

Requirements for iterative linear equation solvers in problems of solid- and structural mechanics

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MTU60: Let's make it sparse, Prague, Czech Republic, Jan 31 - Feb 2, 2019

Happy birthday Mirek!



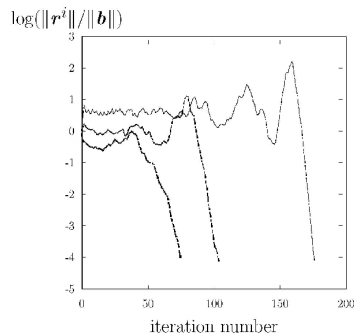
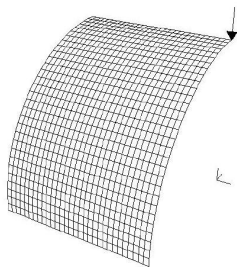
Veräjämäki May 27, 2000.

Some history

- ▶ I became interested in iterative linear solvers around 1995.
- ▶ After hitting my head to the wall with X preconditioners I found the paper:
M. Benzi, C.D. Meyer, M. Tuma, A sparse approximate inverse preconditioner for the CG method, *SIAM J. Sci. Comp.*, **17**,1135-1149 (1996) and I felt fascinated about the idea.
- ▶ I sent a mail to Michele (autumn 1996?) and then everything started to evolve fast.
- ▶ Mirek, Michele and I wrote our first journal paper and it was published 1998 in *Commun. Numer. Methods Eng.*
- ▶ I met Mirek first time face to face in Prague May 1999 and Michele in Finland July 2004.
- ▶ Mirek visited Helsinki in May 2000.

It started with shells

Bending dominated loading, 30×30 uniform mesh, stabilized quadrilateral MITC4 shell elements 5489 unknowns. Convergence of the PCG depends highly on the “thinness” of the shell, here $t/R = 0.1, 0.01, 0.001$ and convergence with the IC(0)-preconditioner shown below.



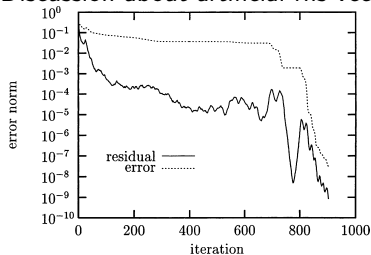
M. Benzi, RK, M. Tuma, An assessment of some preconditioning techniques in shell problems, *Communications in Numerical Methods in Engineering*, **14**, 1998, 897-906

In 1999 it continued with solids etc.



Veräjämäki May 27, 2000.

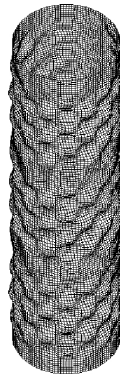
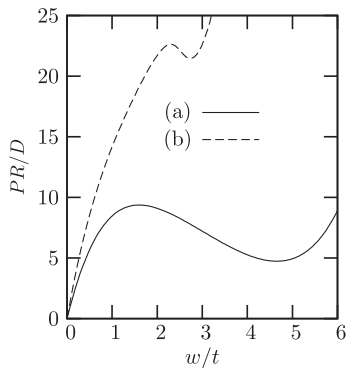
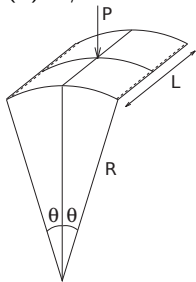
Block versions of the stabilized AINV
Discussion about artificial rhs-vectors



M. Benzi, RK, M. Tuma, Stabilized and block approximate inverse preconditioners for problems in solid and structural mechanics, *Computer Methods in Applied Mechanics and Engineering*, **190**, 2001, 6533-6554

Why I am interested in shells? - Shells are prone to stability problems

$R/L = 4$
(a) $R/t = 100$
(b) $R/t = 400$



Path-following methods

The *non-linear* mapping $\mathbf{f}$ defines the equilibrium path in the displacement $\mathbf{q}$ and load parameter λ space:

$$\mathbf{f}(\mathbf{q}, \lambda) \equiv \mathbf{r}(\mathbf{q}) - \lambda \mathbf{p}_r(\mathbf{q}) = \mathbf{0} \quad (1)$$

and constitutes the balance between internal- and external forces.

