Equidimensional modelling of flow and transport processes in fractured porous systems I

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Flow and transport in fractured porous media play an important role for many environmental applications, e.g. the design of disposal systems for hazardous waste. The different hydraulic properties of the fractures and the surrounding rock matrix have a strong influence on the behaviour of the physical processes existing on site.
In the two papers of this conference, we will present a new numerical concept to describe saturated flow and transport processes in arbitrarily fractured porous media. We will use an equidimensional approach where fracture and matrix are discretized with elements of the same dimension. To solve the problem, we developed a two–level multigrid method based on a hierarchical decomposition into a fracture problem and a matrix problem. This decoupled treatment of fracture and matrix allows us to handle the locally governing physical processes appropriately. In this paper we will also present convergence comparisons with classical multigrid and algebraic multigrid methods (AMG). In *Neunhäuserer et al.* (this issue, part II) we will discuss the effect of equidimensionality on the modelling results and the influence of the chosen transport discretisation technique.

1. INTRODUCTION

The simulation of groundwater flow and solute transport behaviour in fractured subsurface systems is of major importance when investigating the longterm safety of legacies and waste disposal sites, the remediation of contaminant sites, or the safety of aquifers used as drinking–water reservoirs. The complex geometry as well as the vastly different hydraulic properties of fractures and the porous matrix lead to very heterogeneous flow and transport conditions. Fractures representing distinctive pathways allow for fast contaminant transport through the system, resulting in early breakthrough times. From the fractures, the contaminant enters the surrounding matrix by diffusive or dispersive processes. It is stored in the matrix and released slowly back into the fractures, thus causing a longterm contamination of the system. Numerical concepts employed to describe fractured porous formations have to take these heterogeneous conditions into account.

In this paper we consider a discrete model for the flow in porous media in two space dimensions. Matrix as well as fractures are represented by quadrilaterals (equidimensional modelling). This contrasts to most of the previous works on this field where fractures are usually represented by 1d–elements (2–D) or 1d–and 2d–elements (3–D) (cf. e.g. *Helmig*[6], *Barlag* [2]). Though well–working in a number of applications this lower dimensional approach does not provide local mass conservation and does not allow to follow unambiguous streamlines in and out of the fracture. This might be a drawback in some situations. It will be shown by numerical experiments in part II that our equidimensional approach might end up with different results in simulation. In part I of this paper, we will concentrate on numerical computation of the flow field, in particular on steady state flow. The resulting flow field will be used for an ideal tracer transport to be considered in part II. A triangulation of the fractures with a reasonable number of nodes leads to long, thin elements. Though almost degenerate elements are not a problem from the approximation point of view (cf. e.g. *Jamet* [8]), they cause severe problems in the iterative solution of the discretized problems. For example, classical multigrid methods usually fail for vanishing width of fractures. Additionally jumping coefficients along the fracture–matrix interface have to be taken into account.

In part I of this paper we present a two–level multigrid approach based on hierarchical decomposition of the original equation and a special multigrid method involving additional corrections at the fracture–matrix interface in the smoothing step of the resulting matrix problem. It turns out in numerical experiments that the convergence of our two–level multigrid method is robust with respect to vanishing width of fractures and jumping coefficients.

2. GOVERNING EQUATIONS

We consider saturated Darcy flow in a confined aquifer. Incompressibility of the fluid and nondeformability of the fractured porous medium are assumed. Then the continuity equation

$$S_0 \frac{\partial h}{\partial t} + \nabla \cdot \underline{v}_f = f, \tag{1}$$

in combination with Darcy's law

$$\underline{v}_f = -\underline{\underline{K}}_f \cdot \nabla h \tag{2}$$

leads to a linear parabolic equation for the piezometric head h. S_0 represents the specific storage coefficient, t the time, $\underline{v}_f$ the Darcy velocity, f external sources and sinks and $\underline{\underline{K}}_f$ the hydraulic conductivity tensor. The coefficients of $\underline{\underline{K}}_f$ are uniformly bounded functions on Ω and $\underline{\underline{K}}_f$ is symmetric and uniformly positive definite. We will use the formulation with unknown pressure $p = \rho g (h - z)$ and given fluid density ρ, gravity g and geodetic altitude z. Furthermore, we will restrict ourselves to the steady state solution

$$\nabla \cdot (\underline{\underline{K}}_f \nabla p) + \rho g \nabla \cdot (\underline{\underline{K}}_f \nabla z) + \rho g f = 0 \tag{3}$$

3. HIERARCHICAL DECOMPOSITION AND ROBUST SMOOTHER

We consider the flow in the pressure-formulation (3). For simplification we assume homogenous Dirichlet boundary conditions.

