On the continuous problem context of matrix computations

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ILAS, Braunschweig, August 2011

Main point

In mathematical modeling of real world phenomena, the computed algebraic approximations must be related to the underlying mathematical model.

Accuracy of algebraic computations can not be evaluated using purely algebraic tools.

Thanks

André Gaul,
Jan Papež.

Model boundary value problem

$$-\Delta u \;=\; 16\eta_1\eta_2(1-\eta_1)(1-\eta_2)$$

on the unit square with zero Dirichlet boundary conditions. Galerkin finite element method (FEM) discretization with linear basis functions on the regular triangular grid with the mesh size $h = 1/(m+1)$, where m is the number of inner nodes in each direction. Discrete (piecewise linear) solution

$$u_h \;=\; \sum_{j=1}^{N} \zeta_j\,\phi_j(\eta_1,\eta_2)\,.$$

Computational error

$$\underbrace{u - u_h^{(n)}}_{\text{total error}} \;=\; \underbrace{(u - u_h)}_{\text{discretisation error}} \;+\; \underbrace{(u_h - u_h^{(n)})}_{\text{algebraic error}}\;.$$

Algebraic error?

Should we solve the discretized linear algebraic system accurately in the presence of modeling (not mentioned above) and discretization errors?

No, it is enough to assure that the algebraic error does not significantly affect the whole picture.

How to do it? What does it mean that the algebraic approximation is accurate enough?

Our first thought is to apply backward error theory.

Backward error

Giving an approximation x_n , how close is the perturbed problem

$$(A + \Delta A)\, x_n = b + \Delta b$$

which is solved exactly by x_n , to the original problem $Ax = b$, which is solved approximately by x_n ? Normwise relative backward error

$$\beta(x_n) \;\equiv\; \min\{\, \beta \;:\, (A + \Delta A)\, x_n = b + \Delta b\, , \|\Delta A\| \leq \beta \|A\|\, ,\; \|\Delta b\| \leq \beta \|b\| \,\}\, ,$$

satisfies

$$\beta(x_n) = \frac{\|b - Ax_n\|}{\|b\| + \|A\|\;\|x_n\|} = \frac{\|\Delta A_{\min}\|}{\|A\|} = \frac{\|\Delta b_{\min}\|}{\|b\|}\, .$$

Componentwise relative backward error takes care for the structure.

Alternative: Energy norm of the error

Theorem

Up to a small inaccuracy proportional to machine precision,

$$
\begin{aligned}
\|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|\nabla(u_h - u_h^{(n)})\|^2 \\
&= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 .
\end{aligned}
$$

Using zero Dirichlet boundary conditions,

$$
\|\nabla(u - u_h)\|^2 = \|\nabla u\|^2 - \|\nabla u_h\|^2 .
$$

Energy norm of the error and CG

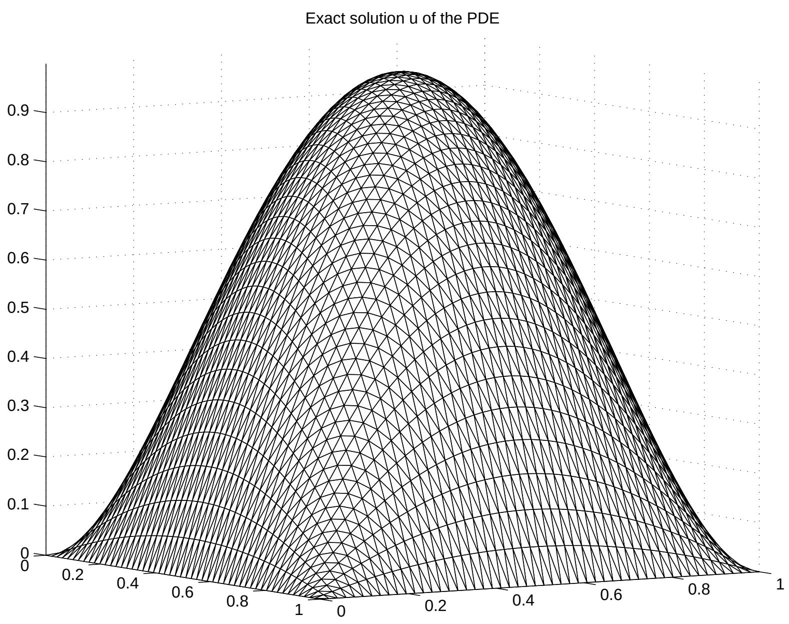
Theorem shows that the (squared) energy norm of the total error $u - u_h^{(n)}$ consists of two distinct components:

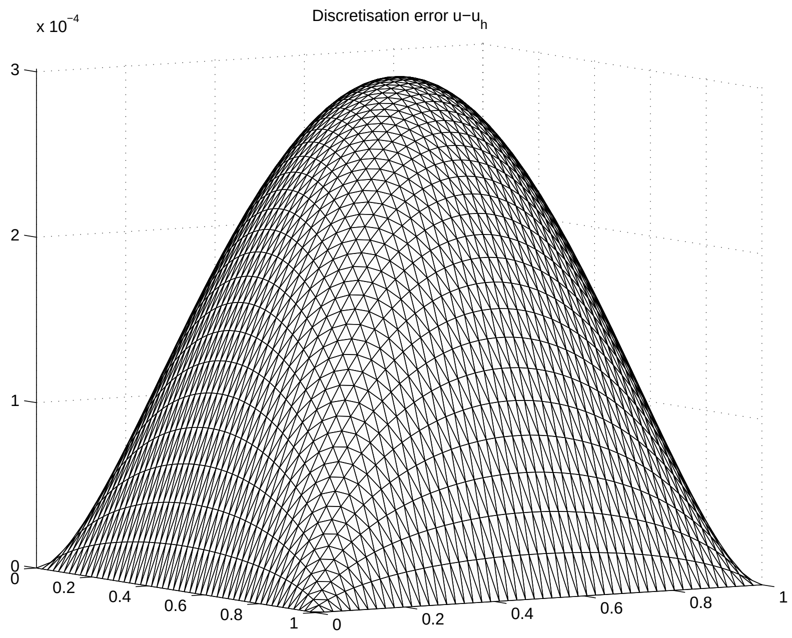
- the (squared) energy norm of the discretization error $u - u_h$,
- the (squared) energy norm of the algebraic error $u_h - u_h^{(n)}$.

In solution of real world problems errors in all stages of the solution process should be in balance.

CG is linked with the Galerkin FEM discretization.

