High Performance Computing Techniques for the FEM Simulation in Solid Mechanics

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Overview

Overview

1. Motivation
2. Concepts of FEAST
   - Meshing Concept
   - Adaptivity Concept
   - Solution Concept
3. Treating Elasticity Problems with FEAST
4. Numerical Results

Motivation

Efficiency of iterative solution methods is influenced by

- physical parameters
- algorithmic parameters
- mesh quality
- number of parallel processors

Distinguish between three aspects:

- processor efficiency
- numerical efficiency
- parallel efficiency

Motivation

Develop a solution method for problems in
Computational Solid Mechanics (CSM)
with

high efficiency in all three aspects
and
low dependency on the listed influences

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Realisation with

FEAST

Finite Element Analysis and Solution Tool

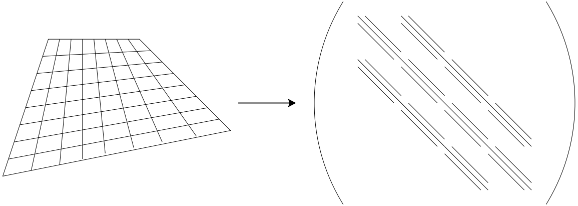
`http://www.feast.uni-dortmund.de`

Overview

FEAST's Meshing Concept

'data moving $\gg$ data processing'

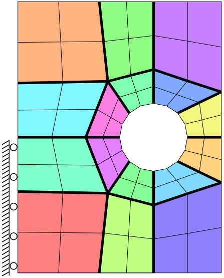
- unstructured meshes $\Rightarrow$ indirect adressing
  $\Rightarrow$ expensive memory access $\Rightarrow$ poor MFLOP/s rates
- FEAST uses generalised tensor product meshes

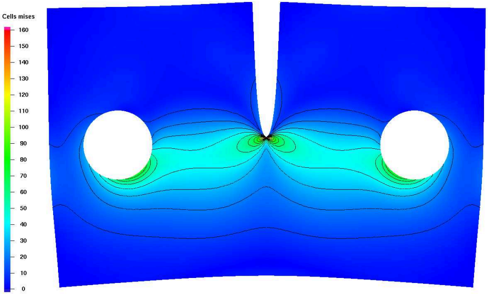


- rowwise numbering
  $\Rightarrow$ exactly 9 matrix bands for bilinear elements
- direct adressing, caching
- optimised Linear Algebra routines
  (SPARSE BANDED BLAS)

FEAST's Meshing Concept

More complex domains by joining several TP meshes ('macros')



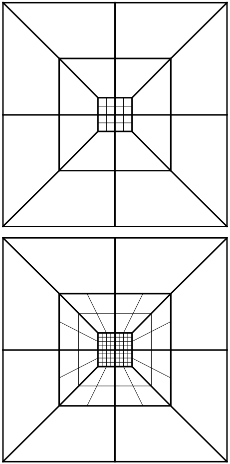


Here:

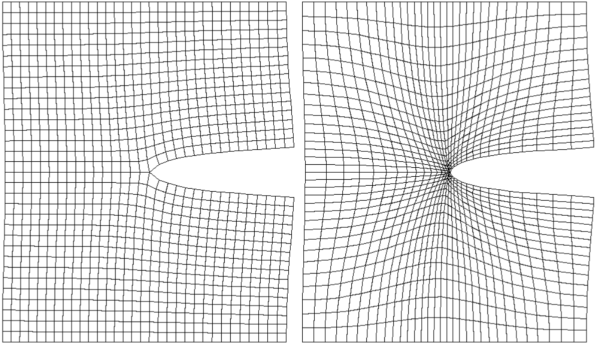
- 64 macros (=64 local matrices), each macro refined 10x
- distributed over 16 processors
- $\Rightarrow 1.34 \cdot 10^8$ DOFs in total

FEAST's Adaptivity Concept

Patch-wise Hanging Nodes:



Mesh Deformation:



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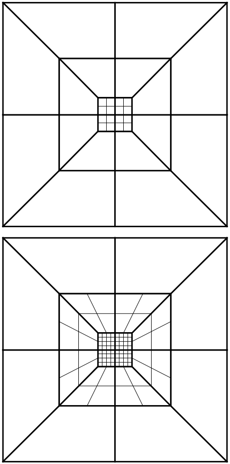

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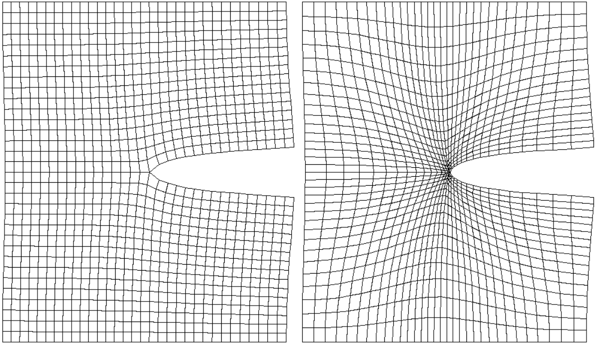


TP property fulfilled!

