Model-assisted effective large scale matrix computations

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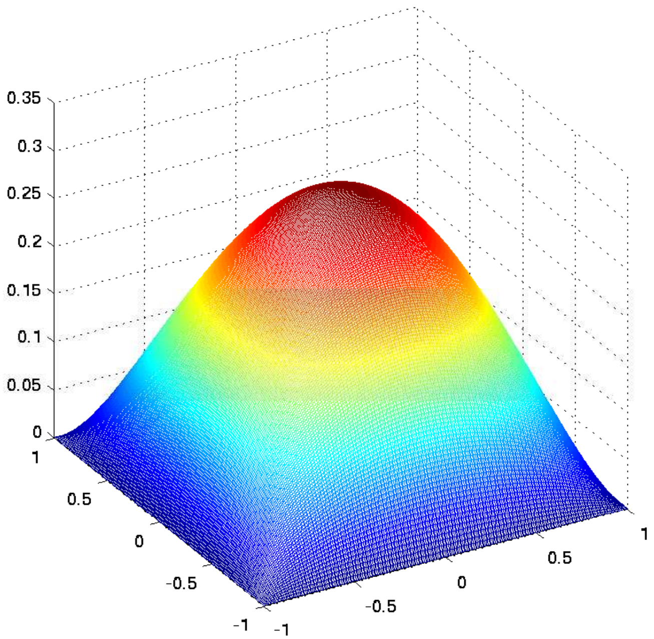
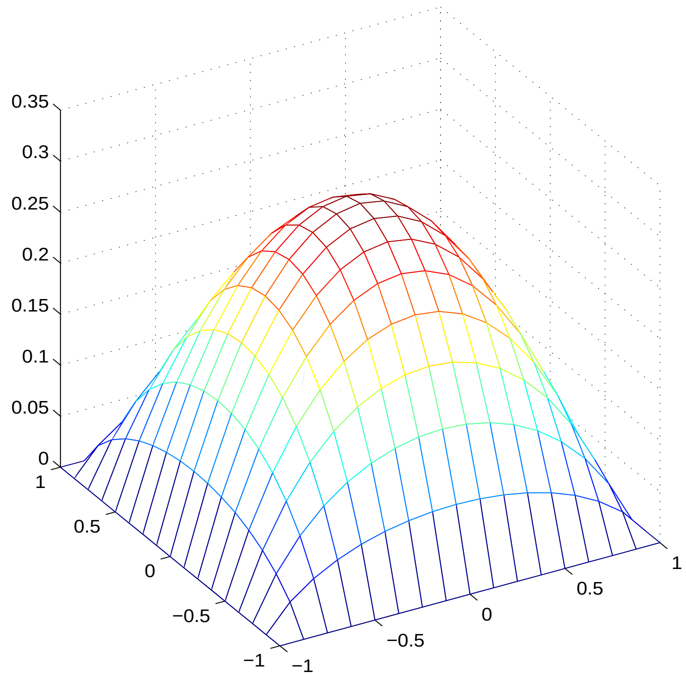
An intuitive relation





$$-\Delta u = f, \quad (x, y) \in (-1, 1)^2$$

$$u = 0 \quad \text{on} \quad \partial[-1, 1]^2$$

Given $\mathbf{A} \in \mathbb{R}^{n \times n}, \mathbf{f} \in \mathbb{R}^n$

Find $\mathbf{u} \in \mathbb{R}^n$ s.t. $\mathbf{A}\mathbf{u} = \mathbf{f}$

A slow start

Solution of a (square) algebraic linear system of large dimension.

Find $\mathbf{u} \in \mathbb{R}^n$ *such that*

$$\mathbf{A}\mathbf{u} = \mathbf{f}$$

with $\mathbf{A}$ *symmetric and positive definite:* $\langle \mathbf{x}, \mathbf{A}\mathbf{x} \rangle > 0 \; \forall \mathbf{x} \neq 0$

Very large dimension $\Rightarrow$ iterative procedure

Given an initial guess $\mathbf{u}_0 \in \mathbb{R}^n$ ($\mathbf{u}_0 = 0$ in the following), generate sequence

$$\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \ldots, \mathbf{u}_m, \ldots \rightarrow \mathbf{u}$$

“Projection” methods (or, reduction methods)

- Approximation vector space K_m. At each iteration m

$$\{\mathbf{u}_m\} \text{ such that } \mathbf{u}_m \in K_m$$

K_m: dimension[a] m, with the “expansion” property:

$$K_m \subseteq K_{m+1}$$

- Computation of iterate. Galerkin condition:

$$\text{residual} \quad \mathbf{r}_m := \mathbf{f} - \mathbf{A}\mathbf{u}_m \quad \perp \quad K_m$$

$\Rightarrow$ This condition uniquely defines $\mathbf{u}_m \in K_m$

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(Conjugate Gradients, Hestenes & Stiefel, ’52)

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Optimality property of Galerkin projection method

Let $\mathbf{u}^\star$ be the true solution. Galerkin property:

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is equivalent to:

$$\mathbf{u}_m \quad \text{solution to} \quad \min_{\mathbf{u} \in K_m} \|\mathbf{u}^\star - \mathbf{u}\|_{\mathbf{A}}$$

where $\| \cdot \|_{\mathbf{A}}$ is the energy norm, namely $\|\mathbf{x}\|_{\mathbf{A}}^2 := \langle \mathbf{x}, \mathbf{A}\mathbf{x} \rangle$

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Note: $\|\mathbf{u}^\star - \mathbf{u}\|_{\mathbf{A}}$ cannot be computed!

But, it can be easily estimated - particularly well if convergence is fast

(Strakoš, Tichy, Meurant, Golub, Arioli, ...)

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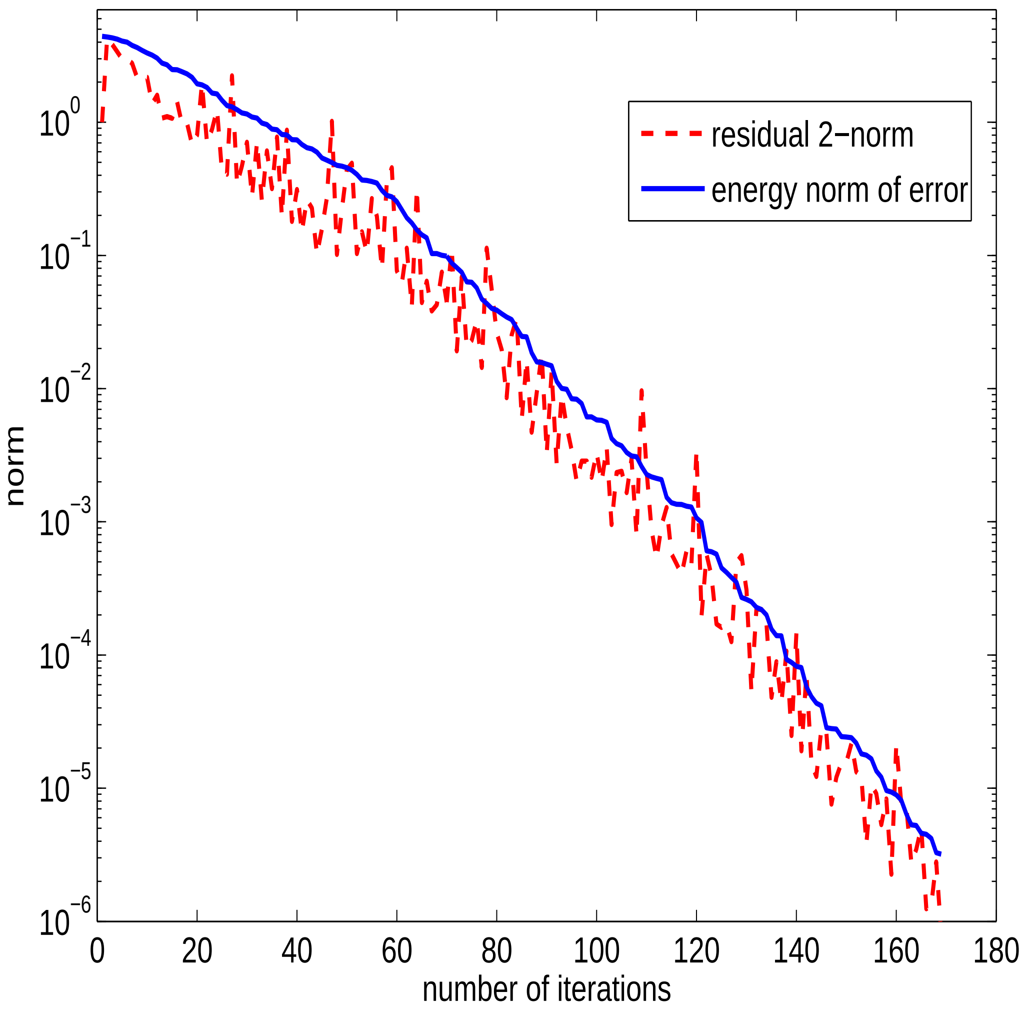
$\Rightarrow$ Use estimate of $\|\mathbf{u}^\star - \mathbf{u}_m\|_{\mathbf{A}}$ as stopping criterion

A typical example



Convergence and spectral properties

- In exact arithmetic (i.e., in theory), finite termination property
- A-priori bound for energy norm of the error:

