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Strategies for an Optimized simulation of granular particles in a Newtonian Fluid, Part 2: Numerical algorithms

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Abstract

We describe our experiences with sparse solvers for the stationary incompressible Navier-Stokes equation on a Friedrichs Keller grid with various boundary conditions. We simulate polygonal granular particles in a surrounding incompressible fluid in a P2P1 Galerkin finite element discretization, whereby Newton-Raphson iteration turns out to be surprisingly robust. For the inversion of the Jacobian, it turns out that from the various sparse algebraic solvers in use in the numerical community, even GMRES does not reach the necessary accuracy, and only BiCGSTAB(l) gives satisfying results.

4 Introduction

The simulation of the interaction between fluids and granular material involves many preliminary steps which simplifies or decrease the degree of freedom of the initial problem. The findings in research introduced in the article are preliminary for the implementation of a full simulation containing polygonal granular particles modeled with the discrete element method and the fluid modeled with the Galerkin finite element discretization of the incompressible Navier Stokes equation.

For an efficient implementation, the use of unstructured grids is necessary, as well as the solution of the nonlinear system of equations resulting from the discretization, with sparse matrix algorithms. In this work, we investigate which of the considerable variety of Krylov-space iterative solvers gives satisfying results for structured grids and is therefore a candidate for the use with unstructured grids.

We are dealing exclusively here with solution of the stationary Navier-Stokes equations, though our final aim is an implementation of the time-dependent equations, because the solution of the stationary problem is necessary to obtain consistent starting values for the time-dependent Navier-Stokes equation in the DAE-formulation (see the first part of this article on the previous pages). From the structure of the problem, it is clear that the non-stationary case is numerically more benign, because the mass-term dominates, where the non-linearities and the stiffness-matrix are rescaled with the time-step and their contribution is much smaller than in the stationary problem.

5 Discretization and Band structure

As the work-horse for this investigation, we choose the Flow5-code by John Burkardt[5], which we re-engineered and optimized for MATLAB. It simulates the incompressible

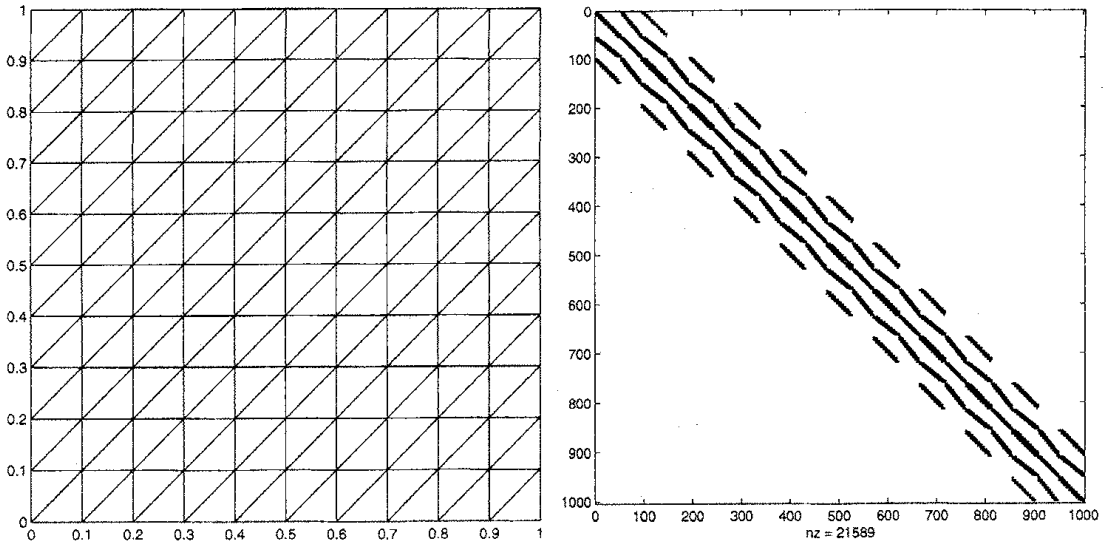

Figure 8: The structure of the Jacobian for the Friedrichs Keller grid (left, here for cavity flow) is a band matrix (right)