To overcome limit points an additional equation is usually augmented to (1), thus we have to solve

$$\begin{cases} \mathbf{f}(\mathbf{q}, \lambda) = \mathbf{r}(\mathbf{q}) - \lambda \mathbf{p}_r(\mathbf{q}) = \mathbf{0} \\ c(\mathbf{q}, \lambda) = 0. \end{cases} \quad (2)$$

Newton's linearisation step results in

$$\mathbf{A} \delta \mathbf{x} = -\mathbf{g}, \quad (3)$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{K} & \mathbf{p}_r \\ \mathbf{c}^T & e \end{bmatrix}, \quad \delta \mathbf{x} = \begin{Bmatrix} \delta \mathbf{q} \\ \delta \lambda \end{Bmatrix}, \quad \mathbf{g} = \begin{Bmatrix} \mathbf{f} \\ c \end{Bmatrix}, \quad \mathbf{K} = \mathbf{f}' = \frac{\partial \mathbf{f}}{\partial \mathbf{q}}, \quad \mathbf{c} = \frac{\partial c}{\partial \mathbf{q}}, \quad e = \frac{\partial c}{\partial \lambda}.$$

Requirements for linear solvers in non-linear analysis

- ▶ Be able to handle indefinite matrices.
- ▶ Symmetry (if existing) of the Jacobian matrix of $\mathbf{f}$ should be exploitable.
- ▶ Information about definiteness (positive definite/indefinite) of the matrix should be extractable.

Stability of equilibrium state ?

Singularity test functions (STF)

- ▶ determinant
- ▶ smallest eigenvalue
- ▶ smallest pivot
- ▶ current stiffness parameter

Requirements for the STF

- ▶ mesh size independent
- ▶ “good predictor”
- ▶ indicates all kind of singular behaviour
- ▶ easy and cheap to evaluate

Check for the positivity

of a matrix $\mathbf{A}$ when applying preconditioned Krylov subspace methods to solve $\mathbf{Ax} = \mathbf{b}$ with accuracy $\|\mathbf{r}_i\| = \|\mathbf{b} - \mathbf{Ax}_i\| < \varepsilon_r \|\mathbf{b} - \mathbf{Ax}_0\| + \varepsilon_a$.

- ▶ λ_i is an eigenvalue of $\mathbf{A}$
- ▶ $\lambda_1 = \min \lambda_i$
- ▶ $|\lambda_1| < \delta$

Conjecture

If $\mathbf{A}$ is indefinite

then there exists with probability $1 - \eta(\delta, \varepsilon_r, \varepsilon_a)$
at least one iterate k such that $\mathbf{d}_k^T \mathbf{A} \mathbf{d}_k < 0$.

To be useful: $\eta \ll 1$ and $\mathbf{A} \mathbf{d}_k$ should be available

1. form $\mathbf{M}$ (or directly $\mathbf{M}^{-1}$),
2. initialize $\mathbf{r}_0 = \mathbf{b} - \mathbf{Ax}_0$, apply preconditioner $\mathbf{d}_0 = \mathbf{M}^{-1} \mathbf{r}_0$, compute $\tau_0 = \mathbf{r}_0^T \mathbf{d}_0$,
3. iterate $i = 0, 1, 2, \dots$ until convergence:
 - 3.1 compute: $\mathbf{s} = \mathbf{A} \mathbf{d}_i$, $a_i = \tau_i / \mathbf{d}_i^T \mathbf{s}$,
 - 3.2 update: $\mathbf{x}_{i+1} = \mathbf{x}_i + a_i \mathbf{d}_i$,
 $\mathbf{r}_{i+1} = \mathbf{r}_i - a_i \mathbf{s}$,
 - 3.3 apply preconditioner: $\mathbf{z} = \mathbf{M}^{-1} \mathbf{r}_{i+1}$,
 - 3.4 compute: $\tau_{i+1} = \mathbf{r}_{i+1}^T \mathbf{z}$, $b_i = \tau_{i+1} / \tau_i$,
 - 3.5 update: $\mathbf{d}_{i+1} = \mathbf{z} + b_i \mathbf{d}_i$.

It works with PCG but not with preconditioned Bi-CGSTAB - Why?

