDEs.

Algebraic preconditioning $\longrightarrow$ Matrices.

Preconditioning $\longrightarrow$ Discretization?

2 Consistency, stability and convergence

Let X_h be a representation of the solution x in V_h .

- Consistency error norm $\|\mathcal{A}_h X_h - b_h\|_{V_h^\#}$. The discretization scheme is consistent if the consistency error norm tends to 0 with h .
- Stability = continuity of the discrete mapping $\mathcal{A}_h^{-1} : V_h^\# \rightarrow V_h$. The discretization scheme is stable if the stability constant $\|\mathcal{A}_h^{-1}\|_{V_h^\#, V_h}$ is bounded uniformly in h . Here

$$\|\mathcal{A}_h^{-1}\|_{V_h^\#, V_h} \leq \frac{1}{\alpha} \, .$$

- The discretization scheme is convergent if the error norm $\|X_h - x_h\|_{V_h}$ tends to 0 with h .

2 Fundamental theorem of numerical PDE analysis

Using

$$\|X_h - x_h\|_{V_h} \le \|\mathcal{A}_h^{-1}\|_{V_h^{\#}, V_h} \, \|\mathcal{A}_h X_h - b_h\|_{V_h^{\#}} ,$$

a discretization scheme which is consistent and stable is convergent.

Instructive (and more general) exposition in Arnold (2012); see also Arnold, Falk and Winther (2010); ...

From the computational point of view, one issue is, however, missing. Here it is assumed that x_h satisfies

$$\mathcal{A}_h x_h = b_h \, .$$

In numerical algebra this reminds of a bound for the forward error using a residual backward error and a conditioning of the problem.
Incorporating algebraic errors?

3 Iterative methods and conditioning

- “[...] useful insight is gained as to the relationship between Hilbert space and matrix condition numbers and translating Hilbert space fixed point iterations into matrix computations provides new ways of motivating and explaining some classic iteration schemes.”
  Kirby, SIREV, 2010

- “[...] in the early sweeps the convergence is very rapid but slows down, this is the sublinear behavior. The convergence then settles down to a roughly constant linear rate [...] Towards the end new speed may be picked up again, corresponding to the superlinear behavior. [...]
  In practice all phases need not be identifiable, nor need they appear only once and in this order.” Nevanlinna, 1993, Section 1.8

- “However, if the operator has a few eigenvalues far away from the rest of the spectrum, then the estimate is not sharp. In fact, a few ‘bad eigenvalues’ will have almost no effect on the asymptotic convergence of the method [...]” Mardal and Winther, NLAA, 2011

3 Self-adjoint $\mathcal{A}$ wrt the duality pairing

CG in Hilbert spaces : $r_0 = b - \mathcal{A}x_0 \in V^{\#}, \quad p_0 = \tau r_0 \in V$

For $n = 1, 2, \ldots, n_{\max}$

$$\alpha_{n-1} = \frac{\langle r_{n-1}, \tau r_{n-1} \rangle}{\langle \mathcal{A}p_{n-1}, p_{n-1} \rangle} = \frac{(\tau r_{n-1}, \tau r_{n-1})_V}{(\tau \mathcal{A}p_{n-1}, p_{n-1})_V}$$

$$x_n = x_{n-1} + \alpha_{n-1} p_{n-1} \,,$$ stop when the stopping criterion is satisfied

$$r_n = r_{n-1} - \alpha_{n-1} \mathcal{A} p_{n-1}$$

$$\beta_n = \frac{\langle r_n, \tau r_n \rangle}{\langle r_{n-1}, \tau r_{n-1} \rangle} = \frac{(\tau r_n, \tau r_n)_V}{(\tau r_{n-1}, \tau r_{n-1})_V}$$

$$p_n = \tau r_n + \beta_n p_{n-1}$$

End

Hayes (1954); ... ; Glowinski (2003); Axelsson and Karatson (2009);
Mardal and Winther (2011); Günnel, Herzog and Sachs (2013)