Navier-Stokes equation

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial x} - \nu\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right] = 0, \tag{8}$$

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial y} - \nu\left[\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right] = 0, \tag{9}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{10}$$

for the velocity-fields u, v in x, y-direction and the pressure field with dynamic viscosity ν in a Galerkin Finite Element Method with P2P1 elements. The discretized problem is a system of nonlinear equations with velocities u_i and v_i x- and y-direction on all i integration points, as well as on the pressures $\hat{p}_k$ on all integration points k (which for the P2P1-elements is only a subset of the i mesh-points of the velocities), so that the vector of all variables

$$X = (u_1, u_2, \ldots u_i, v_1, v_2, \ldots v_i, p_1, p_2, \ldots p_k).$$

The stationary Navier-Stokes equations eqns. (8-10) consist formally a field problem $\mathcal{F}(u, v, p) = 0$, and the corresponding discretized problem

$$\vec{F}(X) = 0,$$

is a conventional root-finding problem for non-linear equations. The iterative solution by the Newton-Raphson method

$$\vec{X}_{n+1} = \vec{X}_n - \left(\nabla\vec{F}(\vec{X}_n)\right)^{-1}\vec{F}(\vec{X}_n) \tag{11}$$

proved to be stable enough during the whole of the investigations; no additional stabilizations had to be introduced, and the convergence was independent from the initial values

X_0. The kernel of the iteration is the solution of the linear system

$$\underbrace{\Delta\vec{X}}_{x} = \left(\underbrace{\nabla\vec{F}(\vec{X}_n)}_{A}\right)^{-1} \underbrace{\vec{F}(\vec{X}_n)}_{b}, \tag{12}$$

where A is matrix of the Jacobian and Δx is the residual of the solution. We have started the Newton-Raphson iteration with constant non-zero initial guesses, the initialization with zero initial guess is both unphysical and gave spurious convergence for some iterative solvers. For most boundary conditions investigated, three iteration steps were enough, after that the solution changed only marginally.

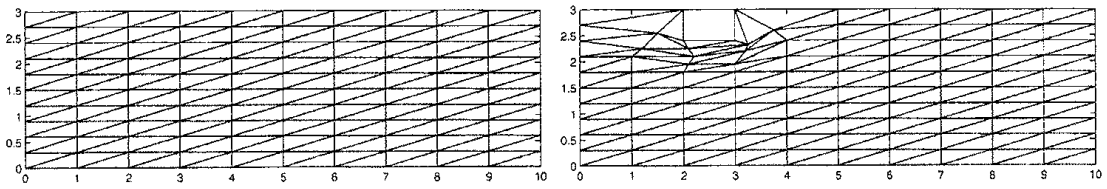

Figure 9: Friedrichs-Keller grids used for the simulation of pipe flow and pipe flow below a protruding step (inflow on the left, outflow on the right, i.e. open boundaries on the left and right end with a nonzero velocity gradient and fixed boundaries on top and bottom). The grid points around the step in the grid on the right were chosen to minimize the dislocation of the other grid points, not to minimize the error in the spacial discretization.

For a finite-element discretization with P2P1-elements, one element has approximately $n = 15$ degrees of freedom, 6 points for u, 6 points for v and 3 points for p, though a point belongs on average to $m = 3$ elements. The dimensions of $\nabla\vec{F}$ for a Friedrichs-Keller-grid (the usual Finite-Element grid, see Fig. 8, left) with $b = (2 \times l_x \times l_y)$ elements has the linear dimension $l = (2 \times l_x \times l_y) \times n/m$. Because there are only entries for adjacent degrees of freedom, the matrix is sparse and banded with bandwidth $(l_x \times l_y)$ (see Fig. 8, right). For the reference runs, we have used the LU-decomposition (for the formulation of $\nabla\vec{F}$ as full matrix) and the incomplete LU-decomposition (threshold 10^{-10}, for the formulation of $\nabla\vec{F}$ as sparse matrix). For general problems with l variables, the number of operations necessary for a solution with the LU-decomposition is of the order of l^3, which would be prohibitive for a general matrix which occurs for unstructured grids. For the banded matrix of the Friedrichs-Keller-Grid, the number of operations is one order of magnitude less, only lb^2.