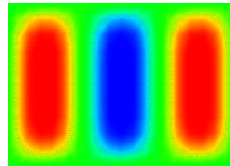
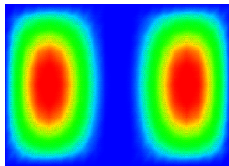
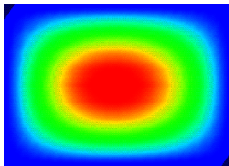
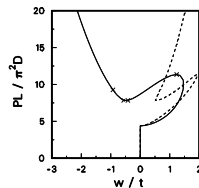
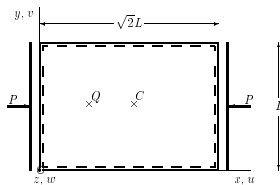
1. form M (or directly M^{-1}),
2. compute $r_0 = b - Ax_0$, choose $\tilde{r}$, compute $\rho_0 = \tilde{r}^T r_0$, set $d_0 = r_0$,
3. iterate $i = 0, 1, 2, \dots$, until converged:
 - 3.1 apply preconditioner: $z = M^{-1}d_i$,
 - 3.2 compute: $v_i = Az$, $a_i = \rho_i / \tilde{r}^T v_i$, $s = r_i - a_i v_i$,
 - 3.3 apply preconditioner: $\tilde{s} = M^{-1}s$,
 - 3.4 compute: $w = A\tilde{s}$, $\omega_i = w^T s / w^T w$,
 - 3.5 update: $x_{i+1} = x_i + a_i z + \omega_i \tilde{s}$, $r_{i+1} = s - \omega_i w$,
 - 3.6 compute: $\|r_{i+1}\|_2$,
 - 3.7 compute: $\rho_{i+1} = \tilde{r}^T r_{i+1}$ and $b_{i+1} = (\rho_{i+1} / \rho_i)(a_i / \omega_i)$,
 - 3.8 update: $d_{i+1} = r_{i+1} + b_{i+1}(d_i - \omega_i v_i)$.

To the next topic - direct solution of singular points

My old favourite - stability analysis



M.C. Escher, Metamorphosis II, 1940.



Stability eigenvalue problem

Definition for critical state: Find displacements $\mathbf{q}_{\text{cr}}$, critical load λ_{cr} and the corresponding eigenmode ϕ such, that

$$\begin{cases} \mathbf{f}'(\mathbf{q}_{\text{cr}}, \lambda_{\text{cr}})\phi &= \mathbf{0} \\ \mathbf{f}(\mathbf{q}_{\text{cr}}, \lambda_{\text{cr}}) &= \mathbf{0} \end{cases} \quad (4)$$

where $\mathbf{f}' = \partial \mathbf{f} / \partial \mathbf{q}$.

System (4) is a non-linear eigenvalue problem, which is **HARD TO SOLVE!**

Solution algorithm for non-linear eigenproblem

Extended system:

$$\mathbf{g}(\mathbf{x}) = \mathbf{g}(\mathbf{q}, \phi, \lambda) = \begin{cases} \hat{\mathbf{f}}(\mathbf{q}, \lambda) \equiv \mathbf{f}(\mathbf{q}, \lambda) + \mathbf{f}_0(\mathbf{q}, \lambda) = \mathbf{0} \\ \mathbf{h}(\mathbf{q}, \phi, \lambda) \equiv \mathbf{f}'(\mathbf{q}, \lambda)\phi + \mathbf{h}_0(\phi, \lambda) = \mathbf{0} \\ \mathbf{c}(\mathbf{q}, \phi, \lambda) = \mathbf{0}. \end{cases}$$

Newton's linearisation step results in

$$\mathbf{A}\delta\mathbf{x} = -\mathbf{g},$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{K}_f & \mathbf{0} & \mathbf{P} \\ \mathbf{Z} & \mathbf{K}_h & \mathbf{N} \\ \mathbf{C}_q & \mathbf{C}_\phi & \mathbf{C}_\lambda \end{bmatrix}, \quad \delta\mathbf{x} = \begin{Bmatrix} \delta\mathbf{q} \\ \delta\phi \\ \delta\lambda \end{Bmatrix}, \quad \mathbf{g} = \begin{Bmatrix} \hat{\mathbf{f}} \\ \mathbf{h} \\ \mathbf{c} \end{Bmatrix}.$$