3 Galerkin discretization and the matrix CG

Let $\Phi_h = (\phi_1^{(h)}, \dots, \phi_N^{(h)})$ be the basis of V_h , $\Phi_h^{\#} = (\phi_1^{(h)\#}, \dots, \phi_N^{(h)\#})$ the basis of its dual $V_h^{\#}$. Using the coordinates in Φ_h and $\Phi_h^{\#}$,

$$\langle f, v \rangle \to \mathbf{v}^* \mathbf{f} \, ,$$

$$(u, v)_V \to \mathbf{v}^* \mathbf{M} \mathbf{u}, \quad (\mathbf{M}_{ij}) = ((\phi_j, \phi_i)_V)_{i,j=1,\dots,N} \, ,$$

$$\tau \to \mathbf{M}^{-1} \, ,$$

$$\mathcal{A}_h \to \mathbf{A}, \quad (\mathbf{A}_{ij}) = (a(\phi_j, \phi_i))_{i,j=1,\dots,N} = (\langle \mathcal{A}\phi_j, \phi_i \rangle)_{i,j=1,\dots,N} \, ,$$

$$b \to \mathbf{b} \, ,$$

we get with $x_n = \Phi_h \, \mathbf{x}_n \, , \; p_n = \Phi_h \, \mathbf{p}_n \, , \; r_n = \Phi_h^{\#} \, \mathbf{r}_n$

3 Preconditioned algebraic CG

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0,$ solve $\mathbf{M}\mathbf{z}_0 = \mathbf{r}_0,\ \mathbf{p}_0 = \mathbf{z}_0$

For $n = 1, \dots, n_{\max}$

$$\alpha_{n-1} = \frac{\mathbf{z}_{n-1}^* \mathbf{r}_{n-1}}{\mathbf{p}_{n-1}^* \mathbf{A} \mathbf{p}_{n-1}}$$

$$\mathbf{x}_n = \mathbf{x}_{n-1} + \alpha_{n-1} \mathbf{p}_{n-1}\,,$$ stop when the stopping criterion is satisfied

$$\mathbf{r}_n = \mathbf{r}_{n-1} - \alpha_{n-1} \mathbf{A} \mathbf{p}_{n-1}$$

$$\mathbf{z}_n = \mathrm{M}^{-1} \mathbf{r}_n\,,$$ solve for $\mathbf{z}_n$

$$\beta_n = \frac{\mathbf{z}_n^* \mathbf{r}_n}{\mathbf{z}_{n-1}^* \mathbf{r}_{n-1}}$$

$$\mathbf{p}_n = \mathbf{z}_n + \beta_n \mathbf{p}_{n-1}$$

End

3 Philosophy of a-priori robust bounds

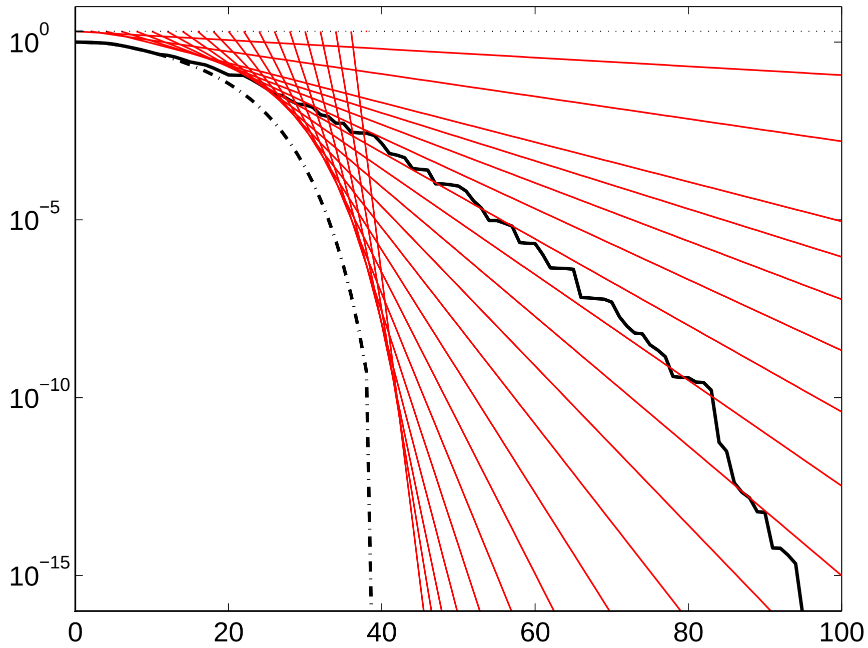
Theorem

$$\kappa(\mathbf{M}^{-1}\mathbf{A}) \,\le\, \frac{C}{\alpha} = \frac{\|\mathcal{A}\|}{\inf_{u \in V,\, \|u\|_V = 1} \langle \mathcal{A}u, u\rangle}$$

“Knowledge of robust estimates not only contributes to the question of well-posedness, but also to discretization error estimates and the construction of efficient solvers for the discretized problem. In the dicretized case, having robust estimates [...] translates to having a [...] preconditioner for the linear operator [...] with robust estimates on the condition number. This would immediatelly imply that Krylov subspace methods like the minimum residual method [...] converge with convergence rates independent on [...] h.”