6 Eigenvalue Analysis

For finite difference discretizations, the discretized solution of the flow-lines corresponds directly to the continuum solution, and the properties can be compared directly. For the Galerkin Finite Element method, which introduces basis functions and additional degrees of freedom via integration, such a comparison is more problematic. One possible strategy is to analyze the problem[26] in terms of the eigenvalue spectrum of the Jacobian. The central, most time consuming part of the GFEM-simulation of the stationary flow is the

solution of the linear system in eq. (12) with the Jacobian $\nabla\vec{F}(\vec{X}_n)$. Because the choice of Krylov-space solvers depends on the eigenvalue spectrum of the matrix of the linear system, it is worthwile to investigate the eigenvalue spectrum of the Jacobian to develop an insight about the convergence of the algorithms depending on the physical problem. It turns out that the eigenvalues of the Jacobian depend crucially on the vorticity in the problem and the eigenvalues change with each Newton-Raphson iteration eq. (11). In the following, we have performed the Newton-Raphson iteration with LU-based inversion of the Jacobian with constant initial vector.

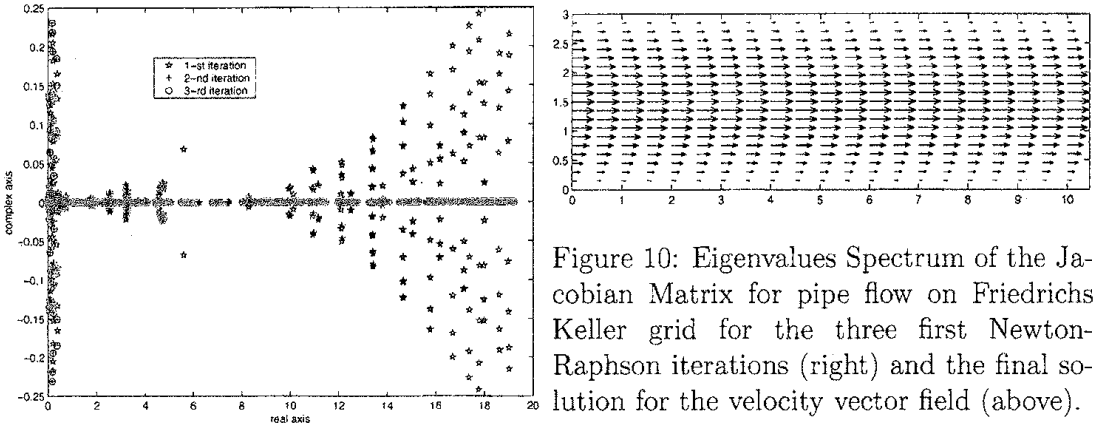

Figure 10: Eigenvalues Spectrum of the Jacobian Matrix for pipe flow on Friedrichs Keller grid for the three first Newton-Raphson iterations (right) and the final solution for the velocity vector field (above).

For the pipe flow (Fig. 9, left), the eigenvalues for the first Newton-Raphson iteration are along the complex axis, along the real axis, and a third group is spread out fan-like symmetrically around the real axis (Fig. 10). With proceeding iterations, the eigenvalues of the fan-like group are drawn towards the real axis. The Newton-Raphson iteration eq. (12) converged basically within three steps to ten digits accuracy , as can be seen by the fact that in the plot of the eigenvalues, (Fig. 10, left), the symbols for the second iteration ("+") are basically in the center of the symbols for the third iteration ("'o"). Convergence within three steps was also observed for the geometries below. For the flow below a step (Fig. 9, right), the eigenvalue distribution is about the same as for the pipe flow, (Fig. 11, note the different scale of the real axis in comparison to Fig. 10.) After the third iteration, some butterfly-like clouds remain relatively far from the real axis. For the pipe-flow below a step, the Jacobian has larger eigenvalues (Fig. 11, left) than the Jacobian for unperturbed pipe-flow (Fig. 10, left), whereas the streamlines for the flow around the obstacle show smaller velocities at the boundary near the obstacle (Fig. 11, right) than for the unperturbed flow (Fig. 10, right). As the Jacobian enters the Newton-Raphson iteration eq. 12 in the denominator, so that its large eigenvalues cause small contributions, plausible to conclude that the small structures in the flow correspond to large eigenvalues in the Jacobean, and vice versa.

