A robust preconditioner for the conjugate gradient method

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- Work context
- Direct solver
- Krylov solver
  - New preconditionner
- Conclusion
- Further development

General context

- General purpose Cast3m computer code developed at CEA for mechanical problem solving by FEM method.
- Used in Nuclear Industry and others.
- Toolbox for researcher
- Blackbox for end user
- Important need for qualification and validation.

Quality criteria for industrial code

– No need for tuning

– Correct solution if correct problem

– Incorrect problem detection

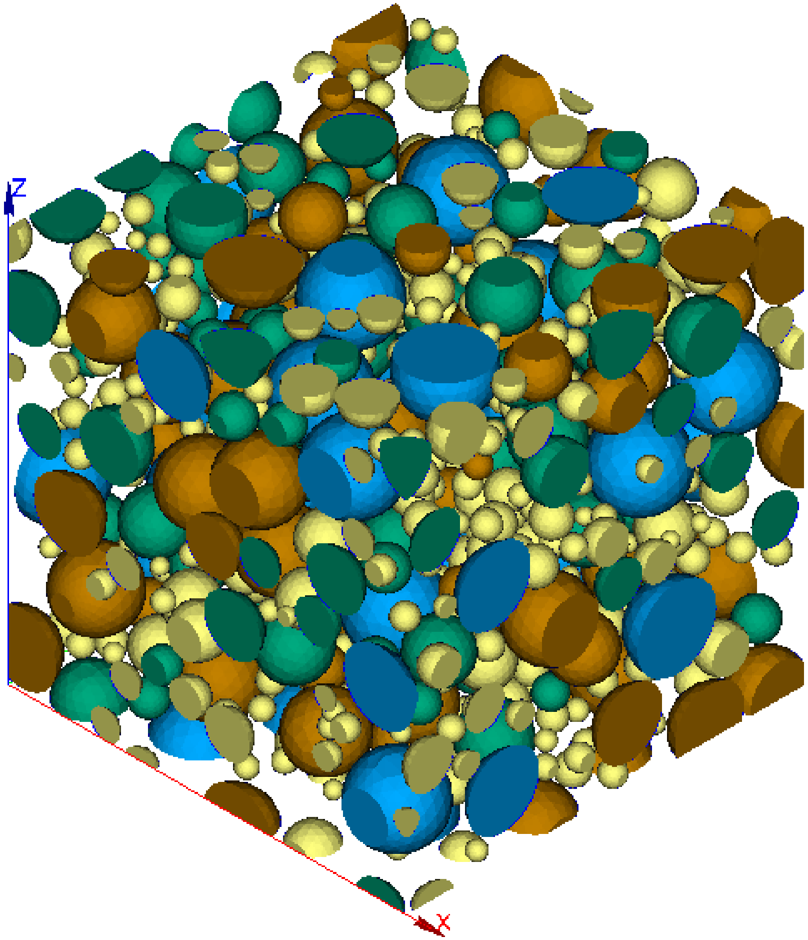
– Predictable time

– No failure

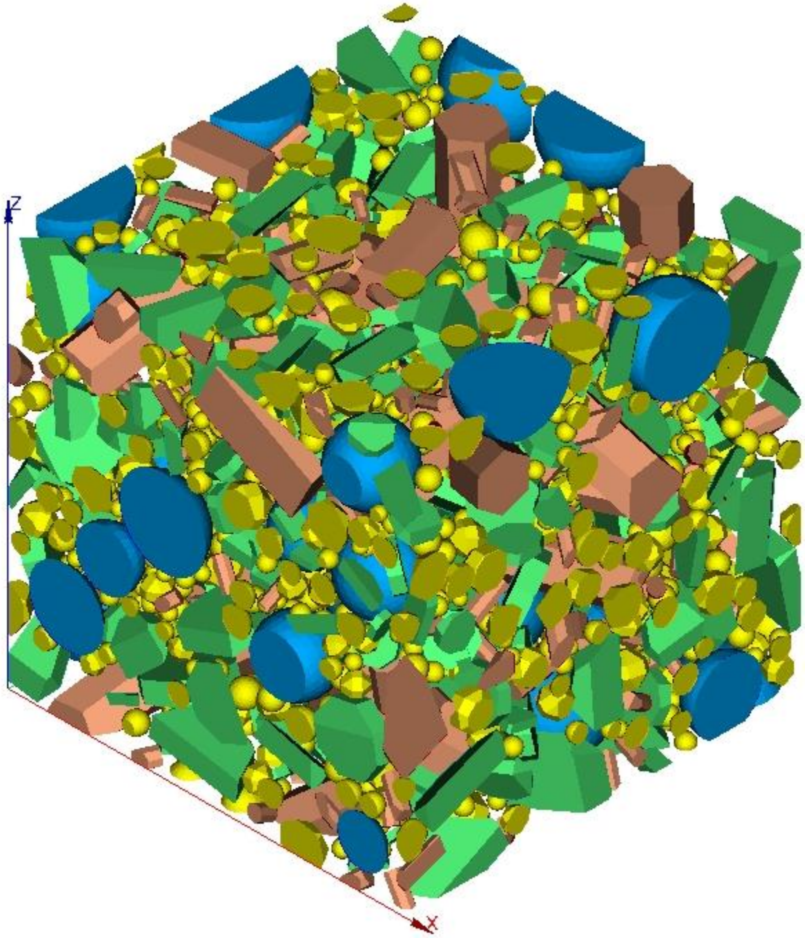
Context

- Cement paste studies – EHPOC project
- Heterogeneous material with inclusions
- High mechanical properties contrast
- REV analysis
- Need for realistic representation of inclusions including sharp edge
- Need for accuracy. Reference calculation
- CAO meshes with the Salome framework