Zullehner, SIAM J. Matrix Anal. Appl. (2011)

3 Liesen, S (2012); Gergelits, S (2013)



Short recurrences always mean in practical computations loss of (bi-)orthogonality due to rounding errors! Principal consequences are not resolved by *the common assumption* that this phenomenon does not take place.

3 Hiptmair, CMA (2006)

Operator preconditioning is a very general recipe [...]. It is simple to apply, but may not be particularly efficient, because in case of the [*condition number*] bound of Theorem ... is too large, the operator preconditioning offers no hint how to improve the preconditioner. Hence, operator preconditioner may often achieve [...] the much-vaunted mesh independence of the preconditioner, but it may not perform satisfactorily on a given mesh."

Mesh independence.

3 Faber, Manteuffel and Parter (1990)

“For a fixed h, using a preconditioning strategy based on an equivalent operator may not be superior to classical methods [...] Equivalence alone is not sufficient for a good preconditioning strategy. One must also choose an equivalent operator for which the bound is small.

There is no flaw in the analysis, only a flaw in the conclusions drawn from the analysis [...] asymptotic estimates ignore the constant multiplier. Methods with similar asymptotic work estimates may behave quite differently in practice.”

Equivalence of operators.

3 Becker, Johnson, and Rannacher (1995)

“ Usually, ad hoc stopping criteria are used, e.g. requiring an initial (algebraic) residual to be reduced by a certain ad hoc factor, but these criteria have no clear connection to the actual error in the corresponding approximate solution, which is the quantity of interest. This leaves the user of iterative solutions methods in a serious dilemma: [...] one has either to continue the iterations until the discrete solution error is practically “zero”, which increases the computational cost with possibly no gain in the overall precision, or take the risk of stopping the iterations prematurely. [...]

A solution to this problem can only be obtained by combining aspects of the underlying partial differential equations and the corresponding finite element discretization with aspects of the iterative discrete solution algorithm. A “pure” numerical linear algebra point of view, for instance based on the condition number of the stiffness matrix, does not appear to be able to lead to a balance of discretization and solution errors.”

4 Babuška and Strouboulis (2001)

“In engineering practice it is not sufficient to estimate only the energy norm of the error because a small value of the global energy norm of the error does not necessarily imply that the error in the outputs of interest is also small (e.g. a 5% relative error in the global energy norm does not imply 5% relative error in the maximum stress in a region of interest). [...] An essential requirement is that the quantity of interest has to be well defined; for example, it is meaningless to ask for an estimate of the maximum error in the derivative, flux, or stress for a problem set in a polygonal non-convex domain, because the exact value does not exists (the derivative, flux, or stress in the neighborhood of a corner point is usually unbounded).”

How to measure *a-posteriori* errors?

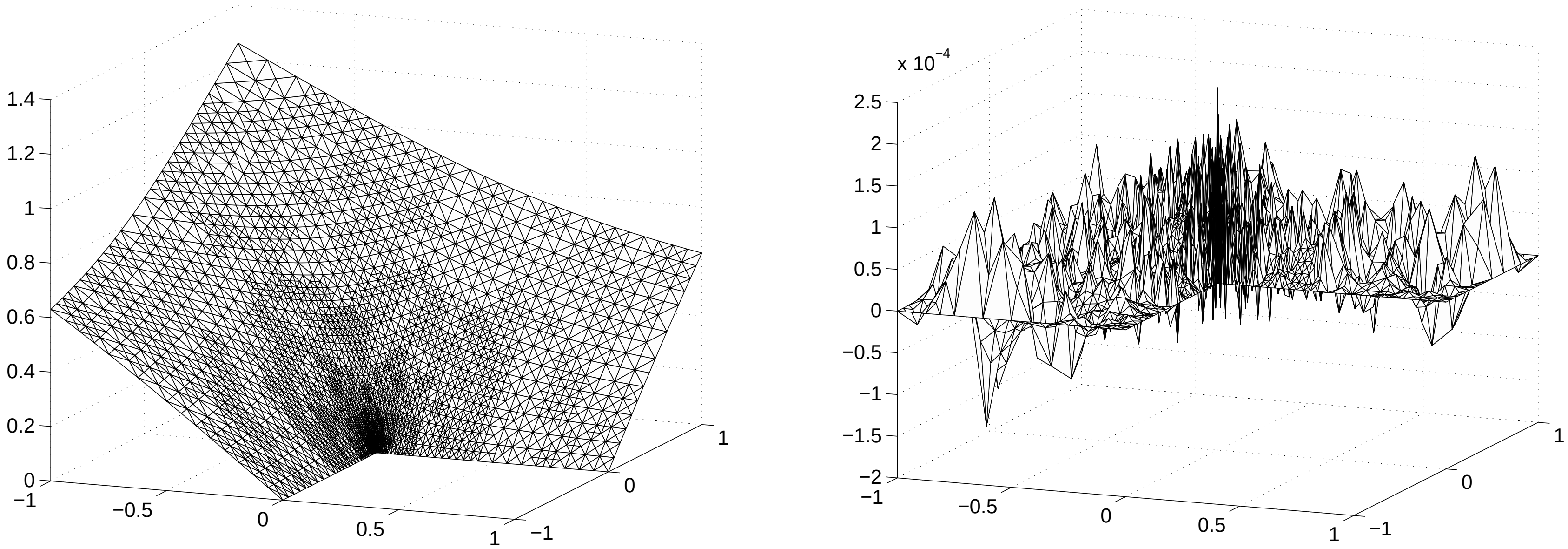
4 Giles and Süli (2002)