In case of cavity flow, at the first Newton-Raphson iteration the eigenvalues are near the axis, and during the iterations spread out into similar butterfly-like structures (Fig. 12, left) as in the case of the flow below a step (Fig. 11). As the similarity between the cavity-flow and the flow below the step, one can conclude that the butterfly-like structures in the eigenvalue spectrum are associated with the vorticity in the system.

In the case of laminar flow with nearly straight streamlines (pipe flow without ob-

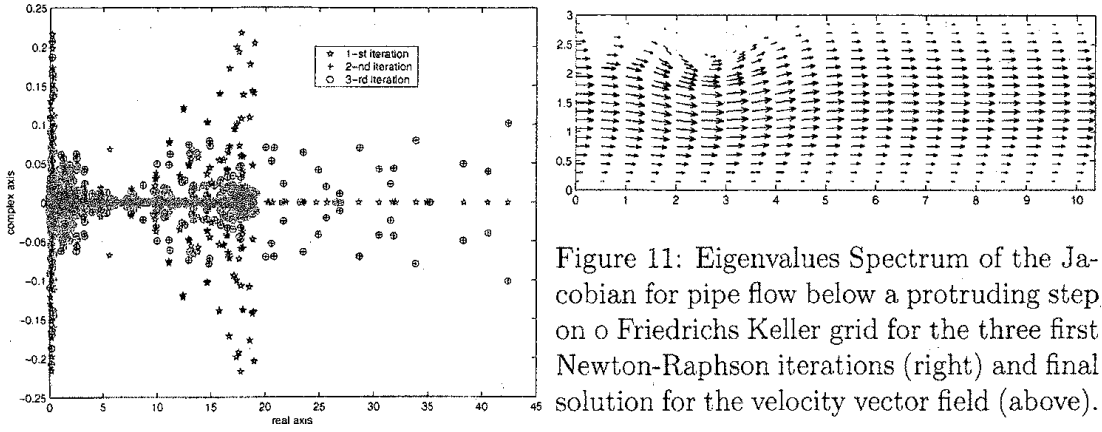

Figure 11: Eigenvalues Spectrum of the Jacobian for pipe flow below a protruding step on o Friedrichs Keller grid for the three first Newton-Raphson iterations (right) and final solution for the velocity vector field (above).

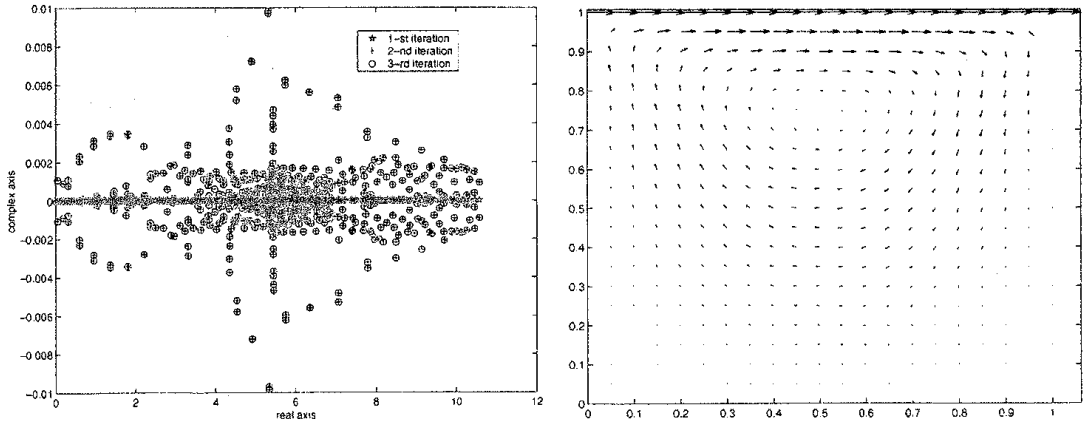

Figure 12: Eigenvalues Spectrum of the Jacobian Matrix for cavity flow using Friedrichs Keller grid and the final solution for the velocity vector field. The upper boundary has a constant flow in x-direction and zero velocity in y-direction imposed, at all other walls fixed boundary conditions are set. The right boundary is at $x = 1.0$, only the vector for the velocity of the upper right boundary point extends beyond.

