IGAS collection of benchmarks, solvers and test results [1]

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Contents:

Draft version: Ostrava, July 1997

[1] This work was supported by Grant COPERNICUS 940820 of the European Commission and Grant GA ČR 105/95/1273 of the Grant agency of the Czech Republic

1 Introduction

Applications of mathematical modelling in geomechanics lead frequently to the solution of large or extremely large linear systems. For this purpose we need high performance iterative solvers and the aim of this paper is testing such solvers. Note that we shall not consider solvers based on direct solution methods because they demand too much memory and the computational (arithmetic) work.

By *iterative solver*, we shall understand some numerical iterative method together with its computer implementation. This imply that the *performance* of the solver will depend on many facts, e.g. on

- adopted iterative method
- the solved problem (we restrict our attention to linear elasticity problems for which the convergence of iterations depends on material coefficients which may include anisotropy or jumps, shape of domain, boundary conditions, etc.)
- the discretization used (FE type, mesh size, mesh anisotropy, system dimension etc.)
- coding (programming language, code optimization, etc.)
- computer hardware (processor, amount of memory, number of processors, etc.)
- operating system
- etc.

Hence, evaluation of performance of solvers is a relatively difficult task which will be solved with the aid of *evaluation methodology* based on construction of a set of suitable test problems (*benchmarks*) and on using an *uniform description* for presentation of the test results.

The presented benchmarks are selected real–life problems arising from geomechanics or problems constructed in such way that they involve characteristic features of real–life problems.

The uniform description which will be described in the next Section was developed during the solution of the HIPERGEOS project, see Minutes of the HIPERGEOS Workshops and [1],[2],[3] and [4] .

The results presented in this report will be further completed by results from testing new sequential and parallel variants of the iterative solver based on [7], see [10]. Moreover, the results presented here will be incorporated into more general HIPERGEOS project report. For this reasons, we shall not evaluate the test results and make conclusions or recommendations in this paper.

Note: The described benchmarks can be distributed in the form: INPUT DATA and CODE FOR GENERATING THE LINEAR SYSTEM, see [1], [3] and [8]. This way of distribution is preferred because the direct distribution of linear system represents unacceptable big amount of data (e.g. 680 MB in case of the Rožínka benchmark, see [5]).

2 Arrangement for uniform description of benchmarks, solvers and tests

2.1 Benchmark presentation

1. Naming
2. Short description. Geometrical data (dimensions).
3. Equations used
4. Material data
5. Boundary conditions
6. Loading
7. Relevant user output (displacements, stresses, etc.)
8. Discretization
9. References for more detailed description
10. Personal contact for assistance with benchmark implementation

2.2 Solver presentation

1. Naming
2. Numerical techniques used for the solver
3. Stopping criteria
4. Main data structures
5. Number of FLOPS per iteration (*)
6. Amount of data transfers per iteration (*)
7. Programming language (P)
8. Single, double precision etc.
9. Authors, references
10. Auxiliary information (e.g. condition numbers), remarks

2.3 Test presentation

1. Benchmark problem
2. Exploited solver
3. Computer (type, processor, RAM)(P)
4. Operating system, compiler
5. Elapsed/CPU times iteration (*)(P) (computed as an average)
6. Convergence history (table - graph) (outer) iteration - (inner iterations) - L2 norm of residual - residual/rhs ratio
7. Example of user output
8. Speed up and other characteristics for parallel processing
9. Auxiliary information (condition numbers, etc.)

Note:
(*) Possibly per one outer iteration without inner iterations and separately per one inner iteration.
(P) In case of parallel computing include also:
2.2.7 tools for parallelization (PVM, MPI etc)
2.3.3 communication links (Ethernet, HPS etc)
2.3.5 with various number of processors.

3 Benchmarks

3.1 Square footing problem

Description : Problem deals with the influence of flexible footing represented by localized pressure to the stress development in a soil medium. The computational domain is a parallelepiped 50x50x40 m which represents one quarter of the overall situation, see Figure below.

