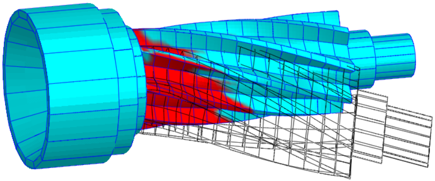
Universität Karlsruhe (TH)
Forschungsuniversität · gegründet 1825

Institut für Angewandte und Numerische Mathematik

The 1000 Processor Challenge

Parallel Multigrid Methods for P.D.E Applications

Christian Wieners



Outline

We demonstrate the performance of state-of-the-art parallel multigrid solution techniques for various application in p.d.e.

The Laplace Problem

Martin Sauter, Wolfgang Müller

The Maxwell Eigenvalue Problem

Alexander Buloyatov

Infinitesimal Plasticity

Stefan Sauter, Katja Jöchen

Cosserat Plasticity

Wolfgang Müller

All computations use the IC1 cluster (SCC Karlsruhe) and the parallel finite element code M++ with standard MPI.

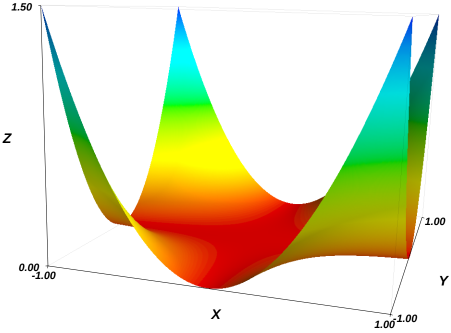
http://www.mathematik.uni-karlsruhe.de/ianm/M++

The “Fruitfly Problem” for Multigrid Methods

We consider the Laplace problem (describing an electro-static field or a temperature distribution) on a square with prescribed boundary values:

$$-\Delta u = f \quad \text{in } \Omega = (-1,1)^2, \qquad u = g \quad \text{on } \partial\Omega .$$

In our test, we approximate $u(x,y) = x^2 y^2$ with bilinear finite elements.



Refinement levels and degrees of freedom (unknowns):

Level	Unknowns
0	4
1	9
⋮	⋮
12	17 M
13	67 M
14	268 M

For every level of refinement, the complexity increases by a factor of 4.

The “Fruitfly Problem” for Multigrid Methods

Parallel performance on refinement level 14 ($\approx$ 268 million d.o.f.)

Procs	RAM (GB)	Solver time	#Iteration	Speed up	Efficiency
128	$\leq$ 2048	32.57 sec.	5		
256	$\leq$ 2048	20.93 sec.	5	1.56	0.78
384	$\leq$ 2048	18.54 sec.	5	1.73	0.58
512	$\leq$ 2048	14.87 sec.	5	2.19	0.55

(speed up and efficiency relative to the results on 128 processors)

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(speed up and efficiency relative to the results on 128 processors)

Solution time for fixed load

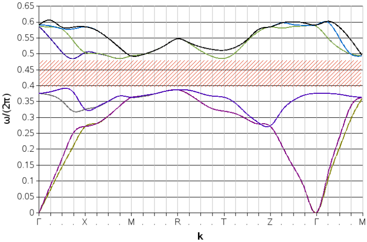
Level	Procs	Solver time	Scale factor
11	8	9.94 sec.	
12	32	10.71 sec.	1.08
13	128	12.01 sec.	1.12
14	512	14.87 sec.	1.24
13	1024	12.50 sec.	

Photonic Crystals: The Maxwell Eigenvalue Problem

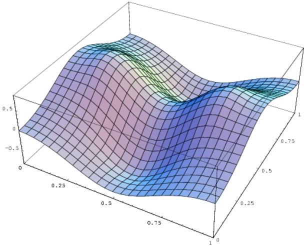
We comput the Block-Floquet mode for $\mathbf{k} = (3, 1, -1)$ in unit cube $\Omega = (0, 1)^3$ with periodic boundary conditions (with $\nabla_{\mathbf{k}} = \nabla + i\mathbf{k}$):

$$\nabla_{\mathbf{k}} \times \varepsilon^{-1} \nabla_{\mathbf{k}} \times \mathbf{H} = \omega^2 \mathbf{H} \qquad \text{in } \Omega,$$