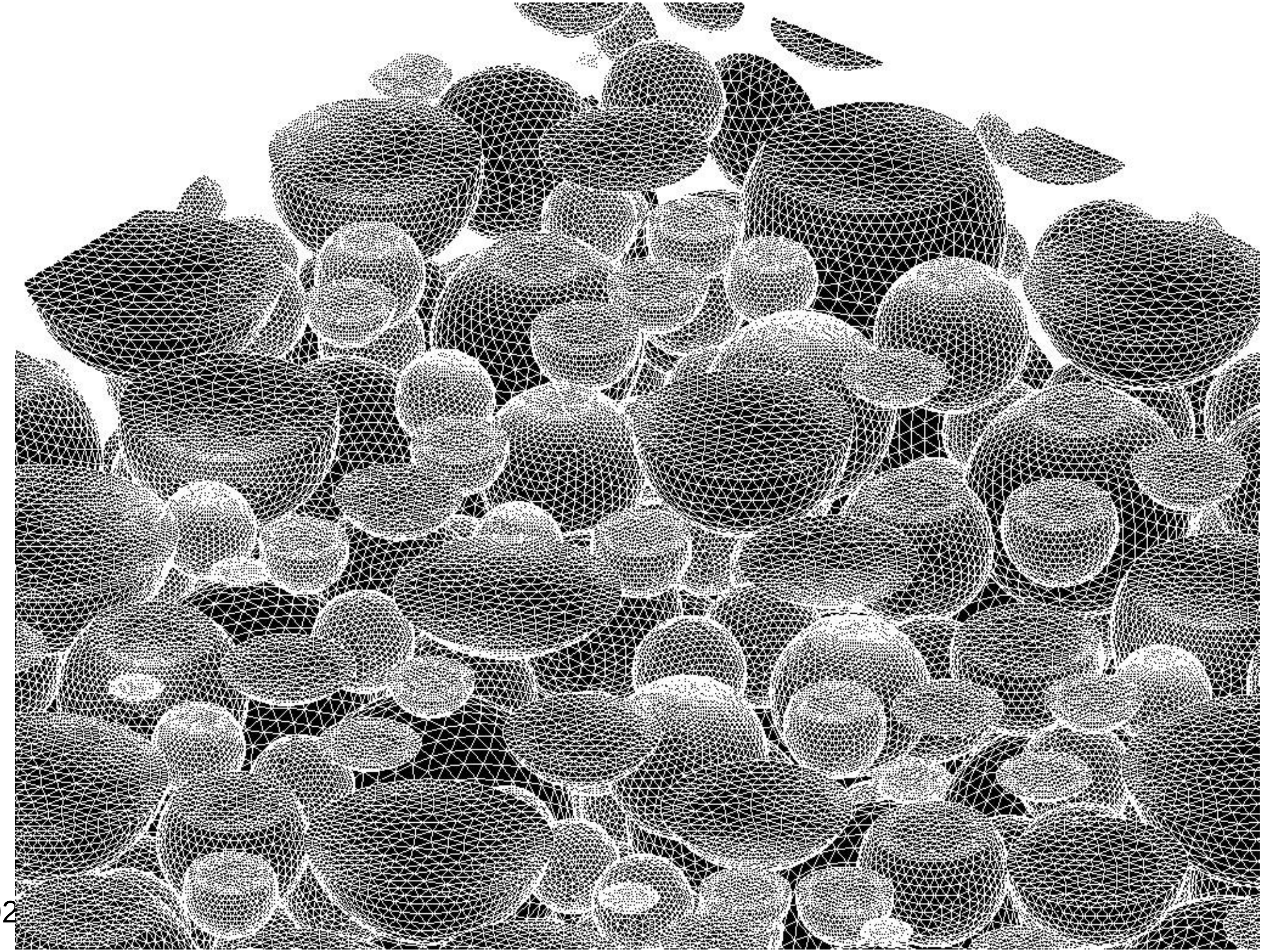
Spherical inclusions



Sharp inclusions



23.5 million tetrahedrons



Solver challenge

- Large number of degrees of freedom
- Very bad matrix conditioning due to
  - Properties contrast
  - Flattened elements
- Various boundary condition including periodic condition of different kind. Use of cinematic constraints with Lagrange multiplier.
- Multiple problem solving on the same matrix.

Direct solver

- Robust and precise
- Nested dissection ordering and sparse Crout solver
- Spatial complexity in $O(n^{4/3})$
- Temporal complexity in $O(n^{5/3})$ for preconditioning (factorization). Parallelizable.
- Temporal complexity in $O(n^{4/3})$ for solving.

Direct solver - 2

- Out of core storage
- Around 100Go of matrix storage for 10.000.000 dof. Practical limit on desktop PC.
- 1d-12 accuracy
- Unilateral constraints available

Krylov method

- Constraint: maintain O(n) spatial complexity
- In core preconditioner storage
- No convergence with ILU(n) or ILUT preconditioner
- No convergence with domain decomposition preconditioner
- Some hope with algebraic multigrid preconditioner, but not yet implemented for mechanic.