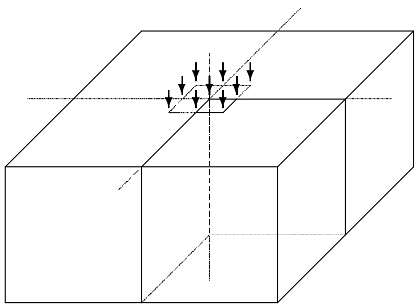

Figure: The square footing problem.

Equations used : equations of elasticity.

Material data : one isotropic material

- soil (E = 14 MPa, $\nu = 0.3$, $\rho = 2.5\,gcm^{-3}$)

Boundary conditions : zero normal displacements and zero tangential stresses on all sides except the top side. Stress on the top side.

Loading : pressure of 2.4 MPa on the square area 5x5 m at the left back corner of the top face (one quarter of footing).

Relevant user output : stresses.

Discretization : rectangular grid 40x40x40 nodes with a grid refinement under the footing. Maximal dimension of hexahedral bricks: 2.5x2.5x1.5 m, minimal dimension: 0.5x0.5x0.5 m.
The discretization is made by the linear tetrahedral finite elements and gives the linear system of 192000 unknowns. The discretization is made by TGRID preprocessor and the linear system is created by FEMSYS code, see [1].

References: [1] R. Blaheta and R. Kohut: *Benchmarks and programs for testing iterative solvers for 3D problems of geomechanics,* Report 9502 (Dept. of Applied Mathematics, Institute of Geonics, Ostrava 1995)

Contact: R. Kohut (kohut@ugn.cas.cz), A. Kolcun (kolcun@ugn.cas.cz)

3.2 Stope stability problem

Description : Problem concerns mining in the coal seam: the computational domain is a cube of 150x150x150 m which contains the characteristic stope mining situation.

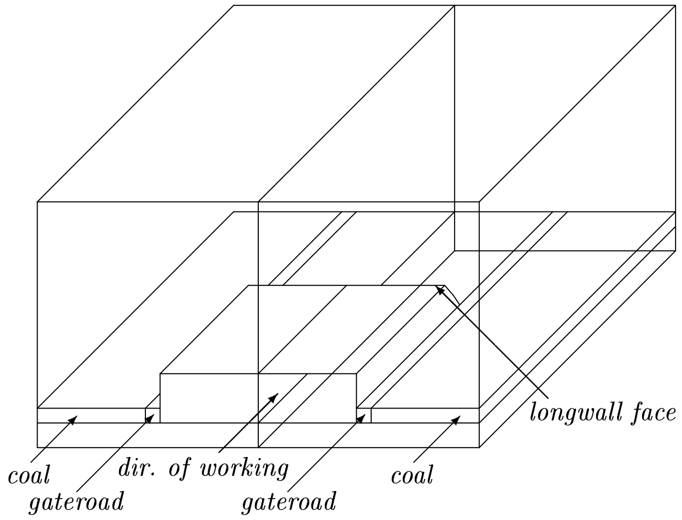

Figure: The stope mining problem.

Equations used : equations of elasticity.

Material data : three isotropic materials:

- rock (E = 8000 MPa, $\nu = 0.2$, $\rho = 2.5\, gcm^{-3}$)
- coal (E = 800 MPa, $\nu = 0.3$, $\rho = 1.3\, gcm^{-3}$)
- goaf (E = 200 MPa, $\nu = 0.4$, $\rho = 2.2\, gcm^{-3}$)

Boundary conditions : zero normal displacements and zero tangential stresses on all sides except the top side. Stress on the top side.

Loading : pressure of 12.5 MPa on the whole top side.

Relevant user output : stresses.

Discretization : rectangular grid of 40x40x40 nodes with the grid refinement in the area of mining. Maximal dimension of hexahedral bricks: 10x15x10 m, minimal dimension: 1x1.5x1.5 m.
The discretization is made by the linear tetrahedral finite elements and gives the linear system of 192000 unknowns. The discretization is made by TGRID preprocessor and the linear system is created by FEMSYS code, see [1].