stacles), the eigenvalue spectrum is "almost purely real". The eigenvalue analysis of the Jacobean initialized with the correct final solution (Hagen-Poiseulle flow) might give the impression that purely real solvers are suitable for the problem. In case of cavity flow, with the approach to the stationary numeric solution the eigenvalues runs away from the real axis, and the necessity for solvers for problems with complex eigenvalue spectrum becomes clear. Because the imaginary part of the eigenvalues can become arbitrary large in the presence of vortices, linear solvers are needed which are explicitly constructed for problems where the corresponding matrix can contain complex eigenvalues.

6.1 Choice of solvers

There are two classes of iterative solvers which can be used on unstructured grids: Stationary/Relaxation methods, which are basically improved versions of the Jacobi-Iteration, and Non-Stationary/Krylov-Space Methods, which are basically improved versions of the

Conjugate Gradient method. The drawback of the original relaxation methods (Jacobi, Gauss-Seidel, Successive Overrelaxation) was the slow convergence due to the small curvature/ large length-scale introduced by the "smoothing" inherent in the relaxation. This problem can be overcome in the Multigrid methods, which solve the equations simultaneously also on coarser grids, so that the information is transferred between the length scales. The appealing feature of transferring length scales of the solution directly in geometrical terms becomes lost when unstructured meshes are used, where so-called algebraic multi grid method have to be use to compensate for the loss of geometrical information in the corresponding matrix. The manuals of such algebraic multi grid packages (e.g. UG[2]) are usually already much thicker than some books on linear algebra, and learning the handling even as black boxes takes considerable time. As we want to put our effort in the solution of the Navier-Stokes equations, not in the underlying algebraic methods, we choose instead Krylov-space solvers for sparse matrix methods, which are based more on algebraic than on geometric considerations. Apart from the fact that the replacement of the LU-decomposition in the original code is straightforward, a further advantage is that there are criteria in terms of eigenvalues, although there is no guarantee of convergence (in the case of Relaxation method, there isn't, either.)

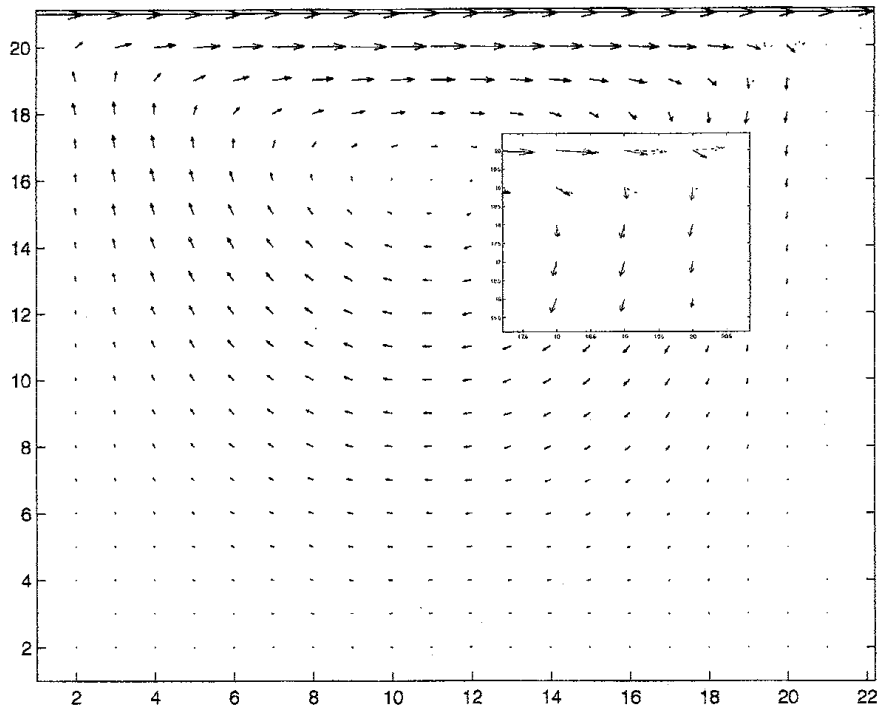

Figure 13: Deviation of the solution for the final Newton-Raphson iteration (dark: correct, with LU, light: incorrect with GMRES) for the velocity field; the insert shows the magnification of the solution in the upper right corner, where the largest error occurs