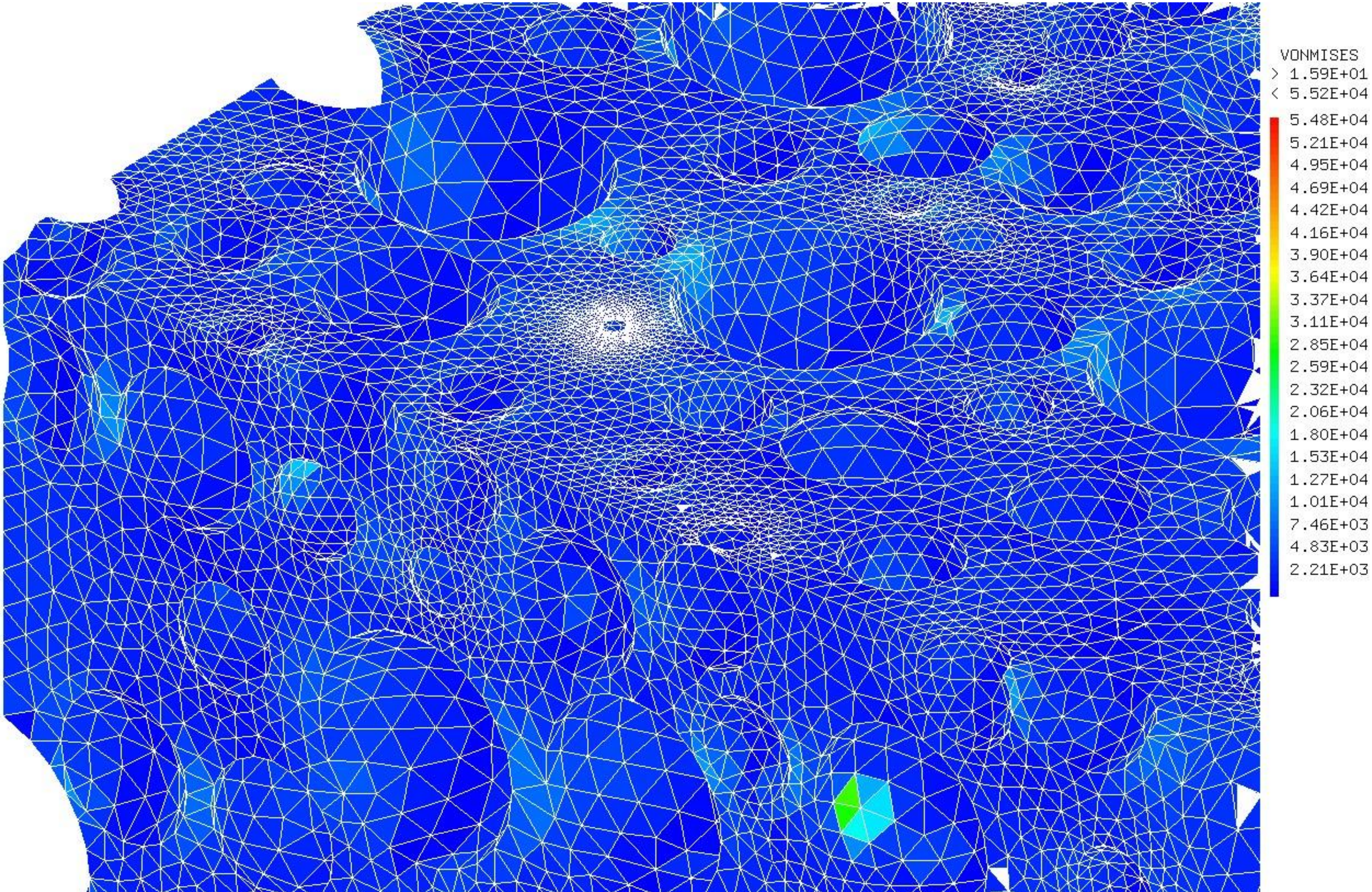
New preconditioner

- ILU(0) far better than ILU(n) for n small when it converges
- Non convergence of Krylov iterations is related to small diagonal terms in the preconditioner
- Idea: control the diagonal terms of the preconditioner by augmentation.
- Risk of numerical instability due to the augmentation.