References: [1] R. Blaheta and R. Kohut: *Benchmarks and programs for testing iterative solvers for 3D problems of geomechanics,* Report 9502 (Dept. of Applied Mathematics, Institute of Geonics, Ostrava 1995)

Contact: R. Kohut (kohut@ugn.cas.cz), A. Kolcun (kolcun@ugn.cas.cz)

3.3 Headgate problems

Description : Problems concern the stability of coal pillars which are periodically distributed in the corridor passing throw a coal seam. Beside the corridor, the situation include a mined out area excavated by the longwall mining technology. Computational domain is a parallelepiped 1800x237x86 m.

We shall consider three variants of the described problem:
A – the whole situation,
B – restricted problem situated in 2/3 of the whole computational domain,
C – restricted problem situated in 1/3 of the whole computational domain.

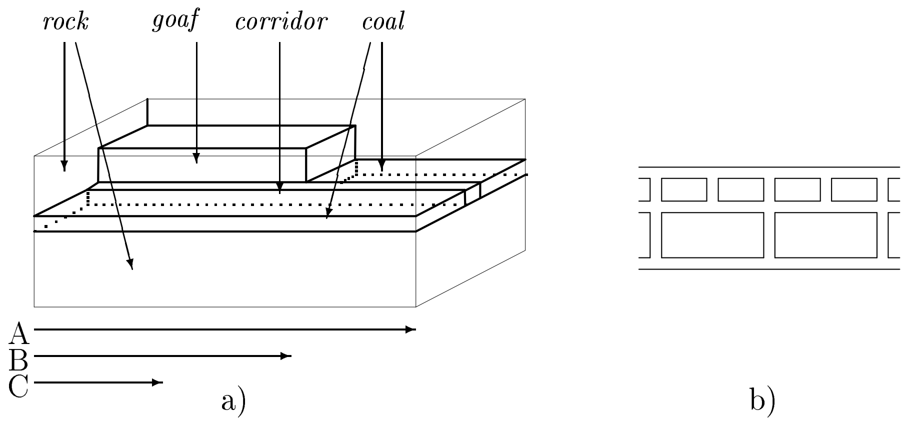

Figure: (a) Headgate problems with extent of the domain for the considered variants A, B and C, (b) top view on the detail of distribution of the coal pillars in the corridor.

Equations used : equations of elasticity.

Material data : three isotropic materials:

- rock (E = 8000 MPa, $\nu = 0.2$, $\rho = 2.5\, gcm^{-3}$)
- coal (E = 800 MPa, $\nu = 0.3$, $\rho = 1.3\, gcm^{-3}$)
- goaf (E = 80 MPa, $\nu = 0.4$, $\rho = 2.2\, gcm^{-3}$)

Boundary conditions : zero normal displacements and zero tangential stresses on all sides except the top side. Stress on the top side.

Loading : pressure of 12.5 MPa on the whole top side.

Relevant user output : stresses.

Discretization : rectangular grids of 302x26x33, 202x26x33, 102x26x33 nodes are used for the variants A, B and C, respectively. The grids are refined in the vicinity of the corridor. Maximal dimension of hexahedral bricks is: 6.1x16x6 m, minimal dimension is: 6.1x5.25x0.6 m.

The discretization is made by the linear tetrahedral finite elements and gives the linear system of 777348, 519948 and 262548 unknowns for the variants A, B and C, respectively. The discretization is made by TGRID preprocessor and the linear system is created by FEMSYS code, see [1].

References: [1] R. Blaheta and R. Kohut: *Benchmarks and programs for testing iterative solvers for 3D problems of geomechanics,* Report 9502 (Dept. of Applied Mathematics, Institute of Geonics, Ostrava 1995)
[2] R. Blaheta: *HIPERGEOS related benchmarks, software and testing,* HIPERGEOS Workshop, Rožnov p. R. 1996

Contact: R. Kohut (kohut@ugn.cas.cz), A. Kolcun (kolcun@ugn.cas.cz)

3.4 Rožínka problem

Description : Problem concerns the mining in uranium ore veins in the deposit Dolní Rožínka. The domain is a parallelepiped 1430x550x600 m. The benchmark represents the solution of the first excavation step with the load induced by the initial stress given according to the performed measurements. See [3] for the details.