“In many scientific and engineering applications ... the objective is merely a rough, qualitative assessment of the details of the analytical solution over the computational domain, the quantitative concern being directed towards a few *output functionals,* derived quantities of particular engineering or scientific relevance.”

Wohlmuth, ENUMATH 2013, Monday Aug. 26; ... ...

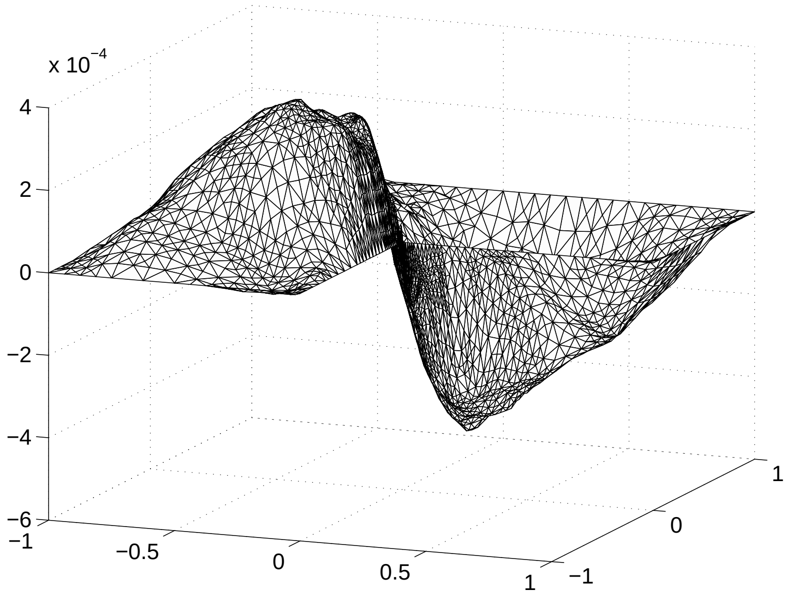
In addition to discretization errors, algebraic errors can also affect the accuracy of the computed approximate solution. What is known on the spatial distribution of the algebraic errors over the computational domain?

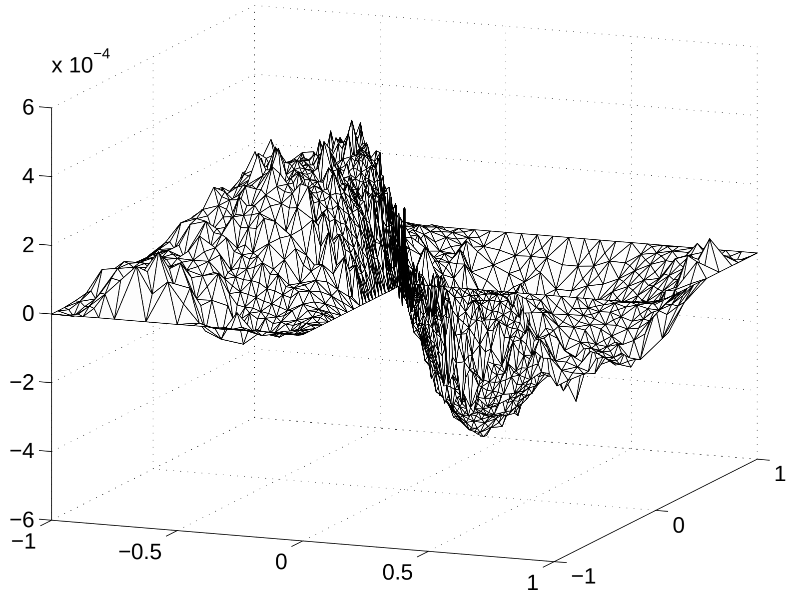
4 L-shape domain, Papež, Liesen, S (2013)