Finite element discretisation. By multiplying the differential equation with an arbitrary v from the solution space $V = \{v \in H^1(\Omega) | v(x) = 0 \ \forall x \in \partial\Omega\}$, integrating over Ω and applying Greens formula we obtain the weak formulation

$$p \in V: \qquad a(p, v) = \ell(v) \qquad \forall v \in V, \tag{4}$$

with

$$a(p, v) := \int_\Omega \nabla p^{\mathrm{T}} \underline{\underline{K}}_f \nabla v \, dx \quad \text{and} \quad \ell(v) := \rho g \int_\Omega (fv + (\underline{\underline{K}}_f \nabla z)^{\mathrm{T}} \nabla v) \, dx. \tag{5}$$

As $\underline{\underline{K}}_f$ is symmetric, uniformly positive definite and uniformly bounded on Ω, the bilinear form $a(\cdot, \cdot)$ is symmetric, positive definite and bounded on V. Hence, for each $f \in L^2(\Omega)$ there exists an uniquely defined weak solution $p \in V$ (cf. e.g. *Braess(1997)*[4]).

For ease of presentation we only consider the 1D case, i.e. $\Omega = (-1, 1)$. 2D calculations will be reported later on. Starting with the grid $\mathcal{N}_0^\varepsilon$ as depicted in figure 1, we construct a sequence of grids $\mathcal{N}_0^\varepsilon \subset \mathcal{N}_1^\varepsilon \subset \cdots \subset \mathcal{N}_j^\varepsilon$ by bisection. The corresponding spaces of linear finite elements $\mathcal{S}_0^\varepsilon \subset \mathcal{S}_1^\varepsilon \subset \cdots \subset \mathcal{S}_j^\varepsilon$ will be used as a starting point for the construction of multigrid methods for the discretized problem

$$p_j^\varepsilon \in \mathcal{S}_j^\varepsilon: \qquad a(p_j^\varepsilon, v) = \ell(v) \qquad \forall v \in \mathcal{S}_j^\varepsilon \tag{6}$$

to be described below.

Hierarchical decomposition. We consider the hierarchical decomposition

$$\mathcal{S}_j^\varepsilon = \mathcal{S}_j^M \oplus \mathcal{S}_j^K \tag{7}$$

into the matrix space $\mathcal{S}_j^M$ and the fracture space $\mathcal{S}_j^K$. In our introductory example $\mathcal{S}_j^K$ is spanned only by the one nodal basis function $\lambda_{0,j}$ associated with the node x_0, while the matrixspace $\mathcal{S}_j^M$ is spanned by the nodal basis functions corresponding to $\mathcal{N}_j^M = \mathcal{N}_j^\varepsilon \backslash \{x_0\}$ (cf. figure 1). According to *Xu* [12] and *Yserentant* [13] the hierarchical decomposition (7) immediately induces the following successive subspace correction method.

Algorithmus 3.2 (Two level iteration)

given: $p_j^\nu \in \mathcal{S}_j^\varepsilon$

$$\text{solve:} \qquad v_j^M \in \mathcal{S}_j^M: \quad a(v_j^M, v) = \ell(v) - a(p_j^\nu, v) \quad \forall v \in \mathcal{S}_j^M \tag{8}$$

$$\text{solve:} \qquad v_j^K \in \mathcal{S}_j^K: \quad a(v_j^K, v) = \ell(v) - a(p_j^\nu + v_j^M, v) \quad \forall v \in \mathcal{S}_j^K \tag{9}$$

new iterate: $p_j^{\nu+1} = p_j^\nu + v_j^M + v_j^K$

Algorithm 3.2 is linearly convergent. Each iteration step requires the solution of the matrix problem (8) and of the fracture problem (9) with unknowns located in the interior of the fractures. Convergence is preserved if the exact solution is replaced by one step of suitable subspace correction methods applied to the two subproblems. The choice of these methods is discussed below.