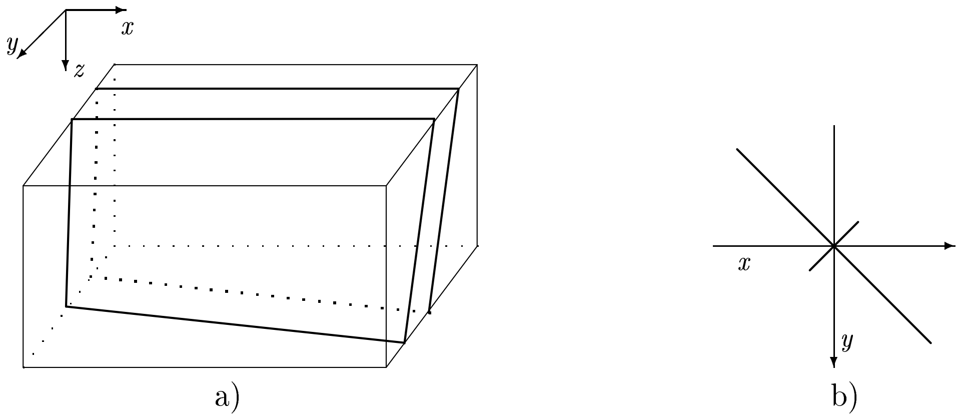

Figure: (a) Computational domain with screwed zone containing three ore veins, (b) principal stresses in the horizontal plane with the size $2\,s_{zz}$ and $0.5\,s_{zz}$ where s_{zz} is the vertical stress given by the weight of rocks.

Equations used : equations of elasticity.

Material data : three isotropic materials:

- rock (E = 20000 MPa, $\nu = 0.25$, $\rho = 2.7\,gcm^{-3}$)
- s-goaf (E = 1250 MPa, $\nu = 0.4$, $\rho = 2.0\,gcm^{-3}$)
- h-goaf (E = 2500 MPa, $\nu = 0.4$, $\rho = 2.0\,gcm^{-3}$)

Boundary conditions : zero normal displacements and zero tangential stresses on all sides except the top side. Zero stress on the top side.

Loading : pressure on the boundary of excavated space computed from given anisotropic initial stress.

Relevant user output : stresses.

Discretization : structured grid (nonorthogonal) with 124x137x76 nodes. Grid refinement in the area of mining. Maximal dimension of hexahedral bricks: 50x86x50 m, minimal dimension: 8x1x5 m.
The discretization is made by the linear tetrahedral finite elements and gives the linear system of 3 873 264 unknowns. The discretization is made by TGRID-2 preprocessor and the linear system is created by FEMSYS code, see [1,2].

References: [1] R. Blaheta and R. Kohut: *Benchmarks and programs for testing iterative solvers for 3D problems of geomechanics,* Report 9502 (Dept. of Applied Mathematics, Institute of Geonics, Ostrava 1995)
[2] A. Kolcun: TGRID - 2 preprocessor for structured non-orthogonal 3D finite element grids, Technical Report (Dept. of Applied Mathematics, Institute of Geonics, Ostrava 1997)
[3] R. Blaheta et al.: *Mathematical Modelling of the Effects of a New Mining Technology at the Uranium Mine Dolní Rožínka,* HIPERGEOS Workshop, Brussels 1997, Report (Dept. of Applied Mathematics, Institute of Geonics, Ostrava July 1997)

Contact: R. Kohut (kohut@ugn.cas.cz), A. Kolcun (kolcun@ugn.cas.cz)

4 Solvers

4.1 PCG–1 solver

Name: PCG-1 (IGAS Ostrava).

Num. techniques : Preconditioned conjugate gradient method.
Preconditioner constructed by displacement decomposition and pointwise incomplete factorization of diagonal blocks.