  If $K_m = \mathrm{span}\{\mathbf{f}, \mathbf{A}\mathbf{f}, \ldots, \mathbf{A}^{m-1}\mathbf{f}\}$, then

$$\|\mathbf{u}^\star - \mathbf{u}_m\|_{\mathbf{A}} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^m \|\mathbf{u}^\star - \mathbf{u}_0\|_{\mathbf{A}}$$

  where $\kappa = \frac{\lambda_{\max}(\mathbf{A})}{\lambda_{\min}(\mathbf{A})}$

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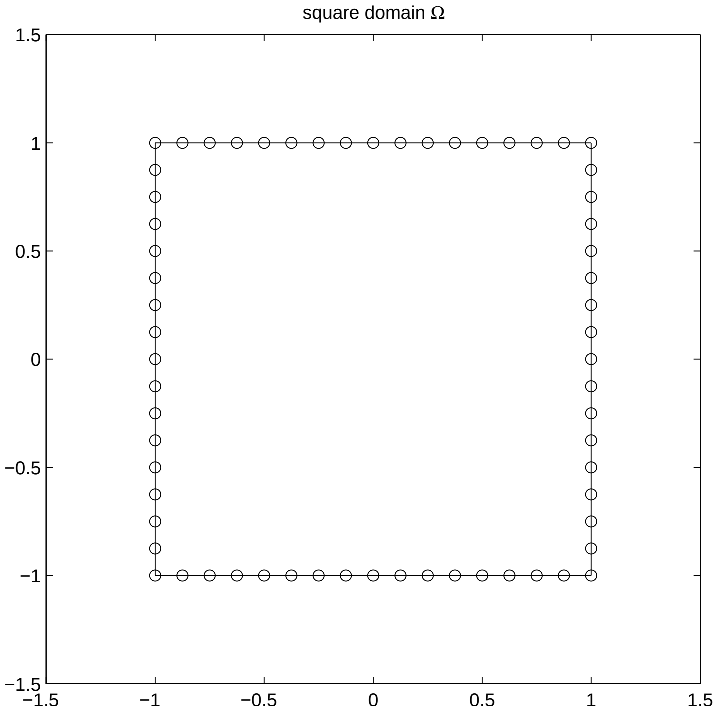
Consequences:

- Convergence: The closer κ to 1 the faster
- Convergence depends on spectral properties, not directly on problem size!

Exploring the intuitive relation. $-\Delta u = f$

V space of continuous solns, V_h discrete space of approximate solns

$V_h \approx V$, V_h e.g., space of piecewise low degree polynomials



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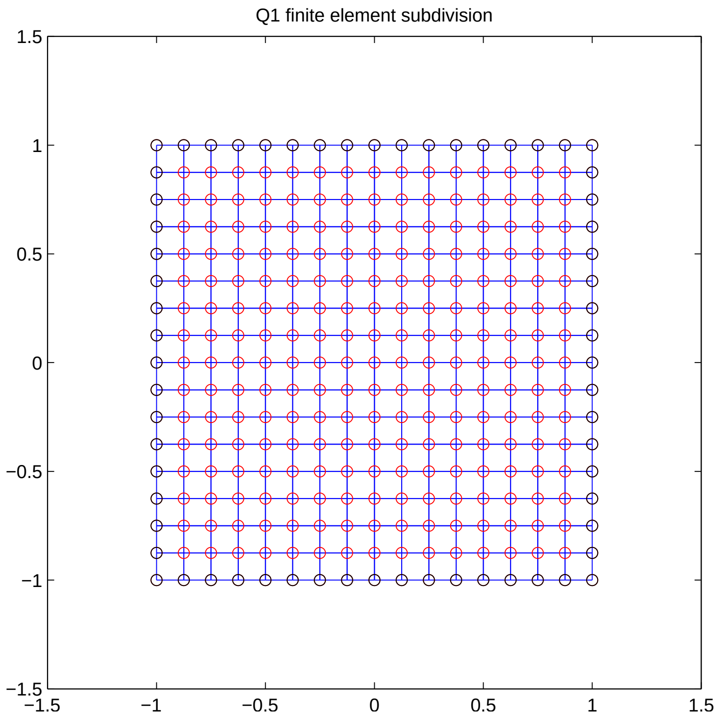

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Continuous weak formulation

Find $u \in V$ s.t. $(\nabla u, \nabla v) = (f, v), \; \forall v \in V_0$ $\qquad (x, y) = \int_\Omega xy$

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Discrete weak formulation

Find $u_h \in V_h$ s.t. $(\nabla u_h, \nabla v_h) = (f, v_h), \ \forall v_h \in V_{h,0}$ $\quad \Leftrightarrow \quad \mathbf{A}\mathbf{u} = \mathbf{f}$

$\{\phi_k\}$ basis for V_h, then $u_h = \sum \phi_k \mathbf{u}(k)$

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Error minimization property

$$\min_{w_h \in V_h} \|\nabla u - \nabla w_h\| \quad \Leftrightarrow \quad \min_{\mathbf{w} \in K_m} \|\mathbf{u} - \mathbf{w}\|_{\mathbf{A}}$$

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So what?

From intuition to practice

1. Spectral properties of $\mathbf{A}$ depend on problem
2. The error energy norms (functional and algebraic) are related

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1. Spectral properties of $\mathbf{A}$ depend on problem. Crucial in

$$\|\mathbf{u}^\star - \mathbf{u}_m\|_{\mathbf{A}} \leq \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m \|\mathbf{u}^\star - \mathbf{u}_0\|_{\mathbf{A}}$$

and $\kappa = O(\frac{1}{h^2})$

h	κ	n	# iterations
2^{-1}	3.33	25	3
2^{-3}	51.71	289	24
2^{-5}	829.86	4225	101

Model-based algebraic acceleration strategies

Spectrally equivalent matrices: $\tilde{\mathbf{A}} \sim \mathbf{A}$ if $\exists$ positive c_1, c_2 such that

$$c_1 \langle \mathbf{x}, \tilde{\mathbf{A}}\mathbf{x} \rangle \leq \langle \mathbf{x}, \mathbf{A}\mathbf{x} \rangle \leq c_2 \langle \mathbf{x}, \tilde{\mathbf{A}}\mathbf{x} \rangle \quad \forall \mathbf{x} \in \mathbb{R}^n$$

... usually, c_1, c_2 do not depend on h

A Realization: Geometric/Algebraic Multigrid

(Brandt, Bramble, Ruge, Stüben, Hackbusch, Trottenberg, Briggs, Henson, McCormick, ...)

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A Realization: Geometric/Algebraic Multigrid

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Formally, if $\tilde{\mathbf{A}} = \mathbf{L}\mathbf{L}^T$ and $\mathbf{M} = \mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-T}$, then $\kappa(\mathbf{M}) = O(\frac{c_2}{c_1})$ and

$$\mathbf{A}\mathbf{u} = \mathbf{f} \qquad \Rightarrow \qquad \mathbf{M}\tilde{\mathbf{u}} = \tilde{\mathbf{f}}, \qquad \mathbf{u} = \mathbf{L}^T\tilde{\mathbf{u}}, \ \mathbf{f} = \mathbf{L}\tilde{\mathbf{f}}$$

h	n	# iterations
2^{-3}	289	7
2^{-5}	4225	8
2^{-8}	66049	9

Exploring the intuitive relation

2. The energy norm of the error:

$$\|\nabla u - \nabla u_h\| \qquad \Leftrightarrow \qquad \|\mathbf{u}^\star - \mathbf{u}_m\|_{\mathbf{A}}$$

Let $u_{h,m} \in V_h$, with coefficients $\mathbf{u}_m$ (similarly for u_h). Then

$$\|\nabla(u - u_{h,m})\|^2 = \|\nabla(u - u_h)\|^2 + \|\mathbf{u}^\star - \mathbf{u}_m\|_{\mathbf{A}}^2$$

with

$$\|\nabla(u - u_h)\| = O(h)$$

(other constants depend, e.g., on the regularity of the solution)

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$\Rightarrow$ Stopping criterion for the iterative method:

$$\|\mathbf{u}^\star - \mathbf{u}_m\|_{\mathbf{A}} = O(h)$$

- Very loose linear system accuracy (cheap...)
- Different perspective from Gauss elimination type solvers

(Arioli, Noulard, Russo, Loghin, Wathen, Jiránek, Strakoš, Vohralík, ...)