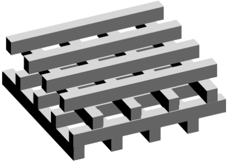
$$\nabla_{\mathbf{k}} \cdot \mathbf{H} = \mathbf{0} \qquad \text{in } \Omega,$$



Band structure of a photonic crystal



Eigenfunction – (Bloch-Floquet mode)



Configuration from Dobson/Pasciak, Comp. Meth. Appl. Math. 1 (2001) 138–153

Photonic Crystals: The Maxwell Eigenvalue Problem

Calculation of the first 7 eigenfunctions ($\approx$ 1 million d.o.f.)

N processors	Total time	Speed up factor
32	5:11 min.	
64	2:53 min.	1.79
128	1:33 min.	1.85
256	1:05 min.	1.42
512	0:47 min.	1.39

Photonic Crystals: The Maxwell Eigenvalue Problem

Calculation of the first 7 eigenfunctions ($\approx$ 1 million d.o.f.)

N processors	Total time	Speed up factor
32	5:11 min.	
64	2:53 min.	1.79
128	1:33 min.	1.85
256	1:05 min.	1.42
512	0:47 min.	1.39

Calculation of the first 7 eigenfunctions on 512 processors

Refinement level	d.o.f.	Total time	Scale up factor
4	13 872	00:18 min.	
5	104 544	00:24 min.	1.32
6	811 200	00:47 min.	1.91
7	6 390 144	03:08 min.	3.98
8	50 725 632	21:31 min.	6.85

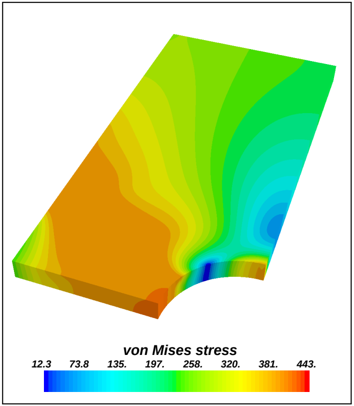
(Every refinement level increases the problem size by a factor of 8.)

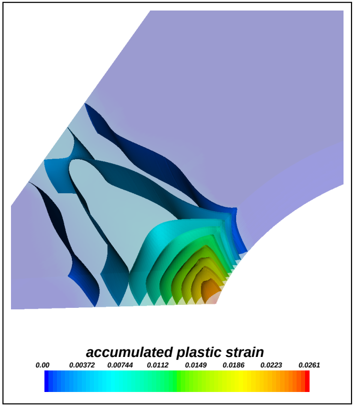
ABAQUS-UMAT-Interface: Classical Plasticity

Von Mises plasticity with isotropic hardening (with displacement vector $\boldsymbol{u}$, stress tensor $\boldsymbol{\sigma}$, plastic strain tensor $\boldsymbol{\varepsilon}_p$ and elasticity tensor $\mathbb{C}$):

$$-\operatorname{div}\boldsymbol{\sigma} = \mathbf{0} \quad \text{in } \Omega, \qquad \boldsymbol{u} = \boldsymbol{g} \quad \text{on } \partial\Omega,$$

$$\boldsymbol{\sigma} = \mathbb{C} : \big(\boldsymbol{\varepsilon}(\boldsymbol{u}) - \boldsymbol{\varepsilon}_p\big), \qquad \dot{\boldsymbol{\varepsilon}} = \lambda \partial f(\boldsymbol{\sigma}), \qquad \dot{\alpha} = \lambda, \qquad f(\boldsymbol{\sigma}, \alpha) = 0.$$





In our test, $\Omega \subset \mathbb{R}^3$ describes an eighth part of a thin plate with a circular hole.