Stopping criterion : (L2 norm of residual) ¡= EPS * (L2 norm of the rhs)

Main data structures : upper triangular part of the symmetric stiffness matrix stored in regular 42 - point stencil in disk memory.

FLOPS per iteration : 114 * NEQ

Data transfers per iteration : Reading of 126*NEQ*4 bytes from disk per iteration.

Language : FORTRAN77.

Precision : Single precision, some operations in double precision.

References : R. Blaheta, R. Kohut: PCG-1 iterative solver. Report DAM 9501, Institute of Geonics, Ostrava 1995.
R. Blaheta: Displacement decomposition - incomplete factorization preconditioning techniques for linear elasticity problems, Numer. Lin. Alg. Appl. 1 (1994), 107-126

Remarks : Two modifications of PCG-1 are also available:
PCG-1 - IC (in core version)
PCG-1 - DP (double precision version)

5 Testing PCG–1 solver

5.1 Square footing

1. Square footing problem

2. PCG-1 code, single precision

3. IBM RS/6000 3CT, Power2 67 MHz, RAM 128 MB

4. AIX version 3.2.5, XL - FORTRAN 77

5. averaged computer times per one iteration

ELAPSED	4.367 s
CPU = USER	3.584 s
SYSTEM	0.721 s

6. convergence history
   RES=l2 norm of the residual, RHS-l2 norm of the right hand side

IT	RES	RES/RHS
1	.34316E+02	.20539E+01
10	.15087E+02	.90302E+00
20	.39690E+01	.23756E+00
30	.91949E+00	.55035E-01
40	.15398E+00	.92162E-02
50	.12476E-01	.74676E-03
60	.16124E-02	.96510E-04
70	.79187E-04	.47396E-05
80	.53887E-05	.32253E-06
90	.10313E-05	.61728E-07
100	.10403E-06	.62263E-08
110	.65181E-08	.39013E-09
120	.26249E-08	.15711E-09
130	.23133E-09	.13846E-10
140	.48782E-10	.29198E-11
148	.16351E-10	.97866E-12

7. List of computed displacements, single precision, accuracy of the iterations EPS=10**-12

DOF	Displacement
1	.00000E+00
2	.00000E+00
3	.25619E+01
4	-.23908E-01
5	.00000E+00
6	.25535E+01
7	-.47122E-01
8	.00000E+00
9	.25319E+01
10	-.70267E-01
11	.00000E+00
12	.25162E+01
13	-.93509E-01
14	.00000E+00
15	.24834E+01

5.2 Stope stability

1. Stope stability problem

2. PCG-1 code, single precision

3. IBM RS/6000 3CT, Power2 67 MHz, RAM 128 MB

4. AIX version 3.2.5, XL - FORTRAN 77

5. averaged computer times per one iteration

ELAPSED	4.332 s
CPU = USER	3.584 s
SYSTEM	0.715 s

6. convergence history
RES=l2 norm of the residual, RHS=l2 norm of the right hand side

IT	RES	RES/RHS
1	.68081E+04	.65454E+00
10	.11483E+05	.11040E+01
20	.32043E+04	.30806E+00
30	.14615E+04	.14051E+00
40	.41444E+03	.39845E-01
50	.58689E+02	.56425E-02
60	.14339E+02	.13785E-02
70	.61179E+01	.58819E-03
80	.18419E+01	.17708E-03
90	.33141E+00	.31862E-04
100	.45968E-01	.44194E-05
110	.56343E-02	.54168E-06
120	.71019E-03	.68279E-07
130	.10126E-03	.97354E-08
140	.75207E-04	.72305E-08
150	.33094E-04	.31817E-08
160	.63512E-05	.61061E-09
170	.10890E-05	.10470E-09
180	.15066E-06	.14485E-10
190	.16625E-07	.15983E-11
193	.86128E-08	.82804E-12