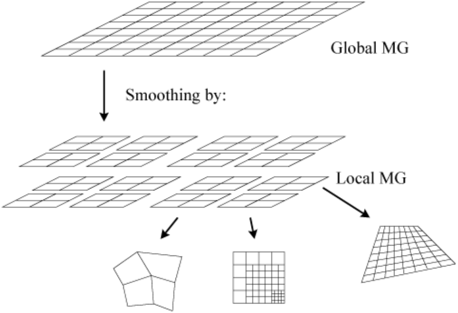
FEAST's Solution Concept

FEAST uses generalised Multigrid/Domain Decomposition methods

ScaRC
Scalable Recursive Clustering

- global MG smoothed by local MG
- locally adapted solution methods
- recursively hide local mesh irregularities
- minimal overlap

$\Rightarrow$ high numerical and parallel efficiency

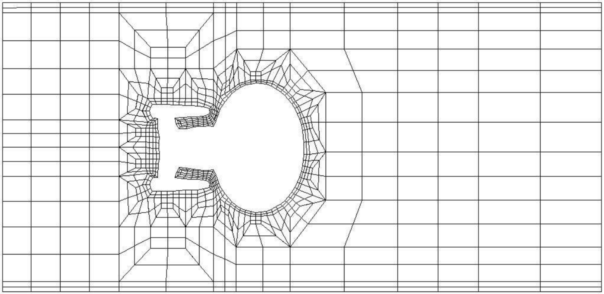


FEAST results (‘Poisson Problem’)

Local MFLOP/s rates:

#DOF	MV (Sparse)	MV (SparseBanded)	
		var	const
65^2	422	1111	1605
257^2	106	380	1214
1025^2	54	362	1140

Sun V40z ‘Opteron’(1800 MHz, peak perf. ≈ 2900 MFLOP/s)



C. Becker, 2006

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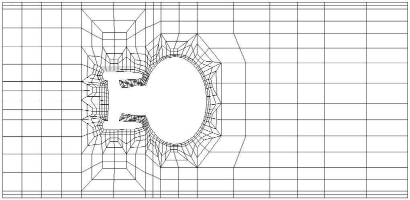
Global (parallel) convergence rates:

#DOF	$AR \approx 10$	$AR \approx 10^6$
211 K	0.17 (**8**)	0.18 (**8**)
844 K	0.17 (**8**)	0.17 (**8**)
3,375 K	0.18 (**9**)	0.19 (**9**)
13,500 K	0.19 (**9**)	0.18 (**9**)

ScaRC-CG solver,
smoothers: 1 glob. ScaRC, 1 loc. MG



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FEAST

'HPC meets Modern Numerics'

$\Rightarrow$ fast and robust solvers for scalar, linear, elliptic equations

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Application to vector-valued, non-linear, time dependent equations in CSM ?

Overview

Example: 2D Linearised Elasticity

- Basic idea: Reduction to solution of scalar problems
- Lamé equation → weak formulation → FE discretisation
- Separate displacement ordering ⇒ block-structured linear system:

$$\begin{pmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{12}^T & \mathbf{K}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}$$

- $\mathbf{K}_{11}$ and $\mathbf{K}_{22}$ correspond to scalar elliptical operators
- Basic iteration: block-preconditioned Richardson method

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \tilde{\mathbf{K}}^{-1}(\mathbf{f} - \mathbf{K}\mathbf{u}^k),$$

e. g. Block-Jacobi $\quad \tilde{\mathbf{K}}^{-1} = \begin{pmatrix} \mathbf{K}_{11}^{-1} & \mathbf{0} \\ 0 & \mathbf{K}_{22}^{-1} \end{pmatrix}$

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Exploit FEAST concepts!

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Exploit FEAST concepts!