and

$$\mathbf{K}_f = \hat{\mathbf{f}}'(\mathbf{q}, \lambda) = \mathbf{K} + \mathbf{f}'_0,$$

$$\mathbf{Z} = (\mathbf{f}'\phi)',$$

$$\mathbf{N} = \partial\mathbf{h}/\partial\lambda,$$

$$\mathbf{C}_q = \partial\mathbf{c}/\partial\mathbf{q},$$

$$\mathbf{K}_h = \partial\mathbf{h}/\partial\phi = \mathbf{K} + \partial_0/\partial\phi,$$

$$\mathbf{P} = \partial\hat{\mathbf{f}}/\partial\lambda,$$

$$\mathbf{C}_\lambda = \partial\mathbf{c}/\partial\lambda,$$

$$\mathbf{C}_\phi = \partial\mathbf{c}/\partial\phi.$$

Block elimination

The solution vector is partitioned as

$$\delta \mathbf{q} = \mathbf{q}_f + \mathbf{Q}_p \delta \boldsymbol{\lambda},$$

$$\delta \boldsymbol{\phi} = \boldsymbol{\phi}_h + \boldsymbol{\Phi}_n \delta \boldsymbol{\lambda}.$$

Vectors $\mathbf{q}_f, \boldsymbol{\phi}_h$ and the $n \times p$ matrices $\mathbf{Q}_p, \boldsymbol{\Phi}_n$ solved from

$$\mathbf{K}_f \mathbf{q}_f = -\hat{\mathbf{f}},$$

$$\mathbf{K}_f \mathbf{Q}_p = -\mathbf{P},$$

$$\mathbf{K}_h \boldsymbol{\phi}_h = -\mathbf{h} - \mathbf{Z} \mathbf{q}_f,$$

$$\mathbf{K}_h \boldsymbol{\Phi}_n = -\mathbf{N} - \mathbf{Z} \mathbf{Q}_p,$$

and for the control parameters

$$\delta \boldsymbol{\lambda} = -(\mathbf{C}_\lambda + \mathbf{C}_q \mathbf{Q}_p + \mathbf{C}_\phi \boldsymbol{\Phi}_n)^{-1}(\mathbf{c} + \mathbf{C}_q \mathbf{q}_f + \mathbf{C}_\phi \boldsymbol{\phi}_h).$$

Suitable strategy if direct linear solver is used.

Iterative solution of the Newton step

Use preconditioned Bi-CGSTAB method (or some other applicable accelerator) for the full non-symmetric equation systems

$$\begin{bmatrix} \mathbf{K}_f & \mathbf{0} & \mathbf{P} \\ \mathbf{Z} & \mathbf{K}_h & \mathbf{N} \\ \mathbf{C}_q & \mathbf{C}_\phi & \mathbf{C}_\lambda \end{bmatrix} \begin{Bmatrix} \delta \mathbf{q} \\ \delta \phi \\ \delta \lambda \end{Bmatrix} = \begin{Bmatrix} \hat{\mathbf{f}} \\ \mathbf{h} \\ \mathbf{c} \end{Bmatrix}.$$

I prefer *monolithic* solution schemes!

RK, M. Tûma, J. Mäkinen, A. Fedoroff, H. Marjamäki, Implementation of a direct procedure for critical point computations using preconditioned iterative solvers, *Computers and Structures*, **108-109**, 2012, 110-117

The crucial thing is the **preconditioner**

$$A = \begin{bmatrix} K_f & 0 & P \\ Z & K_h & N \\ C_q & C_\phi & C_\lambda \end{bmatrix}, \quad M = \begin{bmatrix} M_f & 0 & 0 \\ Z & M_h & 0 \\ C_q & C_\phi & D \end{bmatrix}.$$

$$M^{-1} = \begin{bmatrix} M_f^{-1} & 0 & 0 \\ -M_h^{-1} Z M_f^{-1} & M_h^{-1} & 0 \\ -D^{-1}(C_q M_f^{-1} - C_\phi M_h^{-1} Z M_f^{-1}) & -D^{-1} C_\phi M_h^{-1} & D^{-1} \end{bmatrix}.$$