ABAQUS-UMAT-Interface: Classical Plasticity

Computational Configuration

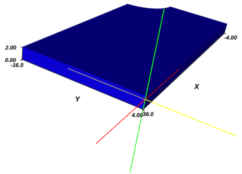
Time steps:	7 linear elastic steps + 4 nonlinear elasto-plastic steps
Linear solver:	Preconditioned GMRES (reduction factor 1e-6)
Preconditioner:	Multigrid W-cycle with Point-Block-Gauss-Seidel smoother and sequential direct solver on level 0

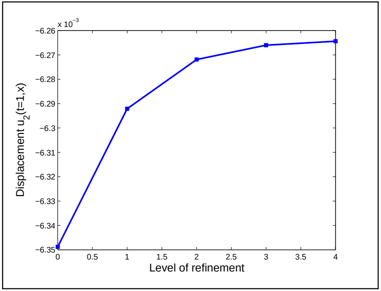
Level	Unknowns	Internal var.	Procs	RAM (GB)	Total time
0	10 845	148 736			
1	74 871	1 189 888	1	≤ 1	5 min.
2	553 707	9 519 104	2	≤ 8	21 min.
3	4 253 139	76 152 832	16	≤ 64	35 min.
4	33 328 035	609 222 656	128	≤ 512	51 min.
5	Not yet available due to memory limitations				

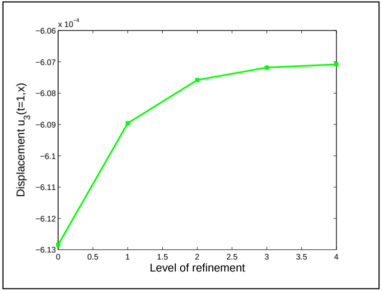
(Every refinement level increases the problem size by a factor of 8.)

ABAQUS-UMAT-Interface: Classical Plasticity

Convergence of the displacement vector $\boldsymbol{u}(t,\boldsymbol{x}) = \big(u_1(t,\boldsymbol{x}), u_2(t,\boldsymbol{x}), u_3(t,\boldsymbol{x})\big)$ at Point $\boldsymbol{x} = (36, 4, 1.5)$ at time $t = 1$ depending on the levels of refinement (note that $u_1(t,\boldsymbol{x})$ is given by the Dirichlet condition).

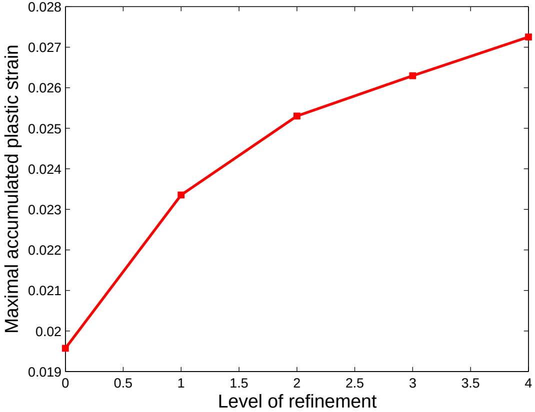






ABAQUS-UMAT-Interface: Classical Plasticity

Maximal accumulated plastic strain depending on the level of refinement.

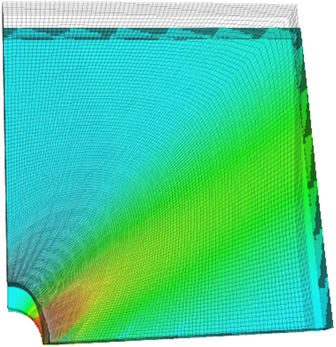


Modern Micro-Plasticity with appended Cosserat Rotations

We consider an extension of the classical plasticity problem:
For given $\boldsymbol{\varepsilon}_p^{n-1}$ and load $\ell_n[\cdot]$ find $(\boldsymbol{u}, \overline{A}) \in \boldsymbol{V}_h(d) \times W_h(d)$ s.t.

$$\begin{aligned} \Big\langle P_{\mathbf{K}}\big(\mathbb{C} : (\boldsymbol{\varepsilon}(\boldsymbol{u}) - \boldsymbol{\varepsilon}_p^{n-1})\big) + 2\mu_c\big(\operatorname{skew} D\boldsymbol{u} - \overline{A}\big), \boldsymbol{\varepsilon}(\delta\boldsymbol{v})\Big\rangle &= \ell_n[\delta\boldsymbol{v}] \\ \mu L_c^2 \langle D\overline{A}, D\delta\overline{A}\rangle - \mu_c\big\langle \operatorname{skew} D\boldsymbol{u} - \overline{A}, \delta\overline{A}\big\rangle &= 0 \end{aligned}$$

where $P_{\mathbf{K}}(\cdot)$ is the nonlinear elasto-plasic response function.