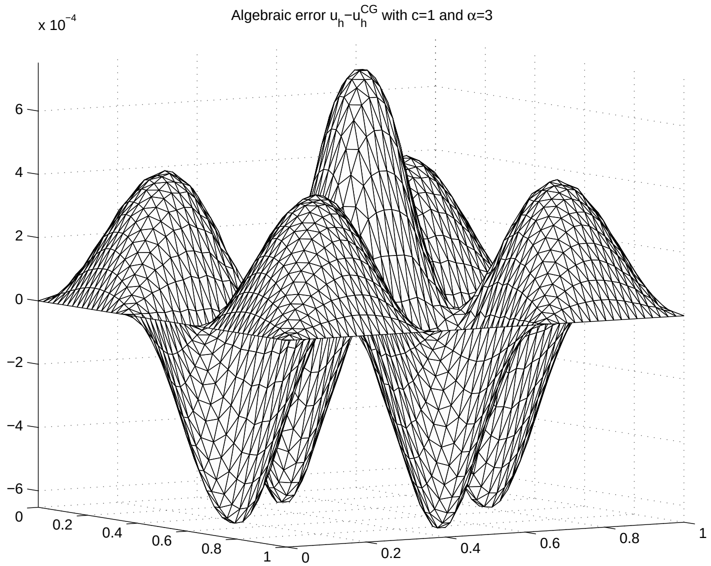
Solution and the discretization error

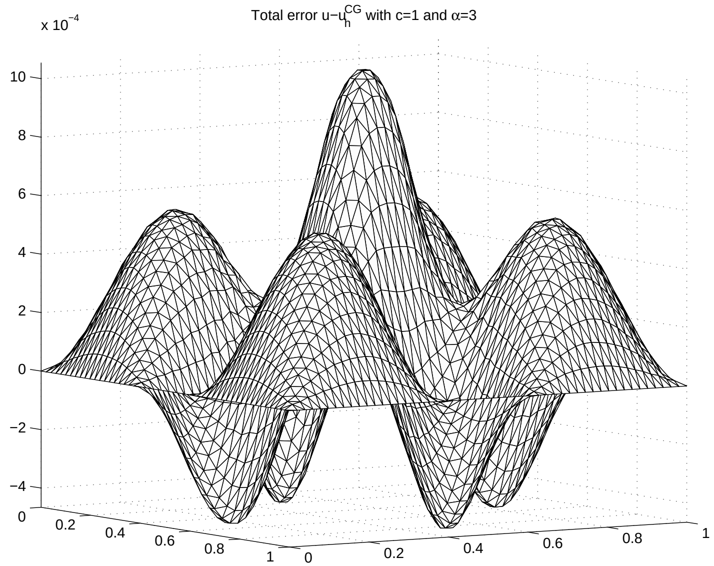




Exact solution u of the Poisson model problem (left)
and the MATLAB `trisurf` plot of the discretization error $u - u_h$ (right).

Algebraic and total errors

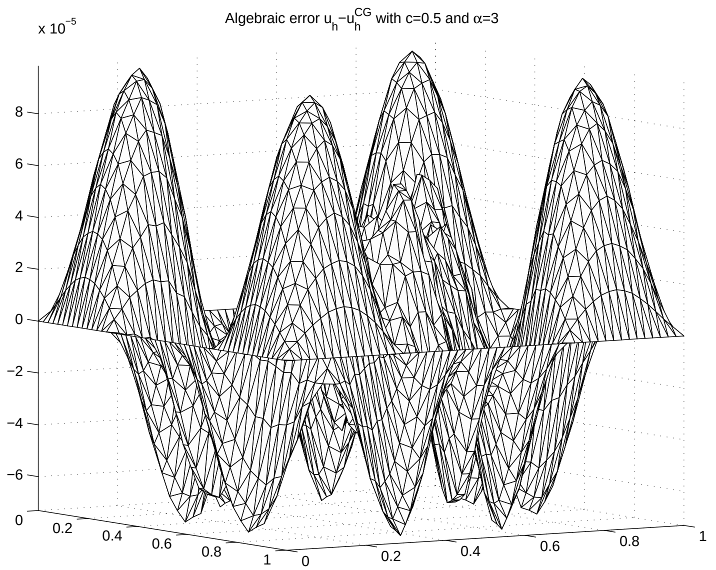


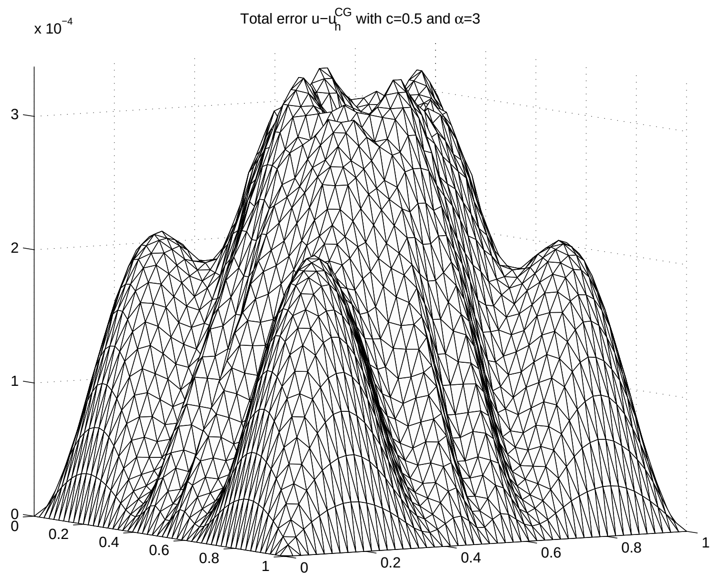


Algebraic error $u_h - u_h^{(n)}$ (left) and the MATLAB `trisurf` plot of the total error $u - u_h^{(n)}$ (right)

$$\begin{aligned}\|\nabla(u-u_h^{(n)})\|^2 &= \|\nabla(u-u_h)\|^2 + \|x-x_n\|_A^2 \\ &= 5.8444e-03 + 1.4503e-05\,.\end{aligned}$$