Preconditioning operation $y = M^{-1}s$

$$\begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{Bmatrix} M_f^{-1} s_1 \\ M_h^{-1} (s_2 - Z y_1) \\ D^{-1} (s_3 - C_\phi y_2 - C_q y_1) \end{Bmatrix}.$$

Error analysis

Accuracy: $\mu_1(\mathbf{A}) = \|\mathbf{A} - \mathbf{M}\|_F$

Stability: $\mu_2(\mathbf{A}) = \|\mathbf{I} - \mathbf{M}^{-1}\mathbf{A}\|_F$

If $\mathbf{K}_f = \mathbf{K}_h = \mathbf{K}$, thus $\mathbf{M}_f = \mathbf{M}_h = \mathbf{M}_1$, results in

$$\mu_1(\mathbf{A}) = \sqrt{2\mu_1(\mathbf{K})^2 + \|\mathbf{P}\|_F^2 + \|\mathbf{N}\|_F^2 + \|\mathbf{C}_\lambda - \mathbf{D}^{-1}\|_F^2},$$

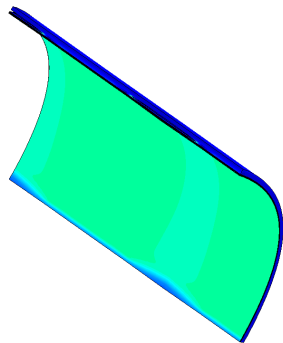
where $\mu_1(\mathbf{K}) = \|\mathbf{K} - \mathbf{M}_1\|$.

$$\mu_2(\mathbf{A}) \leq \eta_1 \mu_2(\mathbf{K}) + \eta_2 \|\mathbf{R}_{13}\|_F + \eta_3 \|\mathbf{R}_{23}\|_F,$$

where

$$\mathbf{R}_{13} = \mathbf{M}_1^{-1}\mathbf{P}, \quad \mathbf{R}_{23} = \mathbf{M}_1^{-1}\mathbf{N} - \mathbf{M}_1^{-1}\mathbf{Z}\mathbf{M}_1^{-1}\mathbf{P}.$$

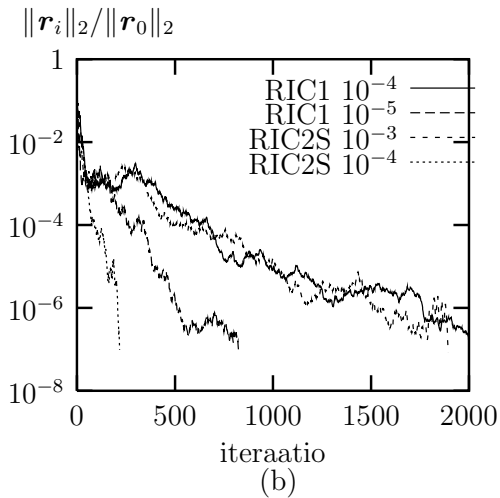
Some examples - Shell type structure analysed as 3D-solid



Smooth Contour Fill (Mean) of Stress tensor, Si-Stress tensor.
Deformation (x763.114): Displacements of Load step , step 1.



(a)



iteration

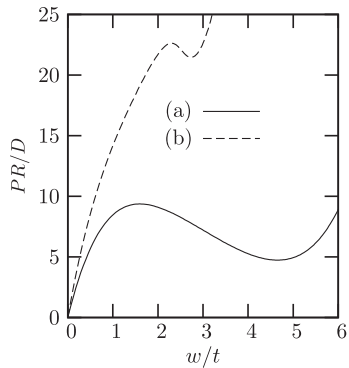
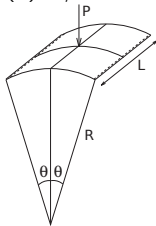
(b)

pohjustin	ψ	ψ_2	prec. dens.	it	p-time	i-time	p+i
RIC1	10^{-4}		3,3	2005	25,9	2360,4	2386,3
RIC1	10^{-5}		8,1	824	95,7	1851,1	1946,8
RIC1	10^{-6}		15,6	297	305,1	660,2	965,3
RIC2S	10^{-3}	10^{-6}	1,1	1864	59,4	779,6	839,0
RIC2S	$2 \cdot 10^{-4}$	10^{-6}	2,7	435	167,5	308,2	475,7
RIC2S	10^{-4}	10^{-6}	3,9	229	273,1	217,5	490,6

Stability analysis of a shallow shell

One layer with 27-node triquadratic 3D-solid elements.