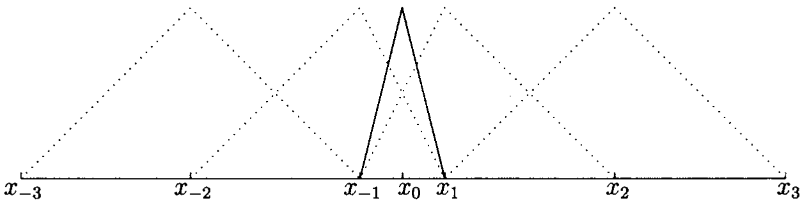

Figure 1. Hierarchical decomposition

Fracture–Problem. For our introductory problem the solution of (9) is trivial. In the 2D case triangulation of fractures by a coarse mesh $\mathcal{T}_0$ leads to long and thin elements. The number of unknowns located in the interior of the fractures is expected to be much smaller than the number of unknowns associated with the matrix. This suggests exact solution of (9) by a direct solver. Anisotropic multigrid with line relaxation (cf. *Wittum (1989)* [11] or *Apel und Schöberl (2000)* [1]) might be considered in more complicated situations.

Matrix–Problem. The construction of suitable iterative schemes for the matrix problem is more complicated. As a first step towards multigrid methods which are robust with respect to jumping coefficients and (in higher space dimensions) to almost degenerate elements, we now describe a multigrid method which will turn out to be robust for $\varepsilon \to 0$. Using the hierarchy of grids $\mathcal{N}_k^M = \mathcal{N}_k^\varepsilon \setminus \{x_0\}$ and the corresponding hierarchy of finite element spaces $\mathcal{S}_k^M$, $k = 0, \ldots, j$, we first consider the classical multigrid method with canonical restriction and prolongation and Gauß–Seidel smoother. For arbitrary intermediate iterate $w \in \mathcal{S}_j^M$ the correction associated with the node $x_{-1} = -\frac{\varepsilon}{2} \in \mathcal{N}_k^M$ (left fracture–matrix interface) on level k is given by

$$z_{-1,k}^\varepsilon = \frac{f(\lambda_{-1,k}) - a(w, \lambda_{-1,k})}{a(\lambda_{-1,k}, \lambda_{-1,k})}. \tag{10}$$

Here $\lambda_{-1,k} \subset \mathcal{S}_k^M$ denotes the nodal basis function on level k corresponding to x_{-1}. It is easily seen that $\varepsilon \to 0$ leads to $\|\lambda_{-1,k}\| = a(\lambda_{-1,k}, \lambda_{-1,k})^{1/2} \to \infty$ giving $z_{-1,k}^\varepsilon \to 0$. As coarse grid corrections at the fracture–matrix interface are vanishing, convergence rates of Gauß–Seidel multigrid deteriorate dramatically for $\varepsilon \to 0$. This property is typical for common multigrid methods.

In order to achieve robust convergence behavior for $\varepsilon \to 0$, we introduce an additional correction at the fracture–matrix interface associated with $\phi_{0,k}^\varepsilon = \lambda_{-1,k} + \lambda_{1,k}$ (cf. figure 2). The additional correction is

$$z_{0,k}^\varepsilon = \frac{f(\phi_{0,k}^\varepsilon) - a(w, \phi_{0,k}^\varepsilon)}{a(\phi_{0,k}, \phi_{0,k}^\varepsilon)}. \tag{11}$$

Note that $\phi_{0,k}^\varepsilon$ tends to the hat function $\phi_{0,k}^0$ as $\varepsilon \to 0$. This is a coarse grid nodal basis function for the reduced grid $\mathcal{N}_k^0 = \mathcal{N}_k \setminus \{x_{-1}, x_1\}$ and $z_{0,k}^0$ is the local Gauß–Seidel correction given by the Gauß–Seidel multigrid method as applied to the reduced problem

$$p_j^0 \in \mathcal{S}_j^0 : \qquad a^0(p_j, v) = \ell(v) \qquad \forall v \in \mathcal{S}_j^0. \tag{12}$$

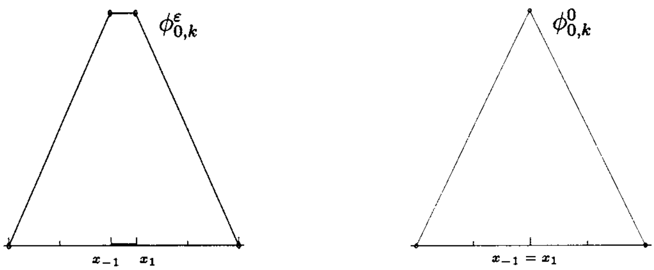

Figure 2. Additional coarse grid correction

The reduced problem (12) describes the situation for the case $x_{-1} = x_0 = x_1$, that is without fracture. Note that $p_j^\varepsilon \rightarrow p_j^0$ w.r.t. the energy norm holds uniformly in j as $\varepsilon \rightarrow 0$.