An application to the Stokes equations

$$\begin{aligned} -\nabla^2 \vec{u} + \nabla p &= \vec{0}, \\ \nabla \cdot \vec{u} &= 0, \end{aligned}$$

on some domain $\Omega \subset \mathbb{R}^n$, with b.c. $\vec{u} = \vec{w}$ on $\partial\Omega$

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With the appropriate choices of bilinear forms and approximation spaces, we obtain:

$$
\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \qquad \Leftrightarrow \qquad \boldsymbol{\mathcal{M}}\,\mathbf{x} = \mathbf{b}
$$

with $\boldsymbol{\mathcal{M}}$ large, real indefinite symmetric matrix

Saddle point algebraic linear system (cf. Benzi & Golub & Liesen, '05)

Iterative solver and accelerator

$$\boldsymbol{\mathcal{M}}\,\mathbf{x} = \mathbf{b}$$

$\boldsymbol{\mathcal{M}}$ is symmetric and indefinite. Petrov-Galerkin condition:

$$\mathbf{x}_m \in K_m, \quad \text{s.t.} \qquad \min \|\mathbf{b} - \boldsymbol{\mathcal{M}}\mathbf{x}_m\|_2$$

$\mathbf{r}_m = \mathbf{b} - \boldsymbol{\mathcal{M}}\mathbf{x}_m$, $m = 0, 1, \ldots$ (Paige & Saunders, '75)

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If $\boldsymbol{\mathcal{P}} = \mathbf{H}\mathbf{H}^T$ is an accelerator (sym. pos.def.),

$$\mathbf{x}_m \in K_m, \quad \text{s.t.} \qquad \min \|\mathbf{b} - \boldsymbol{\mathcal{M}}\mathbf{x}_m\|_{\boldsymbol{\mathcal{P}}^{-1}}$$

where $K_m = \mathbf{H}^{-1}\mathrm{span}\{\mathbf{b}, \boldsymbol{\mathcal{M}}\boldsymbol{\mathcal{P}}^{-1}\mathbf{b}, \ldots, (\boldsymbol{\mathcal{M}}\boldsymbol{\mathcal{P}}^{-1})^{m-1}\mathbf{b}\}$

An accelerator for Stokes mixed approximation

$$\mathcal{M} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix}, \quad \mathcal{P} = \begin{bmatrix} \widetilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \widetilde{\mathbf{S}} \end{bmatrix} \qquad \widetilde{\mathbf{A}} \sim \mathbf{A}, \quad \widetilde{\mathbf{S}} \sim \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$$

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An example: from IFISS 3.1 (Elman, Ramage, Silvester): Lid driven cavity; Q2-Q1 approximation

$\tilde{\mathbf{S}} \rightarrow$ pressure mass matrix
$\widetilde{\mathbf{A}} \rightarrow$ Algebraic MG
(spectrally equivalent matrix)

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2D. Final residual norm $< 10^{-6}$

size($\mathcal{M}$)	its	Time (secs)
578	26	0.04
2178	26	0.14
8450	26	0.50
132098	26	11.17

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Ideal case: $\widetilde{\mathbf{A}} = \mathbf{A}$, $\widetilde{\mathbf{S}} = \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$. Then a "natural" norm:

energy norm in u-space and L_2 norm in p-space:

$$\|\mathbf{x} - \mathbf{x}_m\|^2_{\mathcal{P}_{\text{ideal}}} = \|\mathbf{u} - \mathbf{u}_m\|^2_{\mathbf{A}} + \|\mathbf{p} - \mathbf{p}_m\|^2_{\mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T}$$

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For stable discretization, heuristic relation between error and residual:

$$\|\mathbf{x} - \mathbf{x}_m\|_{\mathcal{P}_{\text{ideal}}} \leq \frac{\sqrt{2}}{\gamma^2} \|\mathbf{b} - \mathcal{M}\mathbf{x}_m\|_{\mathcal{P}^{-1}_{\text{ideal}}}$$

γ inf-sup constant: $\qquad \gamma^2 \leq \frac{\mathbf{q}^T\mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T\mathbf{q}}{\mathbf{q}^T\mathbf{Q}\mathbf{q}}, \quad \forall \mathbf{q} \neq 0$

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Estimating the inf-sup constant

Spectrum of transformed coefficient matrix:

$$\mathrm{spec}(\boldsymbol{\mathcal{M}}\boldsymbol{\mathcal{P}}^{-1}) \subseteq [\Lambda_-, \lambda_-] \cup [\lambda_+, \Lambda_+]$$

with (Elman-Silvester-Wathen, '05)

$$\lambda_- \leq \frac{1}{2}(\delta - \sqrt{\delta^2 + 4\delta\gamma^2}) \qquad \delta \leq \lambda_+$$

where $\delta = \lambda_{\min}(A\widetilde{A}^{-1})$.

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where $\delta = \lambda_{\min}(A\widetilde{A}^{-1})$.

Were these bounds tight (equalities), then

$$\gamma^2 = \frac{\lambda_-^2 - \lambda_-\lambda_+}{\lambda_+}$$

Estimating the inf-sup constant

Assume that these bounds are indeed tight (equalities). Then

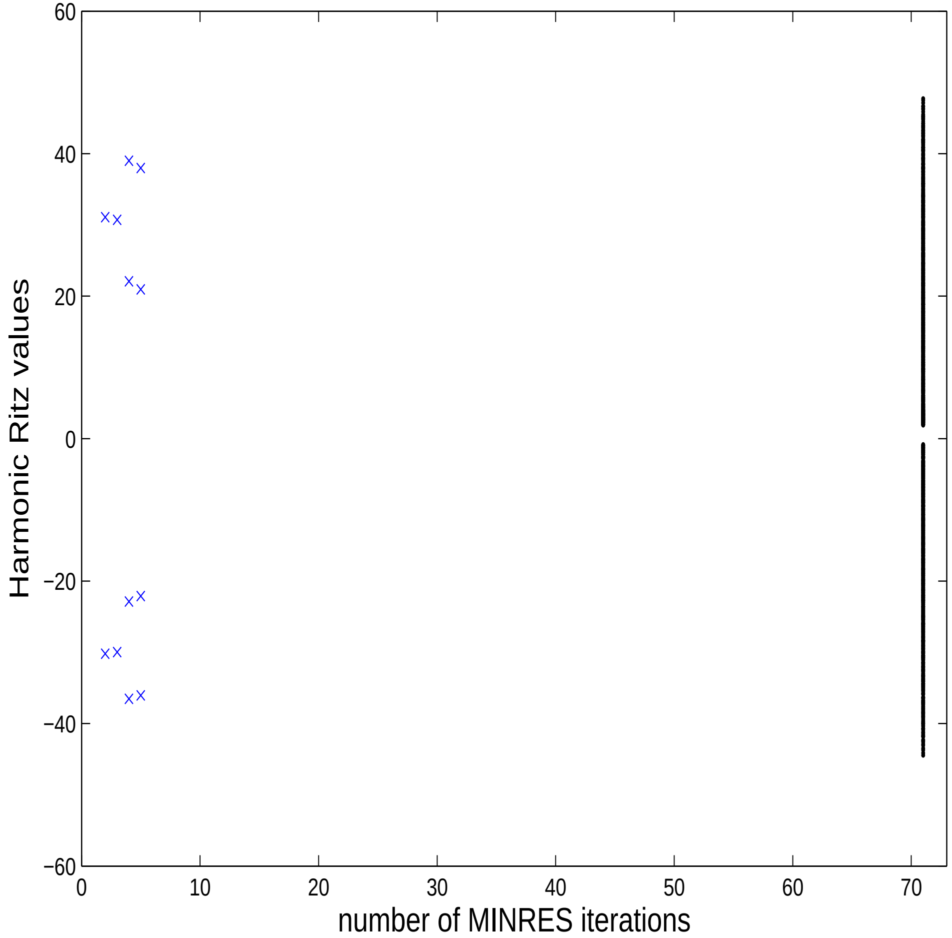
$$\gamma^2 = \frac{\lambda_-^2 - \lambda_- \lambda_+}{\lambda_+}$$

In practice, adaptive estimate with Harmonic Ritz values:

$$\gamma^2 \approx \gamma_m^2 = \frac{(\theta_-^{(m)})^2 - \theta_-^{(m)} \theta_+^{(m)}}{\theta_+^{(m)}}, \qquad mth \text{ MINRES iteration}$$

(Silvester & Simoncini, '11)

Typical convergence pattern



Harmonic Ritz values as iterations proceed

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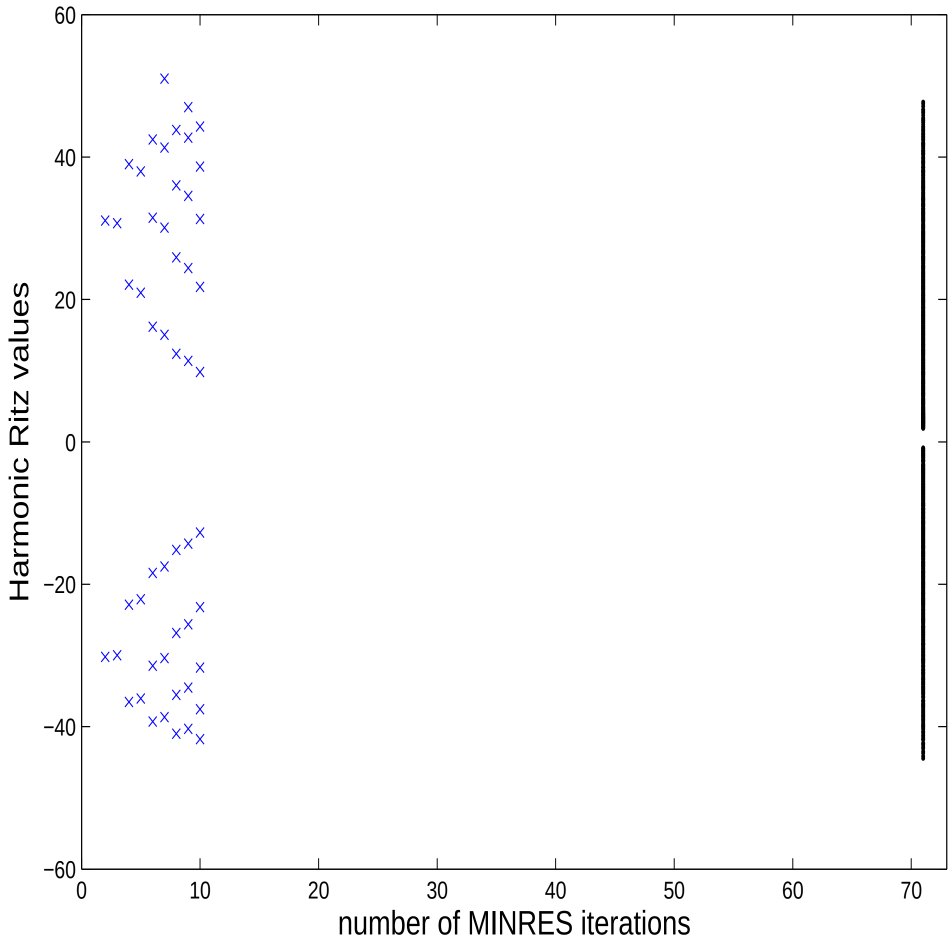