- (a) $R/t = 100, \theta = 0.279$ rad
(b) $R/t = 400, \theta = 0.2$ rad.



Cylindrical shell, 64×64 -mesh, solution times in seconds. BE denotes the block elimination strategy. The preconditioned iterations two values are given: the first one is the preconditioner setup time and the second one is the acceleration iteration time.

method	R/t	preconditioner		av. it.	sol. time
		type	ψ		
BE-SKY	100	-	-	-	10910
BE-SKYB		-	-	-	1670
Bi-CGSTAB		RIC2S _i	10^{-3}	229	360+3861 = 4221
		RIC2S ₀	10^{-3}	166	50+2558 = 2608
		RIC2S ₀	10^{-4}	35	875+1014 = 1889
	SKYB ₀	-	28	179+2754 = 2933	
BE-SKYB	400	-	-	-	1840
Bi-CGSTAB		RIC2S _i	10^{-3}	349	832+7389 = 8221
		RIC2S ₀	10^{-4}	62	991+2219 = 3210
		SKYB ₀	-	42	198+5571 = 5769

HP ProLiant DL785 G5 server with quad-core AMD Opteron 8360 SE (Barcelona) 2.5 GHz processor, 512 GB memory, at the CSC-IT Center for Science at Espoo, Finland.

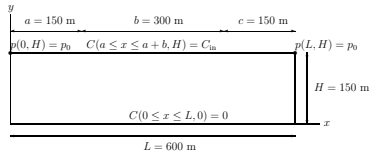
Coupled problems - salt migration known as Elder's problem

Unknowns are pressure p and salt concentration C :

$$\eta \left(\kappa_f \frac{\partial p}{\partial t} + \zeta_c \frac{\partial C}{\partial t} \right) + \eta (\kappa_f \text{grad } p + \zeta_c \text{grad } C) \cdot \mathbf{J}_f + \text{div } \mathbf{J}_f = 0,$$
$$\eta \frac{\partial C}{\partial t} + \text{grad } C \cdot \mathbf{J}_f + (\kappa_f \text{grad } p + \zeta_c \text{grad } C) \cdot \mathbf{J}_c + \text{div } \mathbf{J}_c = 0,$$

with fluxes

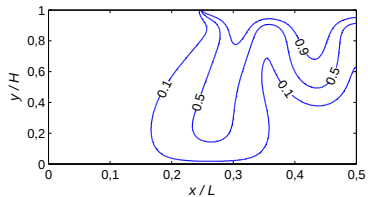
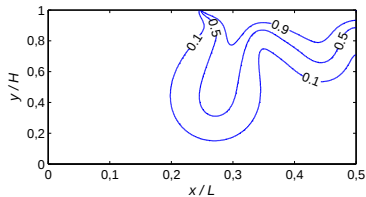
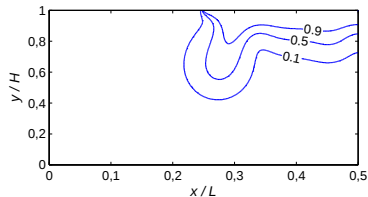
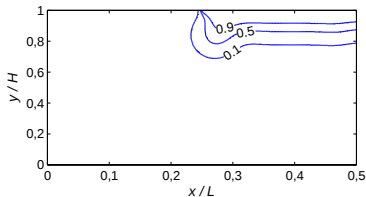
$$\mathbf{J}_f = -\frac{k}{\mu} [\text{grad } p - ((1 - C)\bar{\rho}_w + C\bar{\rho}_c) \mathbf{g}], \quad \mathbf{J}_c = -\eta D [a_1 \text{grad } C - a_0 C(1 - C)(\bar{\rho}_c - \bar{\rho}_w) \mathbf{g}],$$



J. Hartikainen, RK, T. Wallroth. Permafrost simulations at Forsmark using a numerical 2D thermo-hydro-chemical model. Technical Report SKB TR-09-17, 2010.

Elder problem - evolution of salt concentration

After 1,2,3 and 4 years. 88-timesteps, maximum timestep 0.05 year.