Exact solution x (left) and the discretisation error $x - x_h$ (right) in the Poisson model problem.

4 L-shape domain, Papež, Liesen, S (2013)





Algebraic error $x_h - x_h^{(n)}$ (left) and the total error $x - x_h^{(n)}$ (right). Here

$$\|\nabla(x - x_h)\| \ > \ 0.1\, \|\mathbf{x} - \mathbf{x}_n\|_{\mathbf{A}}\, .$$

5 Preconditioning transforms the basis!

Algebraic preconditioning can be viewed as the finite dimensional CG with setting $\mathbf{M} = \mathbf{I}$ (this corresponds in Galerkin discretization of the finite dimensional CG to taking discretization basis Φ orthonormal wrt $(.,.)_V$) applied to

$$\mathbf{B}\mathbf{w} = \mathbf{c}$$

with

$$\mathbf{B} = \mathbf{L}_h^{-1}\mathbf{A}\mathbf{L}_h^{-*}, \quad \mathbf{c} = \mathbf{L}_h^{-1}\mathbf{b}, \quad \mathbf{x} = \mathbf{L}_h^{-*}\mathbf{w}\,, \quad \mathbf{M}_h = \mathbf{L}_h\mathbf{L}_h^{*}\,.$$

Observation:

The associated Hilbert space formulation of CG in V_h corresponds to the transformation of the bases

$$\Phi_t \;=\; \Phi_h\,\mathbf{L}_h^{-*}\,, \quad \Phi_t^{\#} \;=\; \Phi_h^{\#}\,\mathbf{L}_h^{*}\,.$$

5 Preconditioning transforms the basis!

$$\mathbf{B} \equiv (\mathbf{B}_{ij}) = \left(\langle \mathcal{A} \phi_j^{(t)}, \phi_i^{(t)} \rangle \right)_{i,j=1,\ldots,N} = (a(\phi_j^{(t)}, \phi_i^{(t)}))_{i,j=1,\ldots,N},$$

where

$$\phi_\ell^{(t)} = \Phi_h \left(\mathbf{L}_h^{-*} \mathbf{e}_\ell \right), \quad \ell = 1, \ldots, N$$

and the right hand side

$$\mathbf{c} = \Phi_h^{\#} \mathbf{L}_h^{*} \, \mathbf{b} \, .$$

Please recall, e.g., the hierarchical bases preconditioning
Yserentant (1985, 1986), Axelsson, Vassilevski, ... , Gockenbach (2006).

Remark. Equivalently, with the discretization basis Φ_t orthonormal wrt $(.,.)_V$ we get $\mathbf{M} = \mathbf{I}$ and $\mathcal{A}_h \rightarrow \mathbf{B}$. With the choice $(.,.)_V = (.,.)_a$ we get $\mathbf{B} = \mathbf{I}$.

5 Standard argument used in FEM

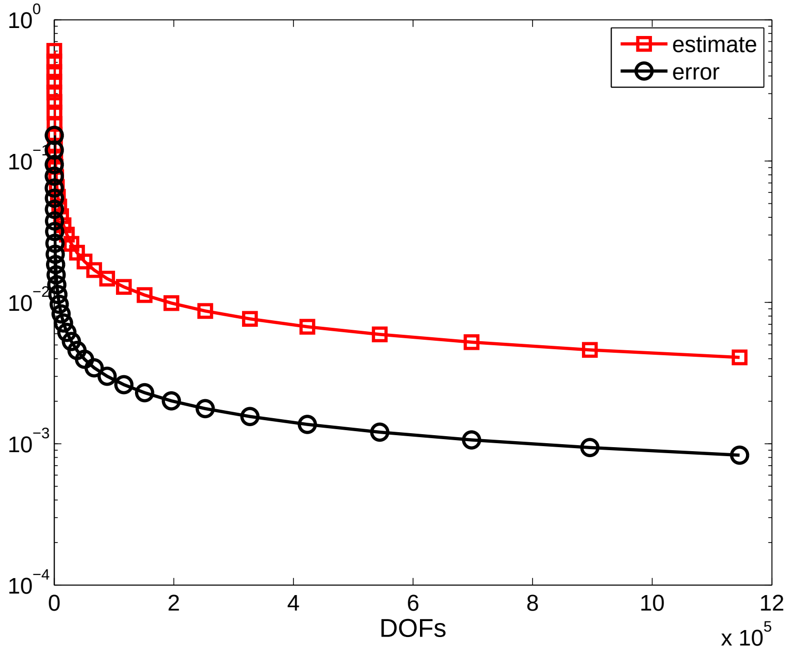
Sparsity of the resulted matrices is always presented as the main advantage of FEM discretizations.