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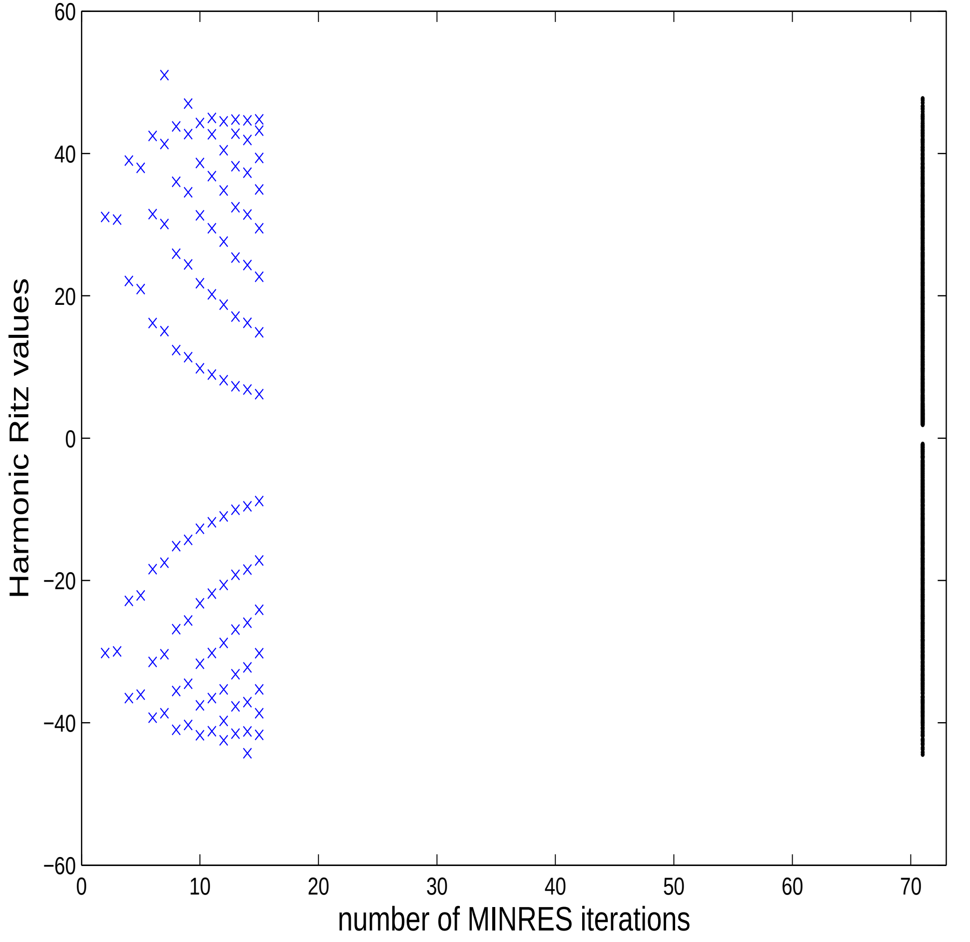

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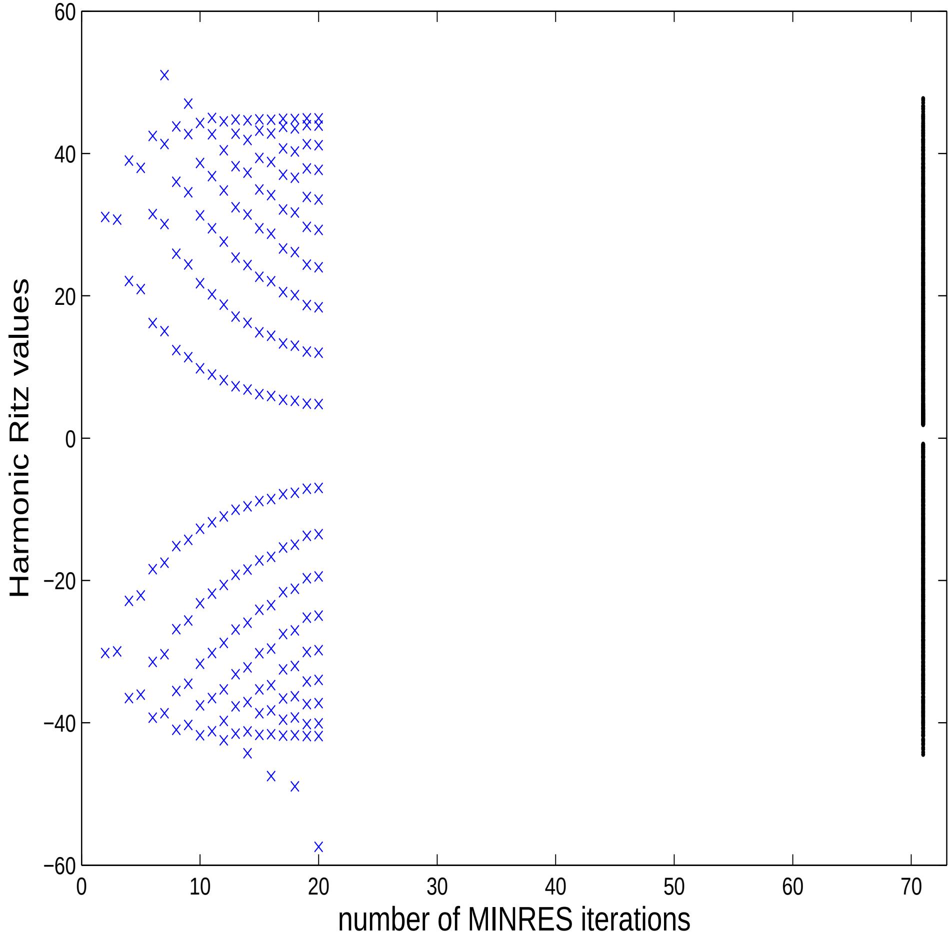

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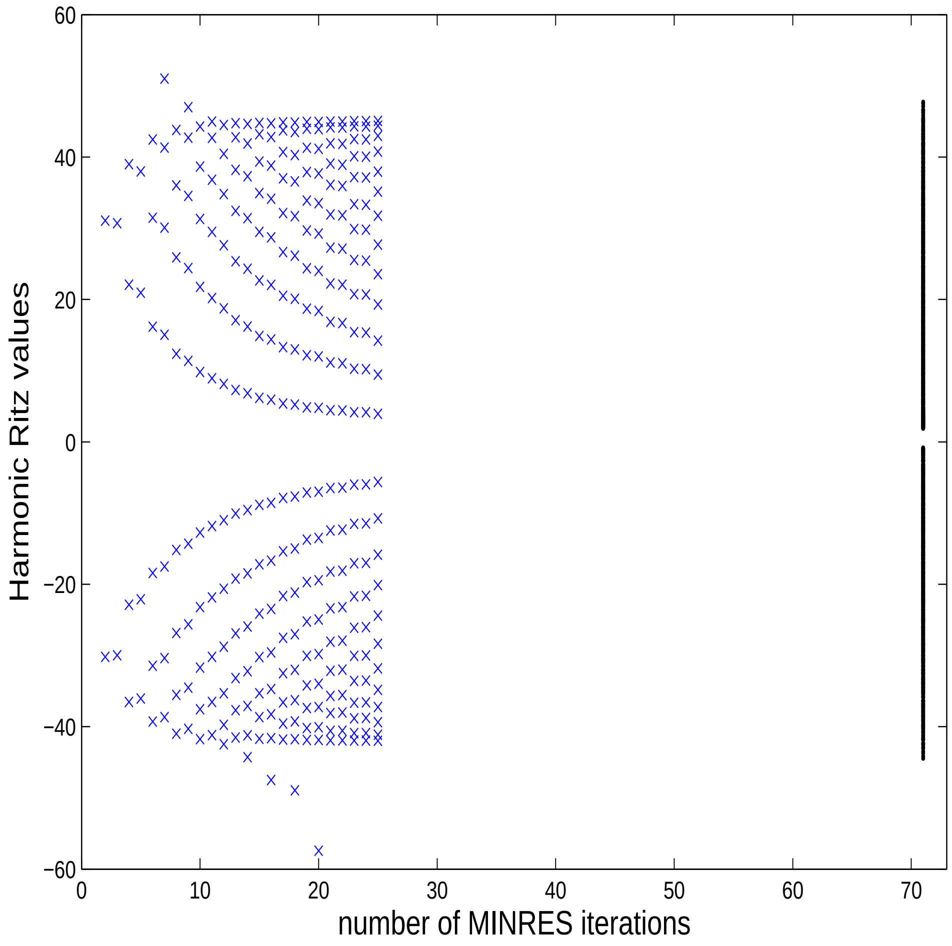
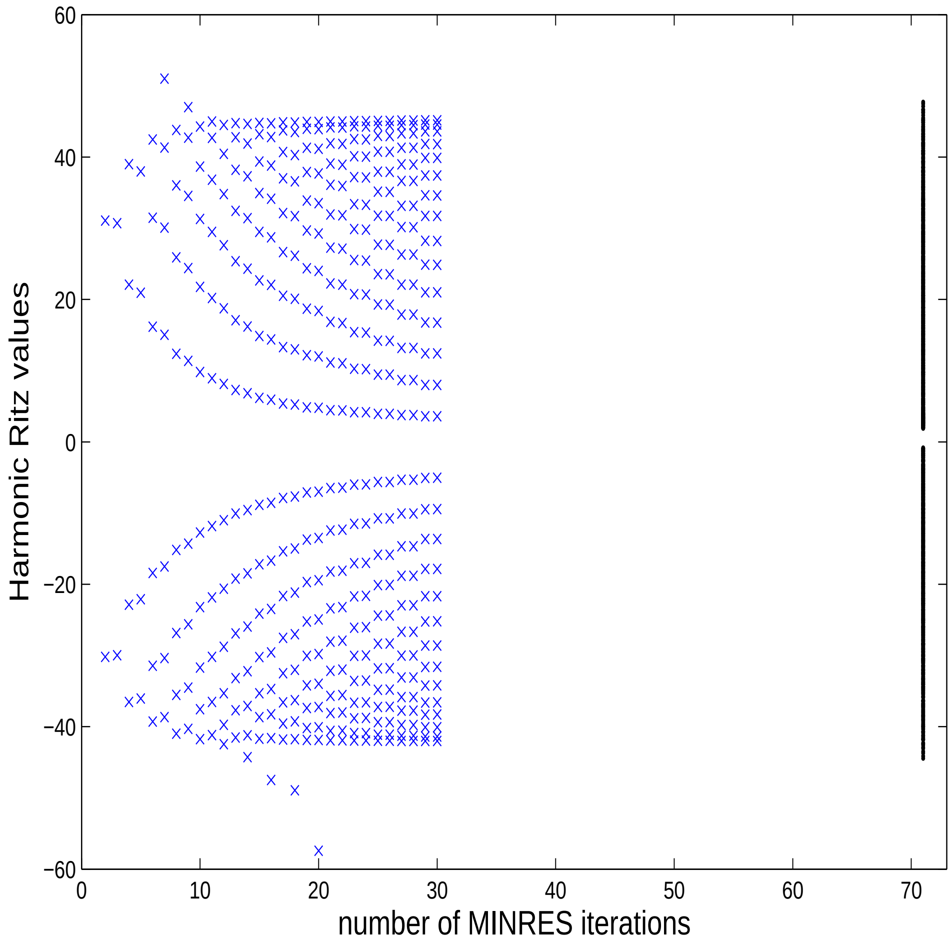
Typical convergence pattern