Algebraic and total errors

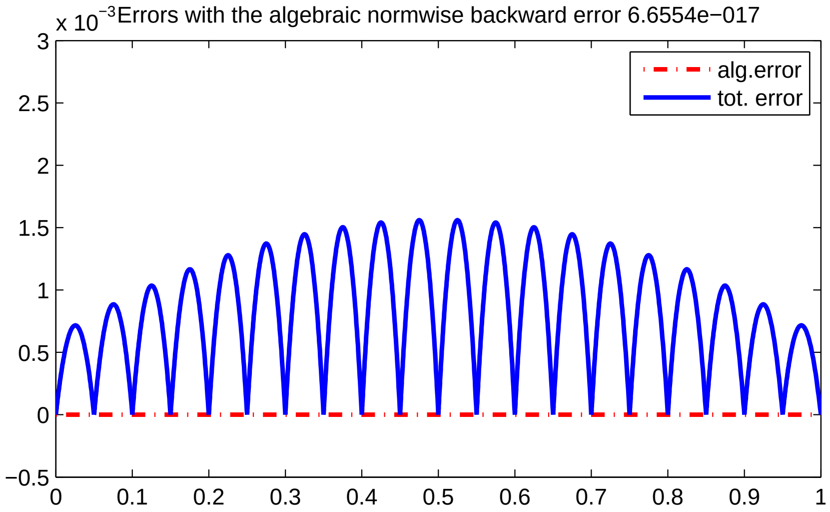


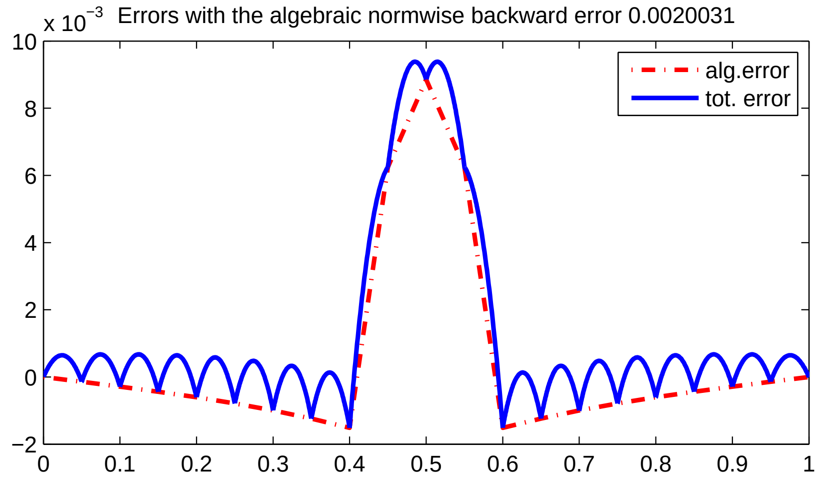


Algebraic error $u_h - u_h^{(n)}$ (left) and the MATLAB `trisurf` plot of the total error $u - u_h^{(n)}$ (right)

$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \\ &= 5.8444e-03 + 5.6043e-07\,. \end{aligned}$$

One can see 1D analogy





The discretization error (left),
the algebraic and the total error (right),
Papež (2011).

Challenges

- Using a formula from literature requires understanding of the whole context.

- Numerical PDE: Matrix computations do not provide exact results. Verification in scientific and engineering computing should take this into account. Whenever possible, one should aim at the local distribution of the total error. Norms can hide important things.

- Algebra: Error should be evaluated in the function space. The backward error analysis and perturbation theory seems not sufficient.

- Both: Local distribution of the discretization and the algebraic errors can be very different. The algebraic computation can not be considered a black box part of the whole solution process. It must be integrated (from both sides) into it.

Liesen and S (2011), Liesen and S (2012?)

Thank you for your kind patience