6.2 Nonstationary Iterative Methods(Krylov Space Methods)

The ancestor of Krylov-Space methods (see Ref. [1] for an overview), which try to solve a linear system $Ax = b$ by minimizing the residuum vector $r = Ax - b$, is the Conjugate Gradient method (GC), which works only for positive definite A. Newer methods have been developed for more general cases. We did not use preconditioners, because for solutions of flow with granular particles in a fluid, this will also be impracticable because it

is unclear what a "good" preconditioner might be. All standard methods like Bi-conjugate Gradient, Conjugate Gradient Squared and Bi-conjugate Gradient Stabilized failed for the solution, both in the MATLAB-implementation as well as in the Implementation of Ref. [1]. Only with GMRES and BiCGSTAB(l)[18], solutions for the Newton-Iteration could be obtained at all.

6.3 GMRES - a surprising failure

The Generalized Minimal Residual Method (GMRES) is widely used in fluid mechanics in the so-called Newton-GMRES-method for the Navier-Stokes equation for compressible flows. For our incompressible problem, it never converged to the exact(LU) solution with more than three digits accuracy. This would not so bad for the velocity in Fig. 13, but it is unacceptable for the pressure in Fig. 14, as the violation of the continuum equation in a DAE-formulation will lead to a degeneration of the solution away from the constraint manifold. We tried out different initial solutions, but this did not improve the convergence in any way. The bad convergence of the Newton-Raphson iteration with GMRES is even more surprising as the Newton-Raphson iteration is a second order method, i.e. it doubles the accuracy of the solution in each iteration. This has the downright magic effect that with a preliminary solution x_n and a Jacobian or its approximant which are correct to k digits in the n-th step, the next solution x_{n+1} will exhibit $2k$ correct number of digits. Not even this formidable property seems to further the accuracy of the solutions obtained with GMRES, so we have to conclude that for our incompressibility problem, GMRES is inherently inapplicable.

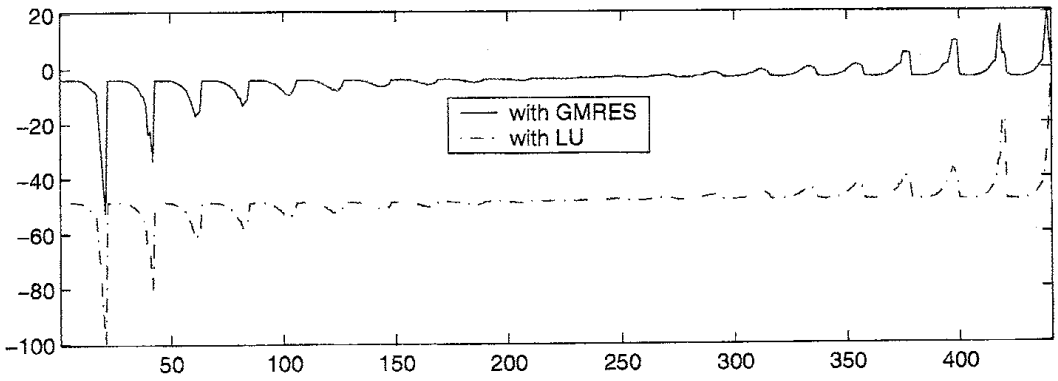

Figure 14: Comparison between pressure vectors obtained via GMRES and LU respectively, for the 3rd iteration of the system in Fig. 8; the GMRES-pressure deviates from the "numerically exact" LU-pressure constantly over the whole grid.