- Acceleration: Krylov-space methods, MG

Nearly Incompressible Material

$$\nu \to 0.5 \quad \Rightarrow \quad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \to \infty$$

Difficulties:

- Increasing degree of anisotropy in the operator

$$-(2\mu + \lambda)\,\partial_{xx} - \mu\,\partial_{yy}$$

- Deterioration of the FE approximation ('volume locking')

Remedy:

- Introduce new variable ('pressure'): $p = -\lambda \operatorname{div} u$

$$\begin{aligned} -2\mu \operatorname{div} \varepsilon(u) + \nabla p &= f, \qquad x \in \Omega \\ -\operatorname{div} u - \frac{1}{\lambda} p &= 0, \qquad x \in \Omega \end{aligned}$$

- $Q_1/Q_1 \Rightarrow$ stabilisation necessary

Solving the Saddle Point Problem

$$\begin{pmatrix} \mathbf{K} & \mathbf{B} \\ \mathbf{B}^\mathsf{T} & \mathbf{C} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}$$

- compressibility and stabilisation terms $\longrightarrow \mathbf{C}$
- Schur complement $\mathbf{S} := \mathbf{B}^\mathsf{T}\mathbf{K}^{-1}\mathbf{B} - \mathbf{C}$

Solving the Saddle Point Problem

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- compressibility and stabilisation terms $\rightarrow$ $\mathbf{C}$
- Schur complement $\mathbf{S} := \mathbf{B}^T\mathbf{K}^{-1}\mathbf{B} - \mathbf{C}$

First solving strategy: Block-Preconditioning approach

- Krylov-space method with block-preconditioner

$$\begin{pmatrix} \tilde{\mathbf{K}} & 0 \\ \mathbf{B}^T & -\tilde{\mathbf{S}} \end{pmatrix}$$

- preconditioners $\tilde{\mathbf{K}}$ and $\tilde{\mathbf{S}}$

Solving the Saddle Point Problem

$$\begin{pmatrix} \mathbf{K} & \mathbf{B} \\ \mathbf{B}^\mathsf{T} & \mathbf{C} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}$$

- compressibility and stabilisation terms $\rightarrow \mathbf{C}$
- Schur complement $\mathbf{S} := \mathbf{B}^\mathsf{T}\mathbf{K}^{-1}\mathbf{B} - \mathbf{C}$

Second solving strategy: Pressure Schur Complement approach

- 'Cancelling' displacements $\mathbf{u} = \mathbf{K}^{-1}(\mathbf{f} - \mathbf{B}\mathbf{p})$

$$\mathbf{S}\mathbf{p} = \mathbf{B}^\mathsf{T}\mathbf{K}^{-1}\mathbf{f} - \mathbf{g}$$

- Basic iteration:

$$\mathbf{p}^{k+1} = \mathbf{p}^k + \tilde{\mathbf{S}}^{-1}(\mathbf{B}^\mathsf{T}\mathbf{K}^{-1}\mathbf{f} - \mathbf{g} - \mathbf{S}\mathbf{p}^k)$$

- Acceleration: Krylov-space method

Preconditioning the Schur complement

Essential for both approaches:
efficient Schur complement preconditioner $\tilde{\mathbf{S}}^{-1}$

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Stationary case:

$$\mathbf{S}^{-1} = (\mathbf{B}^T\mathbf{K}^{-1}\mathbf{B} - \mathbf{C})^{-1}$$

- stabilisation terms are of magnitude $\mathcal{O}(h^2)$
  $\Rightarrow$ can be omitted in preconditioner

$$\tilde{\mathbf{S}}^{-1} := \begin{cases} \left(\frac{1}{2\mu}\mathbf{M}_p\right)^{-1} & \text{if } \nu = 0.5 \\ \left(\left(\frac{1}{2\mu} + \frac{1}{\lambda}\right)\mathbf{M}_p\right)^{-1} & \text{if } \nu < 0.5 \end{cases}$$

Preconditioning the Schur complement

Transient case:

$$\begin{pmatrix} \frac{\rho}{\tau^2\beta}\mathbf{M}_u + \mathbf{K} & \mathbf{B} \\ \mathbf{B}^\mathsf{T} & \mathbf{C} \end{pmatrix}$$

$$\Rightarrow \mathbf{S}^{-1} = \left(\mathbf{B}^\mathsf{T}\left(\frac{\rho}{\tau^2\beta}\mathbf{M}_u + \mathbf{K}\right)^{-1}\mathbf{B} - \mathbf{C}\right)^{-1}$$