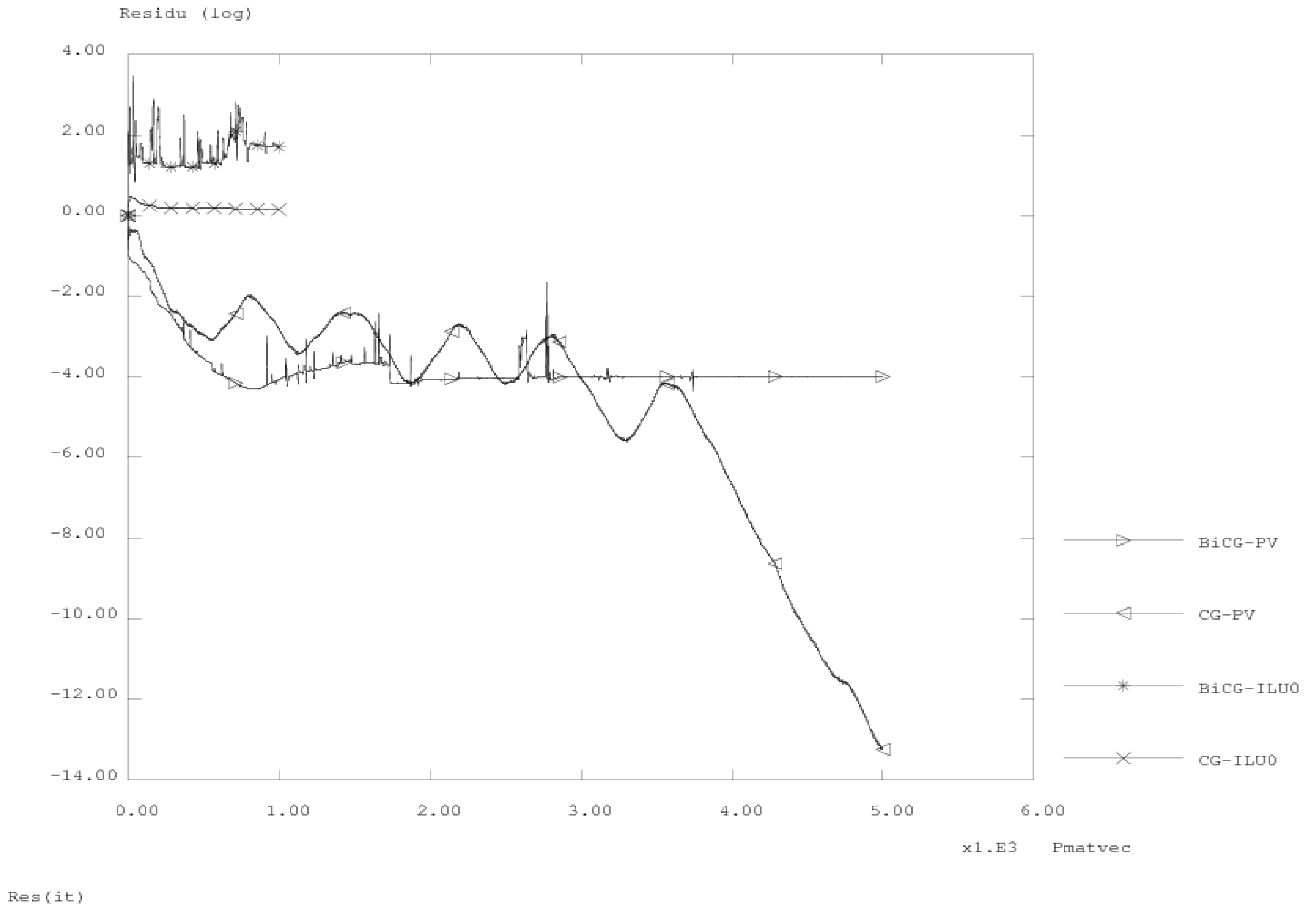
New preconditioner - 2

- Converge in all tested cases!
- Most efficient with conjugate gradient method and RCM ordering
- 1d-15 accuracy
- O(n) space complexity
- $O(n^{4/3})$ temporal complexity approx
- Poor parallelism
- 16 000 000 dof on a 16gB desktop PC