Solution Method

semi–smooth Newton iteration as nonlinear solver combined with Multilevel BiCGStab (V-cycle, damped local pointblock Gauß-Seidel smoother, SuperLU on coarse grid) for linear subproblems

Test configuration

$\Omega = \big([0,10]^2 \setminus B_1(0,10)\big) \times [0,1]$

We calculate 100 time steps until half of the body is plastified.

Modern Micro-Plasticity with appended Cosserat Rotations

Scaling for fixed problem size

#Procs	Time	Speed up
32	2:06h	
64	1:06h	1.91
128	0:35h	1.89
256	0:19h	1.84

Modern Micro-Plasticity with appended Cosserat Rotations

Scaling for fixed problem size

#Procs	Time	Speed up
32	2:06h	
		1.91
64	1:06h	
		1.89
128	0:35h	
		1.84
256	0:19h	

Scaling for fixed processor number

Refinement level	#Cells	#DoF	Time	Scale up
2	16.384	126.750	0:04h	
				4.75
3	131.072	898.614	0:19h	
				7.68
4	1.048.576	6.736.998	2:26h	
				8.60
5	8.388.608	52.107.462	20:55h	

Modern Micro-Plasticity with appended Cosserat Rotations

Scaling for fixed problem size

#Procs	Time	Speed up
32	2:06h	
		1.91
64	1:06h	
		1.89
128	0:35h	
		1.84
256	0:19h	

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3	131.072	898.614	0:19h	
				7.68
4	1.048.576	6.736.998	2:26h	
				8.60
5	8.388.608	52.107.462	20:55h	

Scaling for fixed processor load

Refinement level	#Procs	#Cells	#DoF	Time	Scale up
2	4	16.384	126.750	1:05h	
					1.94
3	32	131.072	898.614	2:06h	
					1.16
4	256	1.048.576	6.736.998	2:26h	

Hardware Comparison IC1 (SCC) – otto (IANM)

	otto.ianm3.uni-karlsruhe.de	ic1.rz.uni-karlsruhe.de
processor	AMD Opteron 2352	Intel(R) Xeon(R) X5355
cpu	2110.840 MHz	2666.663 MHz
cache size	512 KB	4096 KB
address sizes	48 bits physical, 48 bits virtual	36 bits physical, 48 bits virtual
RAM	32 GB per dual board	16 GB per dual-board
InfiniBand	Mellanox EP-DIBS-2400-24	Flextronics F-XR430095
ConnectX	PCI-E HCA MHEH28-XTC	PCIe2.0x8 2,5GT/s

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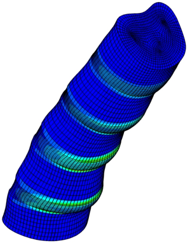
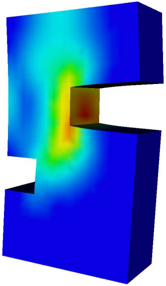
Full plasiticity simulation

level	d.o.f.	procs	otto	ic1
0	3468	1	2:02.89 min.	1:18.49 min.
1	19602	64	3:56.58 min.	3:03.00 min.
2	126750	64	9:03.45 min.	9:29.11 min.
3	898614	64	46:51.00 min.	64:12.00 min.

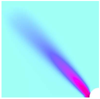
Parallel simulations in Nonlinear Solid Mechanics



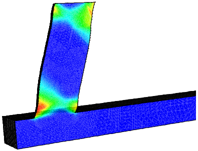
poro-elasticity
in biomechanics



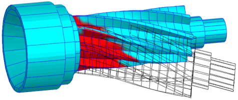
nonlocal plasticity



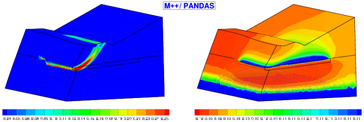
Cosserat plasticity



finite plasticity



Prandtl-Reuss plasticity



poro-plasticity in soil mechanics

Challenge Provide parallel, robust, efficient and reliable linear and nonlinear mesh-independent solution methods for different models.