- Goal: efficiency for all relevant time step sizes τ

Preconditioning the Schur complement

Transient case:

$$\begin{pmatrix} \frac{\rho}{\tau^2\beta}\mathbf{M}_u + \mathbf{K} & \mathbf{B} \\ \mathbf{B}^\mathsf{T} & \mathbf{C} \end{pmatrix}$$

$$\Rightarrow \mathbf{S}^{-1} = \left(\mathbf{B}^\mathsf{T}\left(\tfrac{\rho}{\tau^2\beta}\mathbf{M}_u + \mathbf{K}\right)^{-1}\mathbf{B} - \mathbf{C}\right)^{-1}$$

- Goal: efficiency for all relevant time step sizes τ
- Idea: distinctly precondition

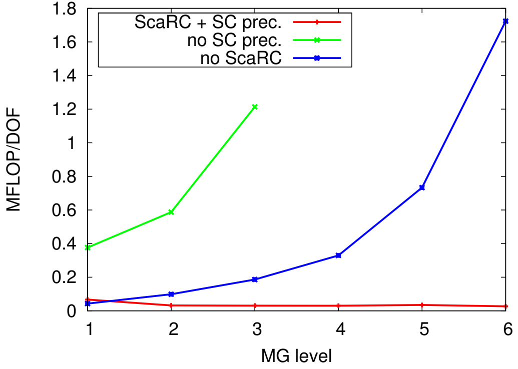
$(\mathbf{B}^\mathsf{T}\mathbf{K}^{-1}\mathbf{B})^{-1}$	with	$\mathbf{M}_p^{-1}$
$(\mathbf{B}^\mathsf{T}\mathbf{M}_u^{-1}\mathbf{B})^{-1}$	with	$\mathbf{P}_p^{-1}$

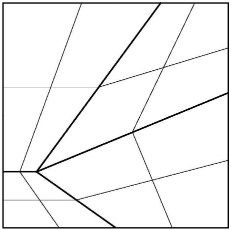
$$\boxed{\tilde{\mathbf{S}}^{-1} := \left(\tfrac{\tau^2\beta}{\rho}\mathbf{P}_p\right)^{-1} + \left(\tfrac{1}{2\mu}\mathbf{M}_p\right)^{-1}}$$

Overview

Results: Preconditioning

Influence of ScaRC and Schur complement preconditioning

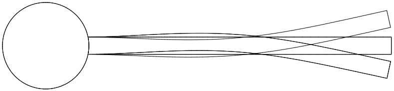




($\nu = 0.5$, block-preconditioned BiCGstab, $\varepsilon_{\text{rel}} = 1.0\text{e-}8$)

Results: Long Beam under Gravity

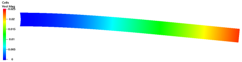
CSM part of Fluid-Solid-Interaction-Benchmark: Beam attached to cylinder in channel (DFG FOR 493)



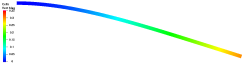
- Comparing three different lengths:

0.08 × 0.02 m

0.32 × 0.02 m

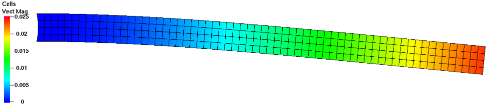


1.28 × 0.02 m

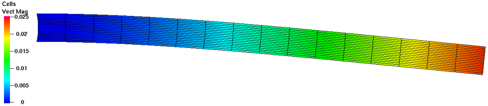


- Comparing two meshings:

isotropic elements:



anisotropic elements:



Results: Long Beam under Gravity

isotropic elements		0.08 x 0.02 m 4 macros		0.32 x 0.02 m 16 macros		1.28 x 0.02 m 64 macros	
Solver	#elem	it	sec	it	sec	it	sec
BiCG BGS	65 K	13	3.6	28	9.1	132	68.6
	262 K	14	14.9	28	32.5	113	167.3
	1049 K	14	62.3	31	142.7	114	608.8

anisotropic elements		0.08 x 0.02 m 1 macro		0.32 x 0.02 m 1 macro		1.28 x 0.02 m 1 macro	
Solver	#elem	it	sec	it	sec	it	sec
BiCG BGS	65 K	14	3.7	33	8.5	149	38.7
	262 K	16	18.9	35	38.4	154	169.1
	1049 K	14	71.9	34	156.3	210	1078.9

- Outer Krylov-subspace scheme with Block-GS preconditioning not sufficient (strong dependence on global anisotropy)