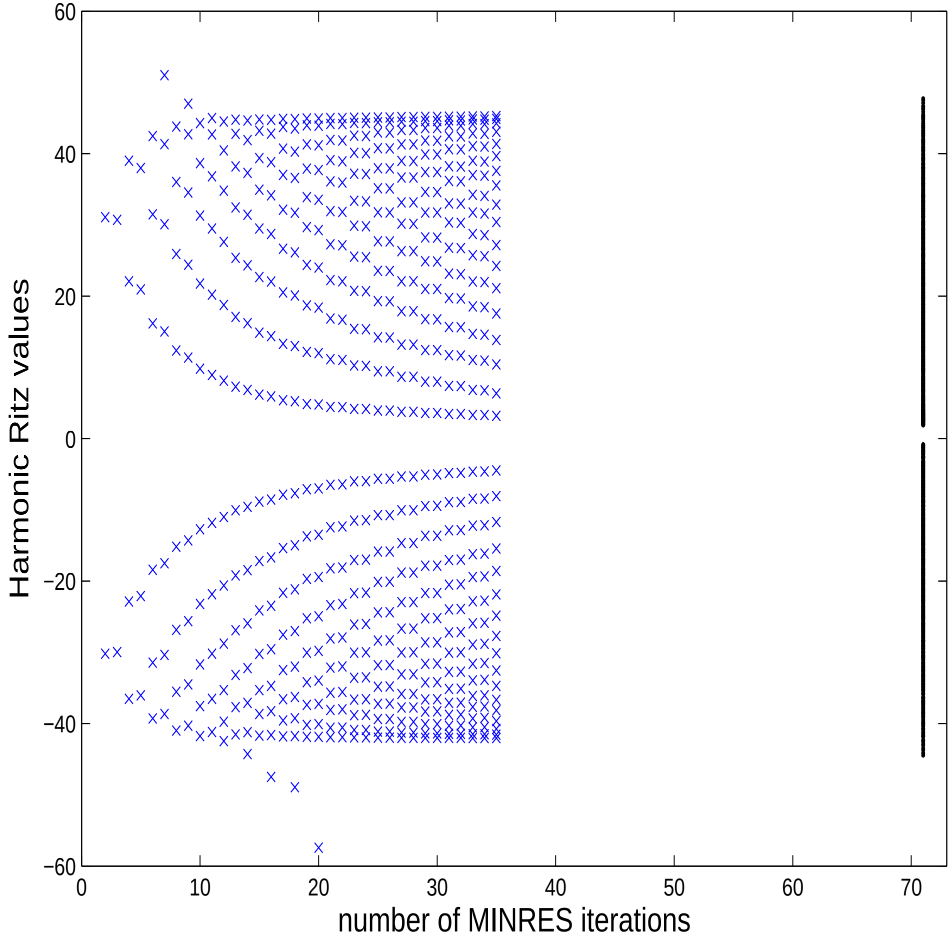
Harmonic Ritz values as iterations proceed

Typical convergence pattern



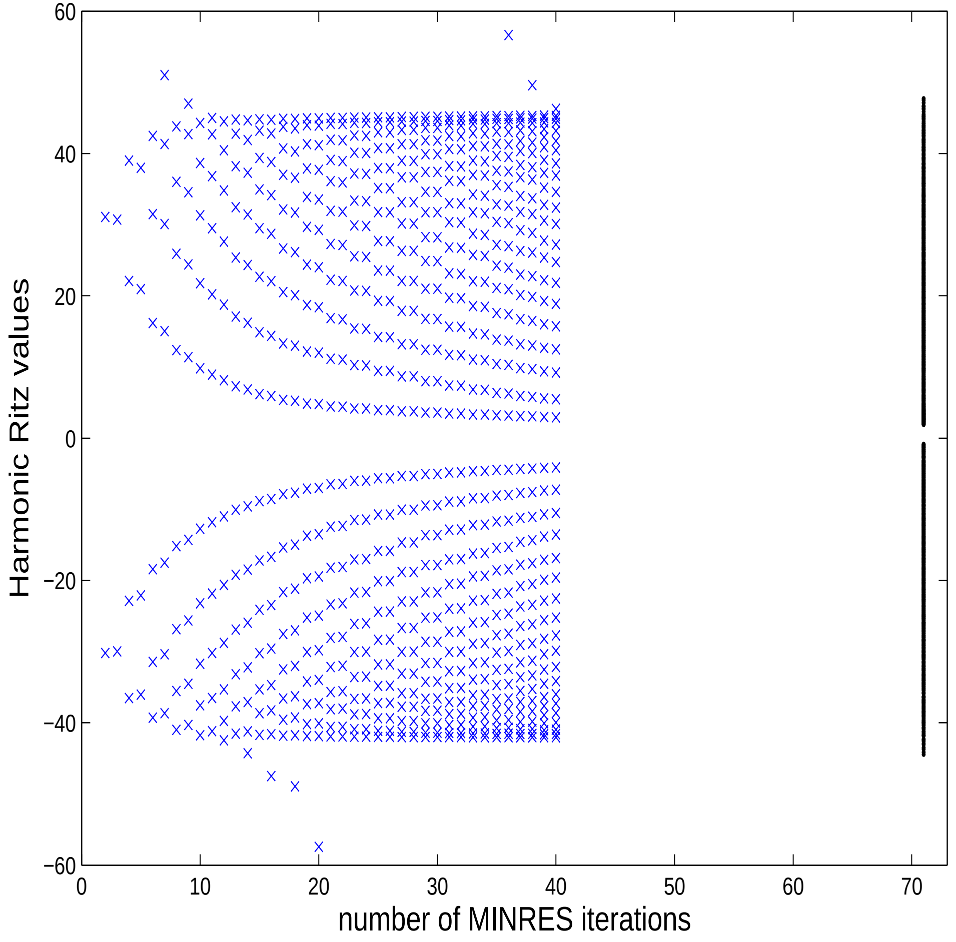
Harmonic Ritz values as iterations proceed