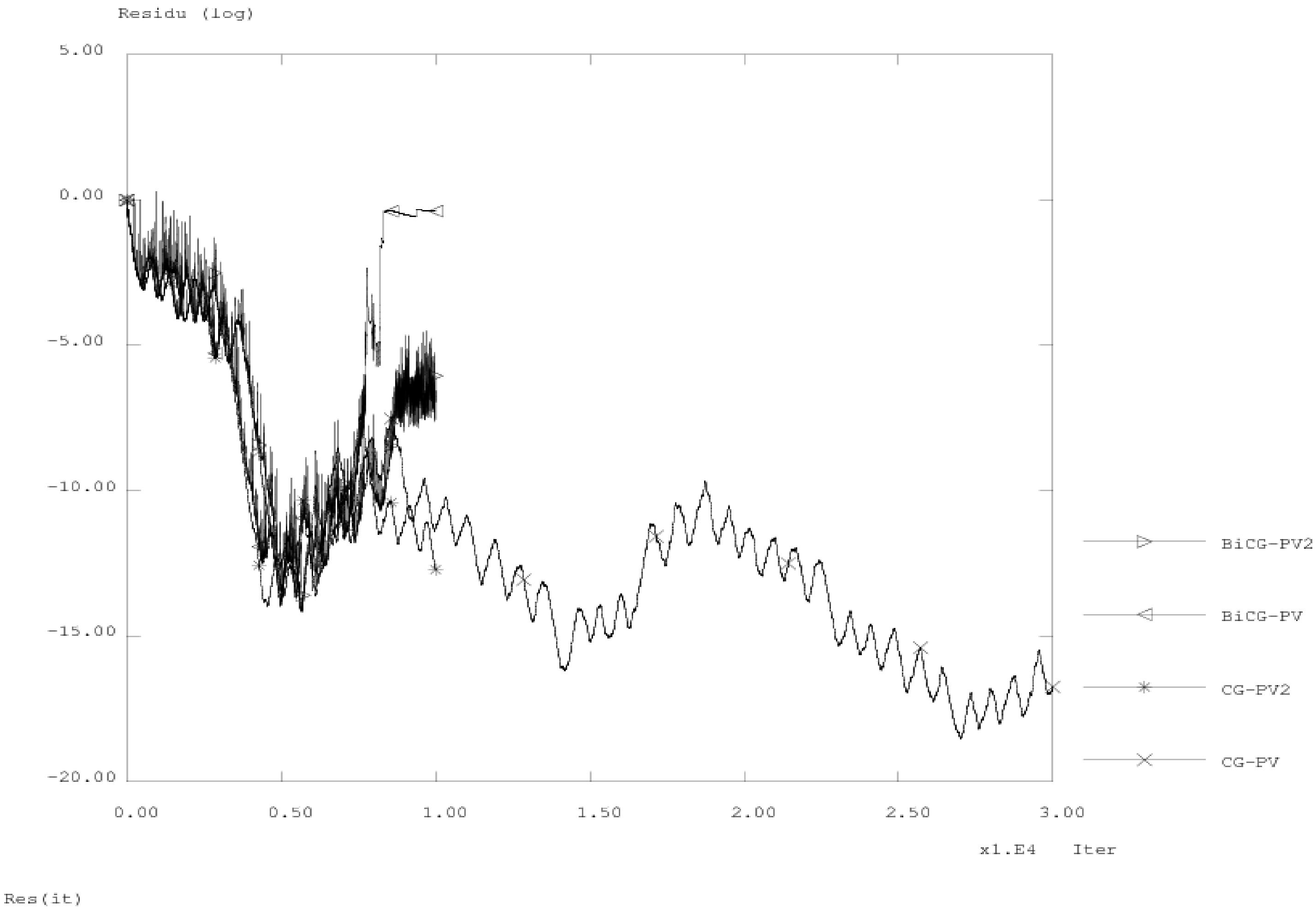
Stresses in matrix



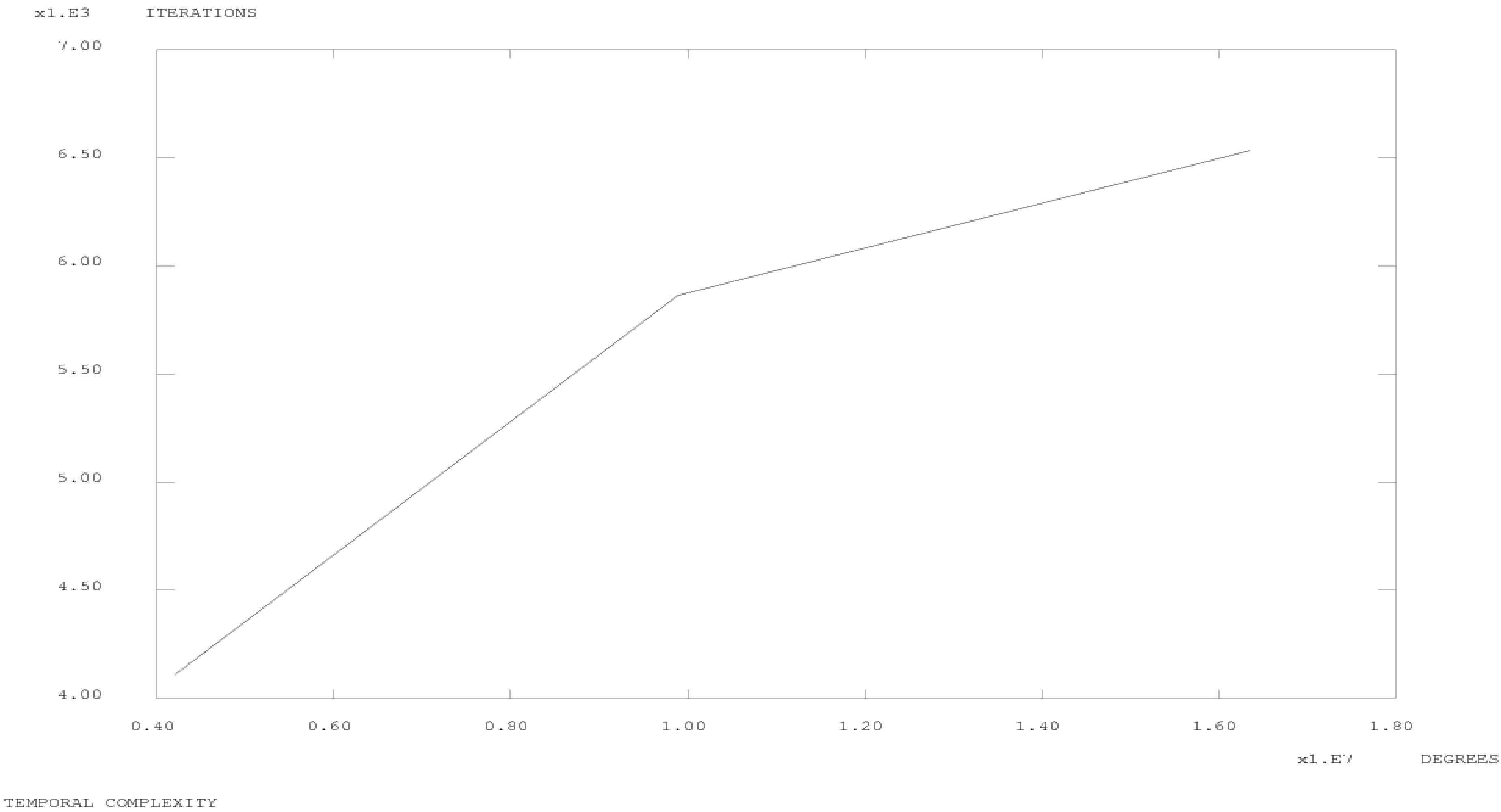
Convergence comparaison



CG versus BiCG



Iterations versus DOF



Shell mesh refinement

- Convergence study
- No refinement in the thickness of the element
- Degradation of the stiffness matrix conditioning
- No convergence of Krylov iteration at some point
- In our case, loss of respect of cinematic constraints (Lagrange multiplier)

New preconditioner - 3

- Idea: exact factorization on constraint unknowns. Incomplete factorization on others
- Applies well in solid mechanic since few filling due to cinematic constraints. To be tested in fluid mechanic with pressure constraint
- Penalization of Lagrange multiplier
- Convergence maintained on highly refined meshes.

Conclusion

- New preconditioner for CG or BiCG method
- RCM ordering
- Augmentation of small diagonal terms
- Penalization of Lagrange multipliers
- Standard in Cast3M FEM code for mechanical analysis

Conclusion -2

- Robust – accurate
- Low programming complexity (one instruction development, 6 months thinking)
- Slower convergence than ILU(0) when ILU(0) works – factor 1.5-2
- No failure (yet)

Further development

- Parallelization by block operations
- Unilateral constraints on Lagrange multiplier
- Automatic switch between ILU(0) and ILU(0)augmented?