7. List of computed displacements, single precision, accuracy of the iterations EPS=10**-12

DOF	Displacement
1	.00000E+00
2	.00000E+00
3	.33318E+00
4	-.31858E-02
5	.00000E+00
6	.33265E+00

```
 7   -.61783E-02
 8    .00000E+00
 9    .33152E+00
10   -.89039E-02
11    .00000E+00
12    .32977E+00
13   -.11270E-01
14    .00000E+00
15    .32742E+00
```

5.3 Headgate problems

1. Headgate problem 102*26*33

2. PCG-1 code, single precision

3. IBM RS/6000 3CT, Power2 67 MHz, RAM 128 MB

4. AIX version 3.2.5, XL - FORTRAN 77

5. averaged computer times per one iteration

```
ELAPSED      6.347 s
CPU = USER   4.913 s
SYSTEM       0.985 s
```

6. convergence history
   RES=l2 norm of the residual, RHS-l2 norm of the right hand side

```
IT        RES         RES/RHS


 1    .30733E+05   .82113E+00
10    .19170E+05   .51219E+00
20    .79898E+04   .21347E+00
30    .16673E+04   .44547E-01
40    .38893E+03   .10391E-01
```

50	.11025E+03	.29457E-02
60	.39725E+02	.10614E-02
70	.13258E+02	.35422E-03
80	.59956E+01	.16019E-03
90	.49697E+01	.13278E-03
100	.18155E+01	.48506E-04
110	.73386E+00	.19607E-04
120	.14086E+00	.37635E-05
130	.40564E-01	.10838E-05
140	.13954E-01	.37282E-06
150	.29281E-02	.78233E-07
160	.83367E-03	.22274E-07
166	.34719E-03	.92763E-08

7. List of computed displacements, single precision, accuracy of the iterations EPS=10**-8

DOF	Displacement
1	.00000E+00
2	.00000E+00
3	.66085E+00
4	-.13796E-03
5	.00000E+00
6	.66076E+00
7	-.25913E-03
8	.00000E+00
9	.66062E+00
10	-.35648E-03
11	.00000E+00
12	.66045E+00
13	-.43035E-03
14	.00000E+00
15	.66026E+00

1. Headgate problem 202*26*33

2. PCG-1 code, single precision

3. IBM RS/6000 3CT, Power2 67 MHz, RAM 128 MB

4. AIX version 3.2.5, XL - FORTRAN 77

5. averaged computer times per one iteration

ELAPSED	11.728 s
CPU = USER	9.717 s
SYSTEM	1.932 s

6. convergence history
   RES=l2 norm of the residual, RHS-l2 norm of the right hand side

IT	RES	RES/RHS
1	.37406E+05	.70758E+00
10	.24102E+05	.45593E+00
20	.11149E+05	.21090E+00
30	.24851E+04	.47009E-01
40	.46333E+03	.87644E-02
50	.13591E+03	.25708E-02
60	.46168E+02	.87332E-03
70	.17885E+02	.33831E-03
80	.14641E+02	.27695E-03
90	.14070E+02	.26616E-03
100	.13256E+02	.25076E-03
110	.53198E+01	.10063E-03
120	.12711E+01	.24045E-04
130	.70439E+00	.13324E-04
140	.33563E+00	.63488E-05
150	.23272E+00	.44021E-05
160	.73680E-01	.13938E-05
170	.29039E-01	.54932E-06
180	.87208E-02	.16496E-06

190	.22443E-02	.42453E-07
200	.68885E-03	.13030E-07
202	.52047E-03	.98454E-08

7. List of computed displacements, single precision, accuracy of the iterations EPS=10**-8

DOF	Displacement
1	.00000E+00
2	.00000E+00
3	.66086E+00
4	-.13461E-03
5	.00000E+00
6	.66078E+00
7	-.25243E-03
8	.00000E+00
9	.66064E+00
10	-.34642E-03
11	.00000E+00
12	.66046E+00
13	-.41692E-03
14	.00000E+00
15	.66027E+00