Typical convergence pattern



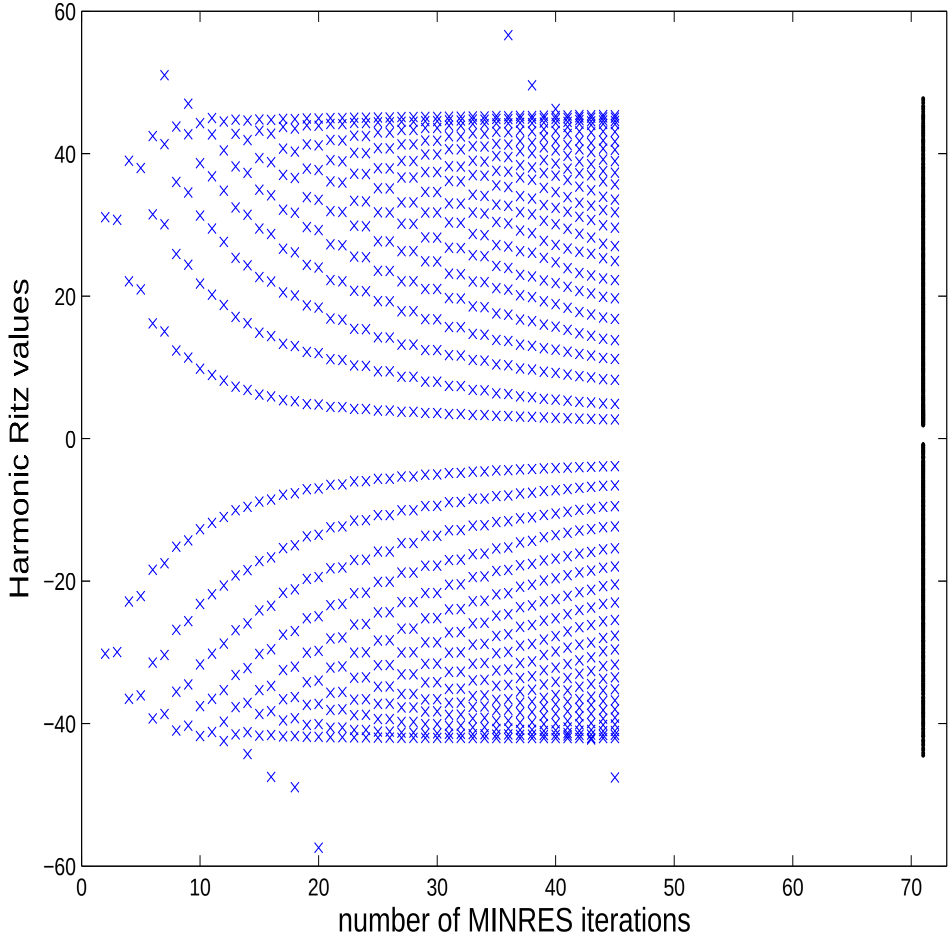
Harmonic Ritz values as iterations proceed

Typical convergence pattern



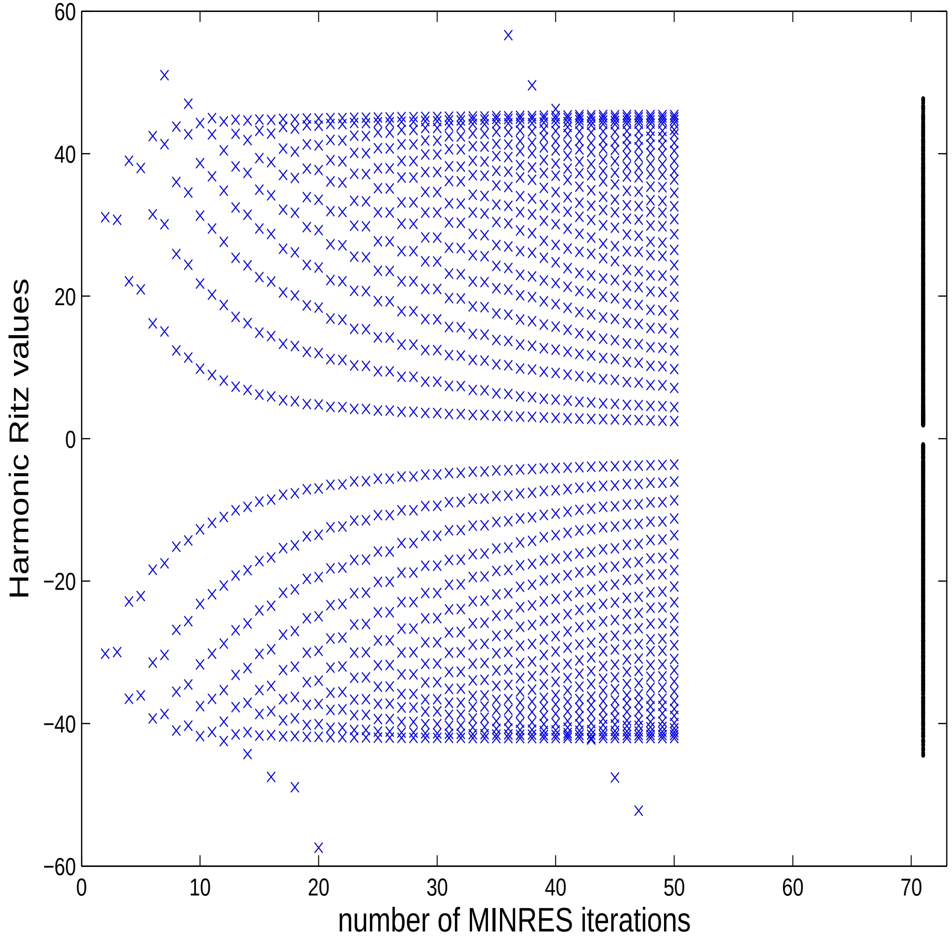
Harmonic Ritz values as iterations proceed

Typical convergence pattern



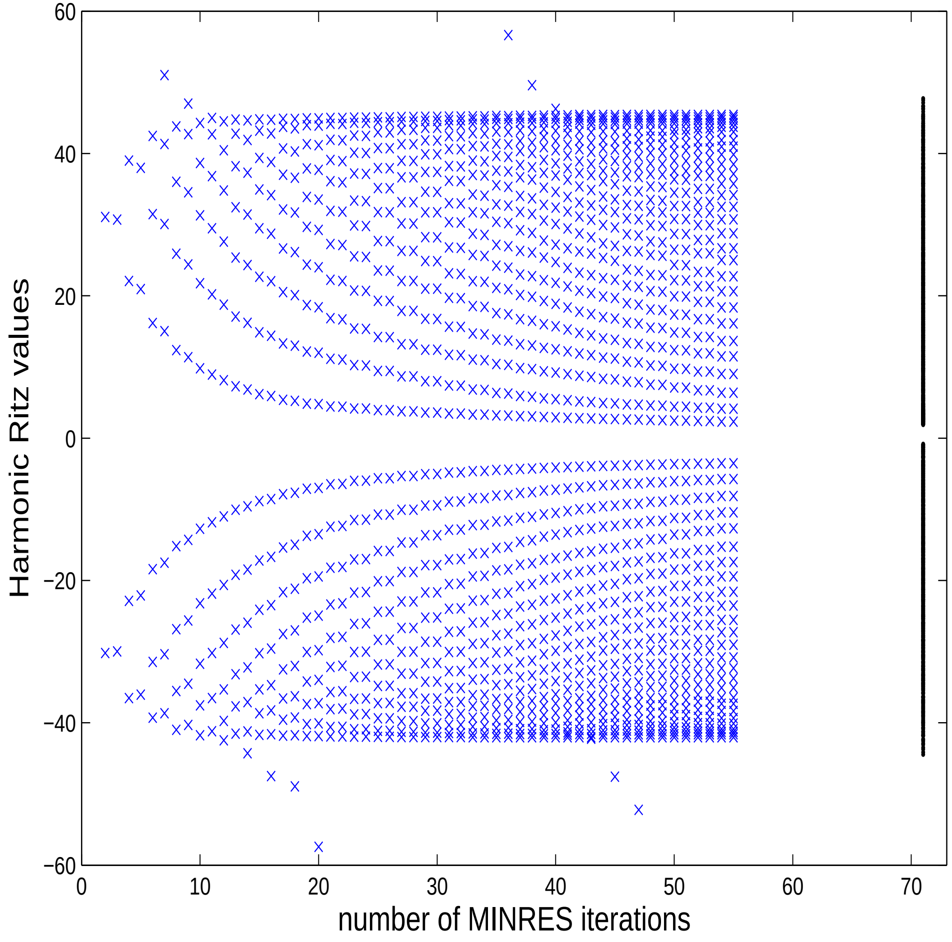
Harmonic Ritz values as iterations proceed