6.4 BiCGSTAB(l)- the successful solver

BiCGSTAB(l) - Bi-Conjugate Gradient Stabilized(l)[18], is newer than other methods, so it has not yet found its way in standard references like Ref. [1]. It was explicitly built for problems with complex eigenvalues spectra to overcome the problems inherent in BiCGSTAB and GMRES and it was the only iterative linear solver which converged

within the desired tolerance. In contrast to other Krylov-Space methods, BiCGSTAB(l) does not only use the residual $r = Ax - b$, but also the "shadow residual" $\tilde{r} = \tilde{x}^T A - \tilde{b}^T$. Using a zero-vector for the initialization lead to spurious convergence, so instead we choose a constant non-zero vector. We use BiCGSTAB(4) as well as BiCGSTAB(8) and, apart from manually adjustment of the tolerance and the maximum number of iterations, there were no problems with the convergence. BiCGSTAB(l) seems to the best choice for the time-dependent solution of the Navier-Stoke Equation for incompressible flow with vortices or further more solver for the granular-particle - fluid system simulation.

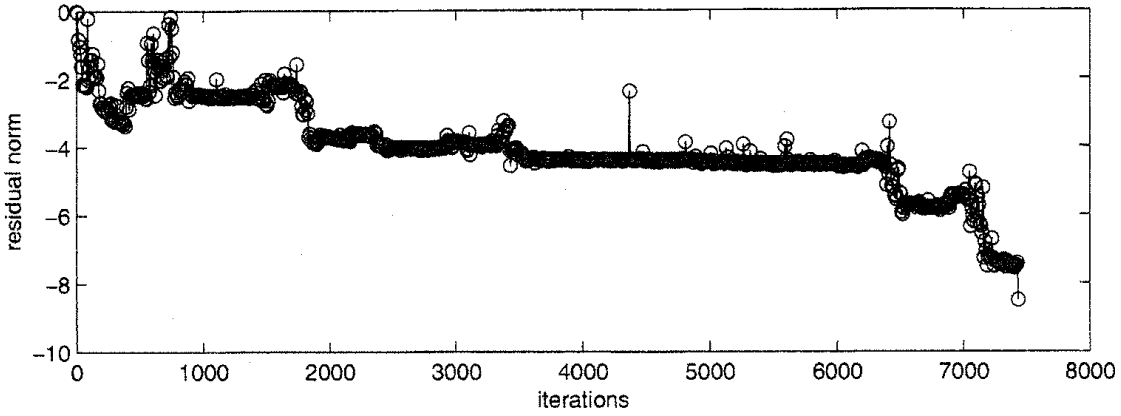

Figure 15: Convergence diagram of BiCGSTAB(4) for the system in Fig. 8

Fig. 15 shows the convergence of the norm of the residual $|r| = |b - Ax^{(i)}|$ with BiCGSTAB(4) to a given accuracy of 10^{-8}. The solver converges to tolerance approximately 10^{-9} after about 8000 BiCGSTAB(l)-iterations . For each Newton-Raphson iteration, e.g. three, these 8000 BiCGSTAB(l)-iterations must be repeated, so that a total of 24.000 BiCGSTAB(l)-iterations is necessary. This looks like a relatively costly performance, but for a simulation of the time-dependent Navier Stokes equation, only for the initial timestep the solution has to be computed from scratch, using this many iterations in the linear solver; for the subsequent time-steps, the previous flow patterns can be used as an initial guess which reduces the number of BiCGSTAB(l)-iterations, and usually, only a single Newton-Raphson iteration is necessary.

7 Summary and Conclusions

We have investigated the solution of the stationary Navier-Stokes equations for the incompressible case with Newton-Raphson solution of the equations resulting Galerkin-Finite element discretization for various geometries and have compared the performance of different linear solvers for the inversion of the Jacobian in the Newton-Raphson procedure. Convergence was reached within three to five iterations. Except GMRES and BiCGSTAB(l), all other solvers among the large variety of Krylov-Space solvers failed to converge or crashed already in the initial problem. Though GMRES is a popular solver for the compressible Navier-Stokes equations, as documented by the existence of the Newton-GMRES-method, GMRES exhibited considerable convergence problems and was insuffi-

cient for all problems we investigated. Only BiCGSTAB(l), with $l \geq 4$ gave satisfying solutions for all test cases in comparison with the "numerical exact" solution for LU-decomposition. The next step in the investigation will be the solution of time-dependent problem for the same boundary conditions, using the stationary solutions obtained in this work as initial guess.

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