1. Headgate problem 302*26*33

2. PCG-1 code, single precision

3. IBM RS/6000 3CT, Power2 67 MHz, RAM 128 MB

4. AIX version 3.2.5, XL - FORTRAN 77

5. averaged computer times per one iteration

```
ELAPSED      55.477 s
CPU = USER   15.036 s
SYSTEM        7.366 s
```

6. convergence history
RES=l2 norm of the residual, RHS-l2 norm of the right hand side

IT	RES	RES/RHS
1	.41791E+05	.64574E+00
10	.25035E+05	.38683E+00
20	.95831E+04	.14807E+00
30	.19967E+04	.30853E-01
40	.52738E+03	.81487E-02
50	.21152E+03	.32683E-02
60	.25938E+03	.40078E-02
70	.29868E+03	.46151E-02
80	.19468E+03	.30081E-02
90	.17150E+03	.26500E-02
100	.11243E+03	.17372E-02
110	.13021E+03	.20119E-02
120	.97488E+02	.15063E-02
130	.47908E+02	.74026E-03
140	.10550E+02	.16301E-03
150	.46230E+01	.71432E-04
160	.20284E+01	.31341E-04
170	.14598E+01	.22555E-04
180	.65504E+00	.10121E-04
190	.23655E+00	.36551E-05
200	.87171E-01	.13469E-05
210	.25180E-01	.38906E-06
220	.76997E-02	.11897E-06
230	.25403E-02	.39251E-07
240	.80727E-03	.12474E-07
242	.61572E-03	.95138E-08

7. List of computed displacements, single precision, accuracy of the iterations EPS=10**-8

```
 DOF    Displacement

   1     .00000E+00
   2     .00000E+00
   3     .66108E+00
   4    -.92467E-04
   5     .00000E+00
   6     .66100E+00
   7    -.16817E-03
   8     .00000E+00
   9     .66085E+00
  10    -.22003E-03
  11     .00000E+00
  12     .66068E+00
  13    -.24842E-03
  14     .00000E+00
  15     .66049E+00
```

5.4 Rožínka problem

```
1. Rozinka problem

2. PCG-1 code, single precision

3. IBM RS/6000 3CT, Power2 67 MHz, RAM 128 MB

4. AIX version 3.2.5, XL - FORTRAN 77

5. averaged computer times per one iteration

   ELAPSED      549.905 s
   CPU = USER    78.872 s
   SYSTEM        47.878 s
```

6. convergence history
RES=l2 norm of the residual, RHS-l2 norm of the right hand side

IT	RES	RES/RHS
1	.32599E+05	.44930E+00
10	.39632E+04	.54622E-01
20	.14912E+04	.20553E-01
30	.65154E+03	.89798E-02
40	.31974E+03	.44068E-02
50	.18855E+03	.25986E-02
60	.13347E+03	.18395E-02
70	.86215E+02	.11882E-02
76	.70192E+02	.96741E-03

7. List of computed displacements, single precision, accuracy of the iterations EPS=10**-3

DOF	Displacement
1	.00000E+00
2	.00000E+00
3	.94191E-03
4	.34793E-03
5	.00000E+00
6	.95255E-03
7	.51286E-03
8	.00000E+00
9	.98697E-03
10	.66124E-03
11	.00000E+00
12	.10305E-02
13	.74898E-03
14	.00000E+00
15	.10653E-02

References

[1] R. Blaheta, R. Kohut: Benchmarks and programs for testing iterative solvers for 3D problems of geomechanics, TR – DAM – 9502, IGAS Ostrava, 1995

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[3] R. Blaheta: HIPERGEOS related benchmarks, software and testing. HIPERGEOS Workshop, Rožnov p. R. 1996

[4] R. Valkenberg: Status of HIPERGEOS benchmarking, HIPERGEOS Workshop, Brussels 1997, see also http://homepages.ulb.ac.be/ rvalkenb/HIPERGEOS/benchmark.html

[5] R. Blaheta et al., Mathematical modelling of the effects of a new mining technology at the uranium mine Dolní Rožínka, Report – DAM – 9702, IGAS Ostrava 1997

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