Typical convergence pattern



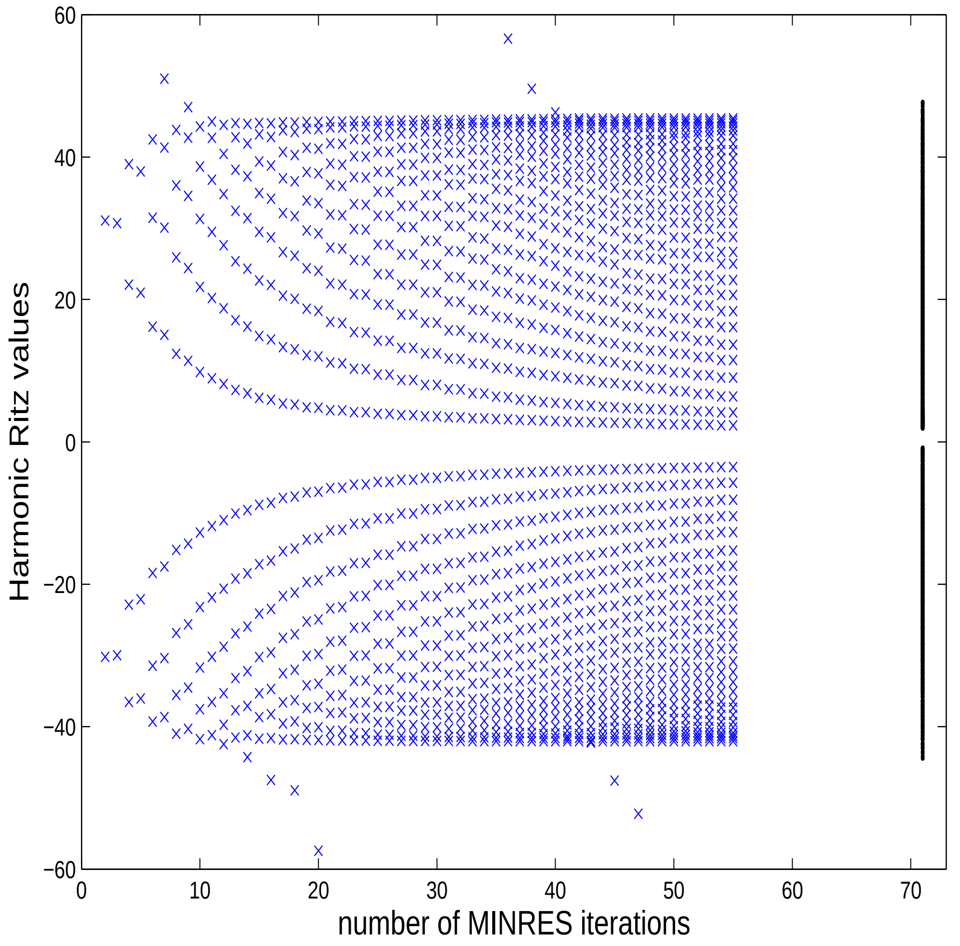
Harmonic Ritz values as iterations proceed

Typical convergence pattern



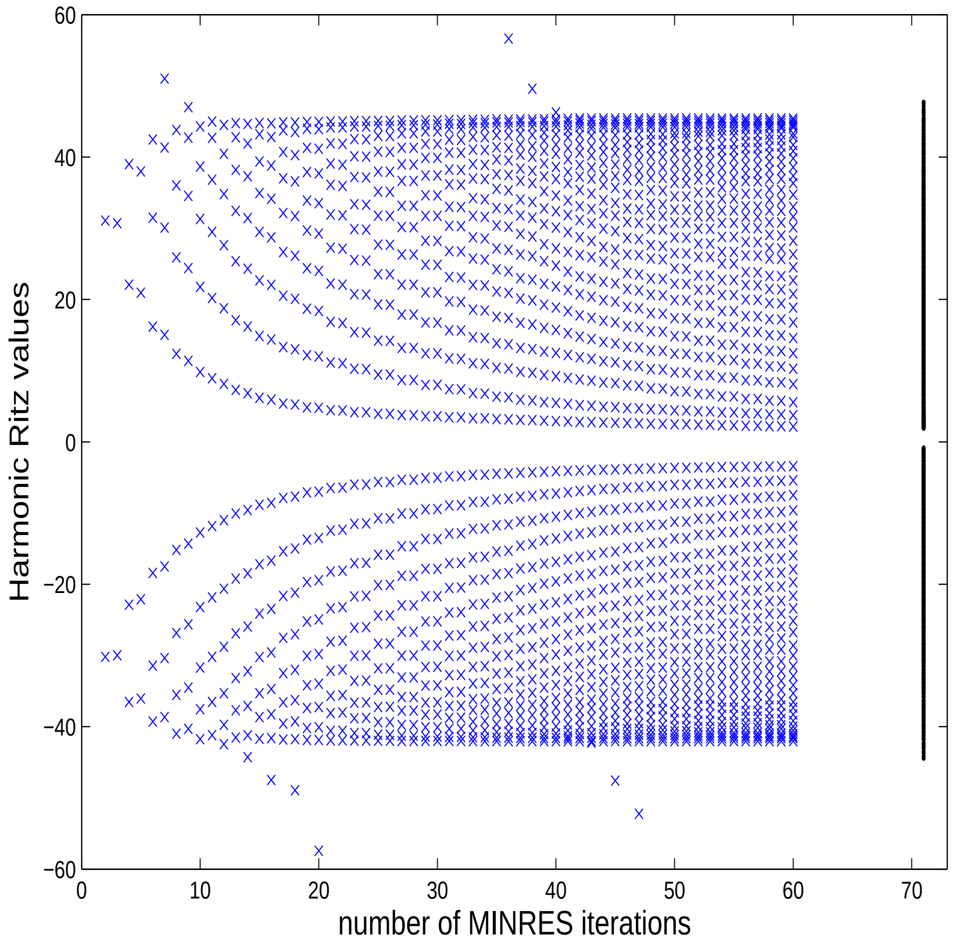
Harmonic Ritz values as iterations proceed

Typical convergence pattern



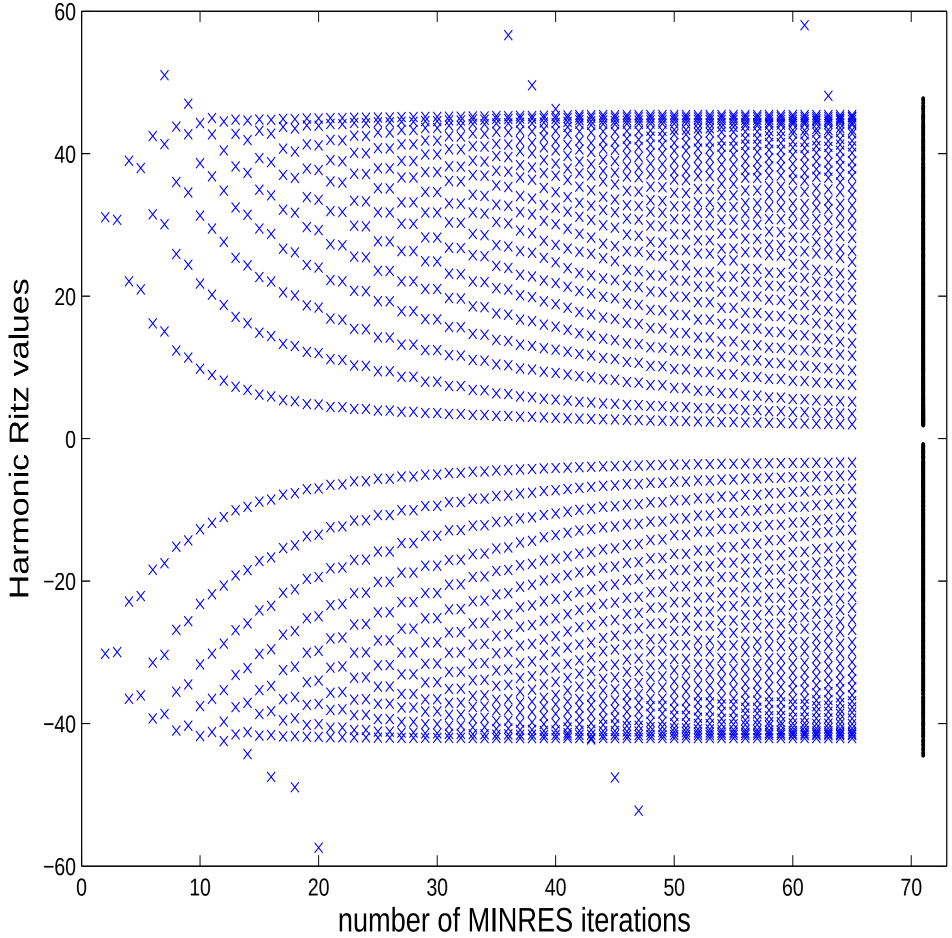
Harmonic Ritz values as iterations proceed

Typical convergence pattern



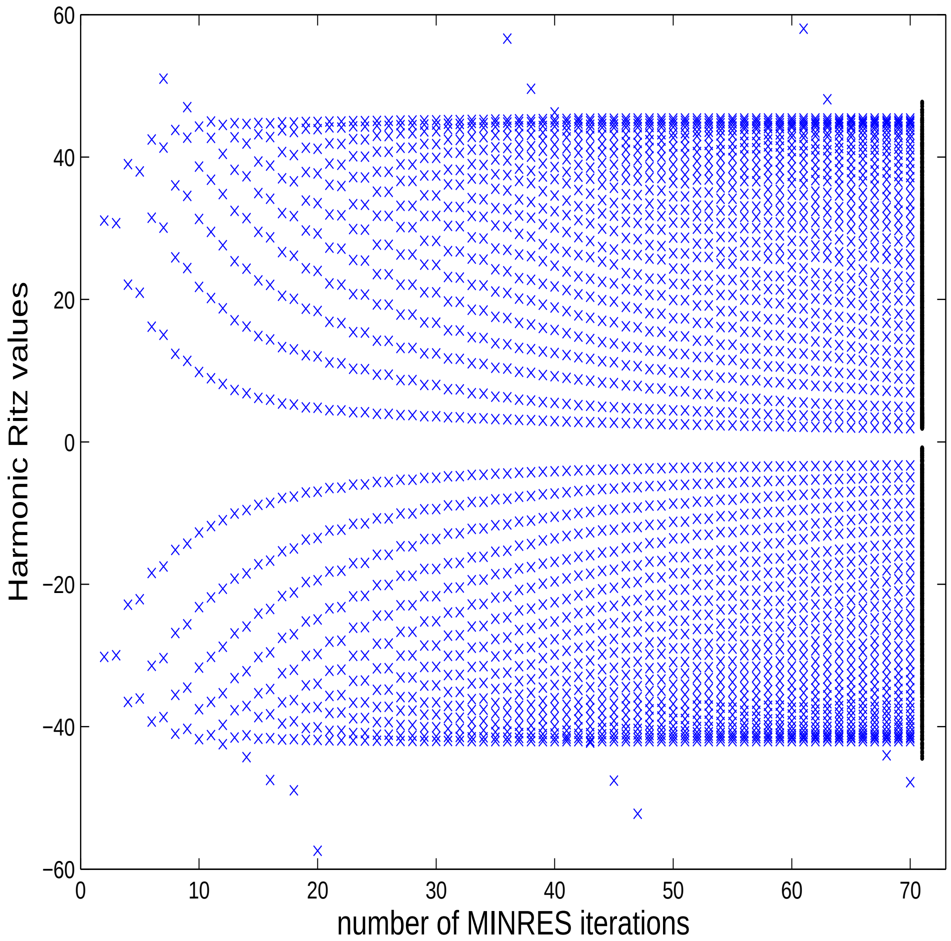
Harmonic Ritz values as iterations proceed