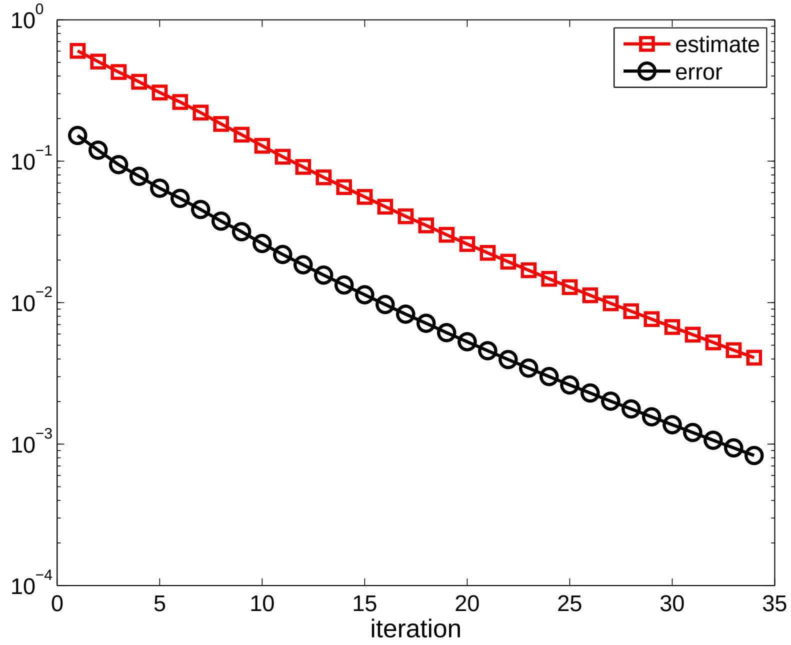
Sparsity means locality of information. In order to solve the problem, we need a global transfer of information. Therefore preconditioning! It is needed on the computational level in order to take care for the trouble caused by the (*computationally*) inconvenient approximation of the mathematical model when the *appropriate globally supported* basis functions are missing.

Preconditioning can be interpreted as an intentional loss of sparsity (loss of locality of the supports of the basis functions).

Sparsity is important for efficiency, but perhaps in a different meaning; see, e.g., Schaeffer, Caflisch, Hauck and Osher (2013).

6 Reaching an arbitrary accuracy?





It seems and it has been proved that an arbitrary prescribed accuracy can be reached using AFEM in a finite number of steps. Here linear FEM; see Morin, Nocheto, and Siebert (2002); Stevenson (2007). Something does not fit $\longrightarrow$ maximal attainable accuracy in matrix computations.

7 Conclusions

Patrick J. Roache's book *Validation and Verification in Computational Science*, 1998, p. 387:

"With the often noted tremendous increases in computer speed and memory, and with the less often acknowledged but equally powerful increases in algorithmic accuracy and efficiency, a natural question suggest itself. What are we doing with the new computer power? with the new GUI and other set-up advances? with the new algorithms? What *should* we do? ... Get the right answer."

7 Our contributions and work to be done

Modest steps in this direction:

- Operator and algebraic preconditioning is related to the discrerization basis.
- Krylov subspace methods viewed as the matching moments model reduction (infinite or finite dimenstional setting).
- *A-posteriori* evaluation of the total error which is based on quantities of interest and includes the algebraic part. Algebraic *a-priori* reasoning is useful, but it addresses different questions. **(CT 3.3, Th 16:30).**
- Adaptivity and stopping criteria for iterative solvers **(STOP, Th 14:00).**
- Numerical stability analysis of adaptive numerical schemes.

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Thank you very much for kind patience!