Results: Long Beam under Gravity

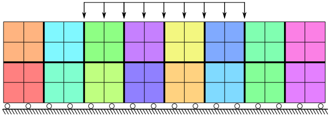
isotropic elements		0.08 × 0.02 m 4 macros		0.32 × 0.02 m 16 macros		1.28 × 0.02 m 64 macros	
Solver	#elem	it	sec	it	sec	it	sec
BiCG BGS	65 K	13	3.6	28	9.1	132	68.6
	262 K	14	14.9	28	32.5	113	167.3
	1049 K	14	62.3	31	142.7	114	608.8
BiCG MG BGS	65 K	4	4.7	5	7.3	6	19.2
	262 K	4	18.5	5	24.2	6	51.8
	1049 K	4	73.7	5	88.9	5	126.5

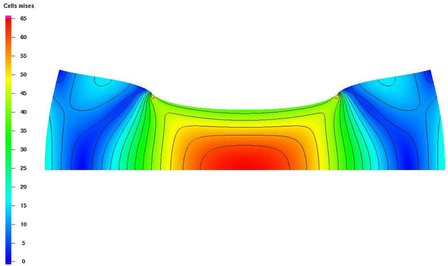
anisotropic elements		0.08 × 0.02 m 1 macro		0.32 × 0.02 m 1 macro		1.28 × 0.02 m 1 macro	
Solver	#elem	it	sec	it	sec	it	sec
BiCG BGS	65 K	14	3.7	33	8.5	149	38.7
	262 K	16	18.9	35	38.4	154	169.1
	1049 K	14	71.9	34	156.3	210	1078.9
BiCG MG BGS	65 K	4	4.2	5	5.2	9	9.4
	262 K	5	19.5	5	21.8	8	34.8
	1049 K	5	83.4	6	102.9	7	129.1

- Outer Krylov-subspace scheme with Block-GS preconditioning not sufficient (strong dependence on global anisotropy)
- Remedy: Use multigrid (applied to the whole system!) as preconditioner

Results: Parallel efficiency

- Compute cluster: 128 nodes, each one equipped with
  2 Intel XEON CPUs (3.4 GHz) and
  1 NVIDIA Quadro FX1400 GPU (350 MHz)
- Linear Elasticity, compressible material, outer BiCGstab solver, $\varepsilon_{\text{rel}} = 10^{-6}$

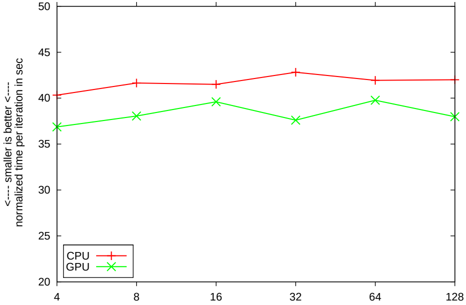




with D. Goeddeke, 2007

Results: Parallel efficiency

	CPU			GPU		
#DOFs	#CPUs	#iters	time	#GPUs	#iters	time
3.36e+7	8	5.5	221.8	4	5.5	202.8
6.71e+7	16	6.5	270.7	8	6.5	247.3
1.34e+8	32	6	249.0	16	6	237.6
2.68e+8	64	6	250.9	32	6	225.6
5.37e+8	128	7	293.6	64	7	278.4
1.07e+9	256	6.5	273.0	128	6.5	246.9



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Outlook

Current state (CSM):

- Finite Deformation (St. VK, Neo-Hooke)
- Compressible + incompressible
- Damped Newton solver, Jacobian via Finite Differences
- Transient computations

Outlook (FSI):

$$\frac{\partial \mathbf{F}(\mathbf{u},\mathbf{v},p)}{\partial(\mathbf{u},\mathbf{v},p)} = \begin{pmatrix} \mathbf{K}_{\mathbf{uu}} & \mathbf{K}_{\mathbf{uv}} & 0 \\ \mathbf{K}_{\mathbf{vu}} & \mathbf{K}_{\mathbf{vv}} & \mathbf{B}_{\mathbf{u}} + \mathbf{B}_{\mathbf{v}} \\ \mathbf{B}_{\mathbf{u}}^T & \mathbf{B}_{\mathbf{v}}^T & \mathbf{C} \end{pmatrix}$$

- Step 1: Applying fully-coupled Vanka-schemes (modified for Q1/Q1)
- Step 2: SC approach + reduction to scalar ScaRC solvers
- Step 3: Efficient Schur complement preconditioner ?!?

Thank you
for your attention!