Typical convergence pattern



Harmonic Ritz values as iterations proceed

Typical convergence pattern

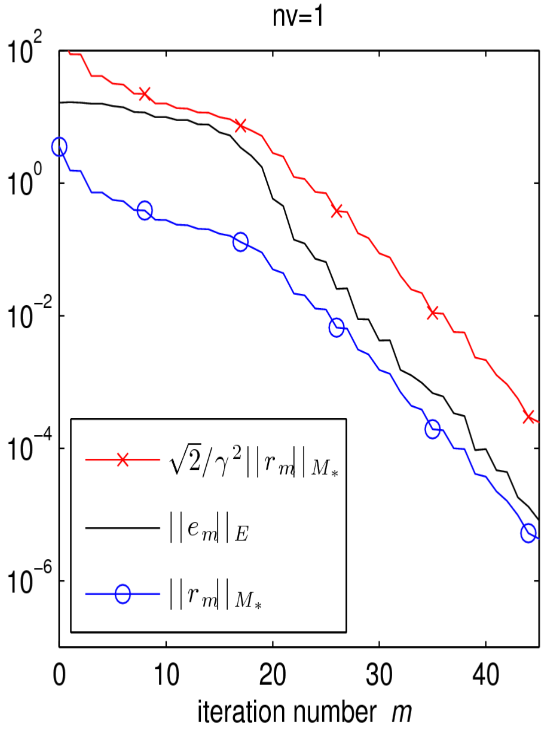


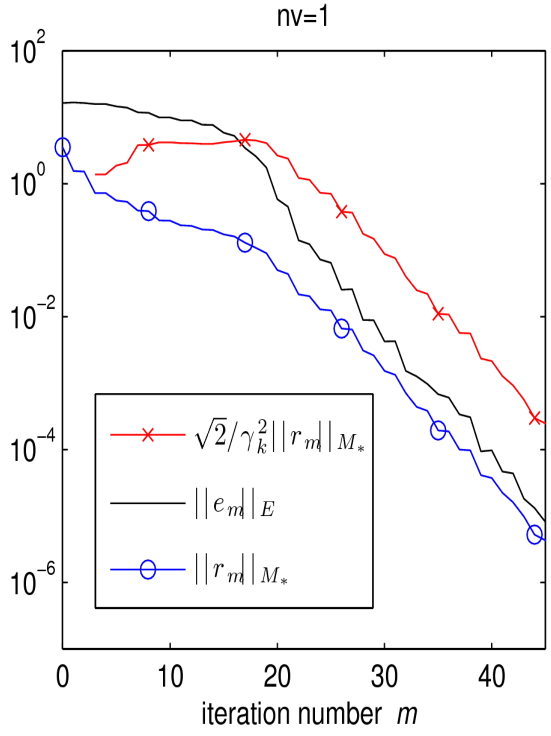
Harmonic Ritz values as iterations proceed

Another IFISS example. Flow over a step.

e_m: error at iteration m $\qquad$ r_m: residual at iteration m

Optimal γ $\qquad$ **Adaptive γ_m**





$E = \mathcal{P}_{\text{ideal}}, \qquad M_* = \mathcal{P}^{-1}$

A model-based stopping criterion

If an a-posteriori discretization error estimate $\eta^{(m)}$ is available, namely

$$c\,\eta^{(m)} \leq \|\nabla(\vec{u} - \vec{u}_h^{(m)})\| + \|p - p_h^{(m)}\| \leq C\,\eta^{(m)}, \quad m = 1, 2, 3 \ldots$$

with $\frac{C}{c} = O(1)$

(Ainsworth, Oden, Kay, Silvester, Elman, Wathen, Liao, Jiránek, Strakoš, Vohralík, ...)

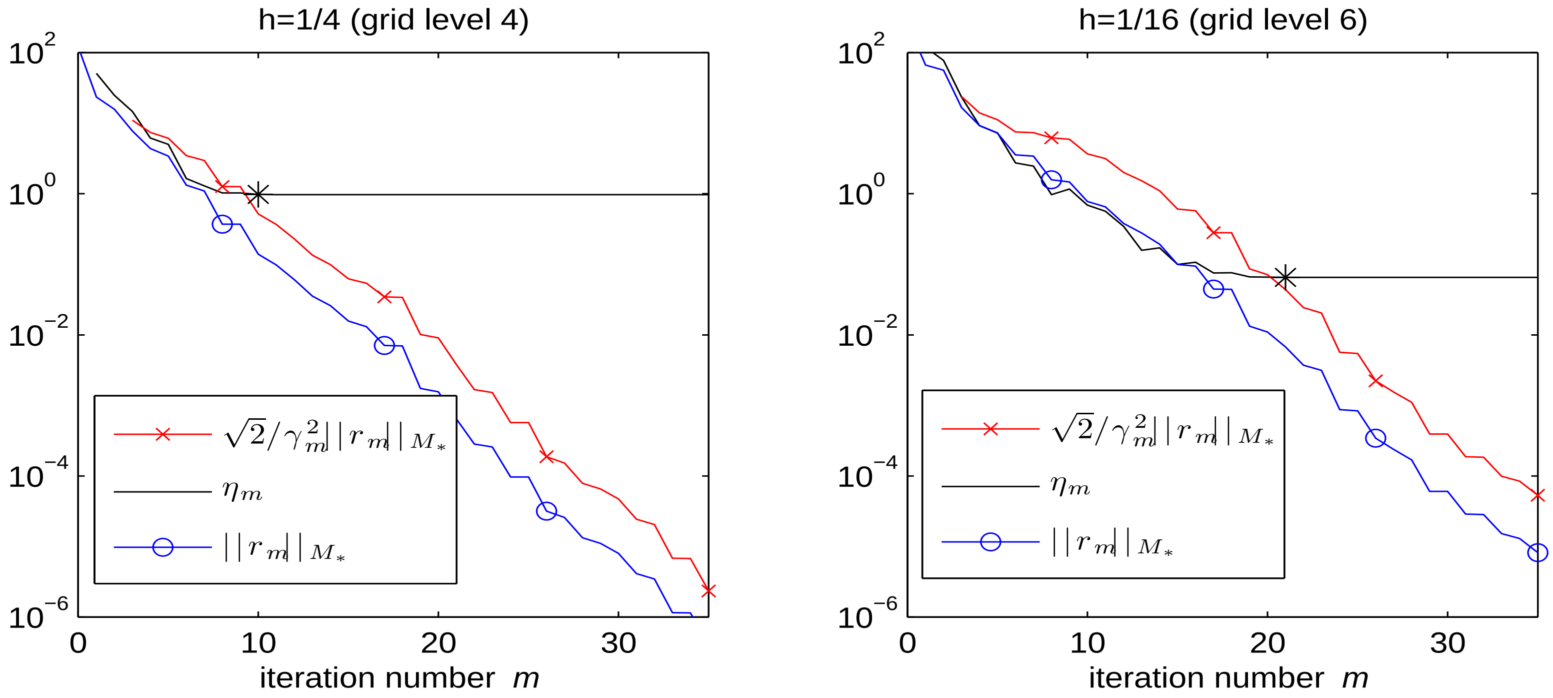
We can devise a stopping criterion:

$$\|\mathbf{x} - \mathbf{x}_m\|_{\boldsymbol{\mathcal{P}}_{\text{ideal}}} \sim \frac{\sqrt{2}}{\gamma_m^2}\|\mathbf{b} - \boldsymbol{\mathcal{M}}\mathbf{x}_m\|_{\boldsymbol{\mathcal{P}}^{-1}} < \eta^{(m)}$$

A model-based stopping criterion

Another IFISS example. Smooth colliding flow.

r_m: residual at iteration m



$$M_* = \mathcal{P}^{-1}$$

Final consideration

Opening the black box may be rewarding, with a mutual gain

References:

* M. Benzi, G.H. Golub and J. Liesen, *Numerical Solution of Saddle Point Problems*, Acta Numerica, 14, 1-137 (2005)

* H. Elman, D. Silvester and A. Wathen, *Finite Elements and Fast Iterative Solvers, with applications in incompressible fluid dynamics*, Oxford University Press, (2005)

* K.A. Mardal and R. Winther, *Preconditioning discretizations of systems of partial differential equations*, Numer. Linear Algebra with Appl., 18, 1-40 (2011)

* D. Silvester and V. Simoncini *An Optimal Iterative Solver for Symmetric Indefinite Systems stemming from Mixed Approximation.* ACM TOMS, (2011)

* Multigrid Website MG-Net, `http://www.mgnet.org` (up to 2010)