Elder's problem -computational statistics

343643 unknowns, 88 time-steps, Newton-Raphson iteration for the non-linear system, ILUT-preconditioner with tolerance ψ

ψ	prec. dens.	ave it	max. it	total. it	ave. p-time	ave. i-time	total p+i
$1 \cdot 10^{-2}$	1,2	38	359	49608	0.7	18.6	28727
$5 \cdot 10^{-3}$	1,5	36	259	37209	0.9	22.0	23895
$1 \cdot 10^{-3}$	2,6	20	121	20367	2.0	19.2	21420
$5 \cdot 10^{-4}$	3,3	18	61	15529	2.7	14.9	15706
$1 \cdot 10^{-4}$	5,4	9	32	8617	6.5	12.9	18424
$8 \cdot 10^{-5}$	5,8	8	29	8060	7.4	11.7	18675
$5 \cdot 10^{-5}$	6,3	7	26	7247	9.0	10.1	20034
$1 \cdot 10^{-5}$	7,3	8	24	6427	12.3	12.9	20642
$1 \cdot 10^{-6}$	8,1	11	24	6171	16.7	18.8	20081

Coupled problems - magnetoelasticity

Many ways to formulate the magnetic problem.

- Using magnetic vector potential $\vec{A}$, such that $\vec{B} = \text{curl } \vec{A}$. Mixed type weak form

$$\begin{aligned}(\text{curl } \vec{A}, \vec{H}) + (\vec{A}, \text{grad } p) &= (\vec{A}, \vec{J}) - [\vec{A}, \vec{H}], \\(\text{grad } \hat{p}, \vec{A}) &= 0,\end{aligned}\tag{5}$$

where the inner products are defined as

$$(\vec{B}, \vec{H}) = \int_{\Omega} \vec{B} \cdot \vec{H} \, dV, \quad \text{and} \quad [\vec{A}, \vec{H}] = \int_{\partial\Omega} \vec{A} \cdot \vec{H} \, ds.$$

In 3D curl-conforming interpolation for $\vec{A}$ should be used and standard C_0 -interpolation for p .

- Using the Lagrangian functional

$$\mathcal{L} = \frac{1}{2}(\text{div } \vec{B}, \text{div } \vec{B}) + (\vec{p}, \text{curl } \vec{H} - \vec{J}).$$

Divergence conforming interpolation for $\vec{B}$ and curl-conforming for $\vec{p}$.

How to solve the curl-curl problem in 3D?

Saddle point problem (5) in the matrix form

$$\begin{bmatrix} \mathbf{H} & \mathbf{C} \\ \mathbf{C}^T & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \mathbf{p} \end{Bmatrix} = \begin{Bmatrix} \mathbf{h} \\ \mathbf{0} \end{Bmatrix}$$

The leading block $\mathbf{H}$ is singular!

Monolithic magnetoelasticity

In strong form

$$\begin{aligned}-\operatorname{div} \boldsymbol{\sigma}(\vec{u}, \vec{B}) &= \rho \vec{b}, \\ \operatorname{curl} \vec{H}(\vec{B}, \vec{u}) &= \vec{J}, \\ \operatorname{div} \vec{B} &= 0,\end{aligned}$$

and using the vector potential approach for the magnetic part gives the following linearized discrete equation system

$$\begin{bmatrix} \mathbf{K} & \mathbf{L} & \mathbf{0} \\ \mathbf{F} & \mathbf{H} & \mathbf{C} \\ \mathbf{0} & \mathbf{C}^T & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \delta \mathbf{u} \\ \delta \mathbf{a} \\ \delta \mathbf{p} \end{Bmatrix} = \mathbf{g}$$

What kind of preconditioner for such a system?

Open source JuliaFEM

See www.juliafem.org! Julia programming language try to combine programming flexibility and high-performance computing.

Eigenvalue analysis for natural frequencies (10 lowest pairs), 12.6 millions unknowns. Solution time 3 h 4 min with 24 x Intel(R) Xeon(R) CPU E5-2690 v3 @ 2.60 GHz with 512 GB total memory.



Tero Frondelius, Jukka Aho. JuliaFEM – open source solver for both industrial and academia use. *Rakenteiden Mekaniikka (Journal of Structural Mechanics)*. **50** (3) 2017, 229-233.

Thank you!



Bohumil Kubišta, Taming snakes

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and my teachers

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