Multigrid method. Our final multigrid method is now obtained by replacing the exact solution of the matrix problem (8) in Algorithm 3.2 by one step of the multigrid method described above. The fracture problem (9) is solved directly.

The resulting multigrid method can be easily extended to higher space dimensions. For example, consider the crossing of two fractures in 2D. Then the additional correction of the form (11) is carried out for $\phi^{\varepsilon}_{0,k} = \lambda_{1,k} + \lambda_{2,k} + \lambda_{3,k} + \lambda_{4,k}$, where $\lambda_{i,k} \subset \mathcal{S}_k^{\mathcal{M}}, i = 1, \ldots, 4$ denote the nodal basis functions associated with the nodes x_i at the corners of the crossing.

4. EXAMPLES

To evaluate our two–level multigrid method we consider the following simplified case of (4) as a model problem (see figure 3)

$$\begin{aligned} -\underline{\underline{K}}_f \Delta p(x) &= f(x) && \text{for} \quad x \in \Omega \\ p &= C_{1,3} && \text{for} \quad x \in \Gamma_{1,3} \quad \text{with } C_i = \text{const} \\ \frac{\partial}{\partial n} p &= 0 && \text{for} \quad x \in \Gamma_{0,2}. \end{aligned}$$

The following convergence rates were computed for a multigrid V–cycle with one pre– and one post smoothing step in the matrix problem.
In figure 4 the convergence rates for different smoothers in the multigrid of the matrix problem of the hierarchical decomposition for a fixed number of unknowns (6821) and variable fracture width are displayed. As expected, the Gauß–Seidel smoother ('– – –') is not applicable for small ε: The convergence rates rapidly tend to 1 for vanishing fracture width. On the other hand, the convergence rates for our two–level multigrid method ('· · ·') seem to be robust with respect to the fracture width. We also tested the incomplete LU–decomposition (ILU, *Wittum*[11]) as a smoother in the multigrid of the matrix problem ('– · –·') but found no convergence for medium fracture widths. Note that the convergence rates of our two–level multigrid method tend to the convergence rates of classical Gauß–Seidel multigrid as applied to the reduced problem without fractures ('—').
Since algebraic multigrid methods where developed for similar examples, we will now compare the convergence behaviour of our method and of the algebraic multigrid method (*Ruge/Stüben* [10] and *Braess* [5]). We will investigate robustness with respect to frac-

ture width, jumps in the hydraulic conductivity and refinement depth.
Again we computed the convergence rates for the simple crossing (cp. figure 3) with a multigrid V–cycle with one pre– and one post smoothing step both for Gauß– Seidel multigrid with additional corrections (matrix problem) and for the AMG (complete problem).

The left picture in figure 5 shows the convergence rates for 26437 unknowns over the

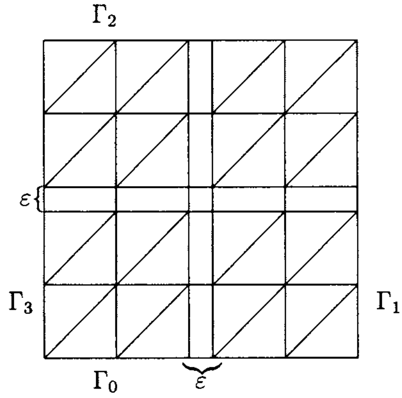

Figure 3. Domain with a simple crossing of two fractures (Coarse Grid of Matrixproblem)

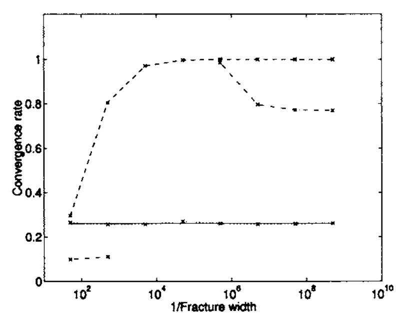

Figure 4. Convergence rates for small ε for different smoothers in the multigrid of the matrixproblem

fracture width ε. The algebraic multigrid method developed by *K. Ruge, J. W. Stueben* [10]('— — —') shows even better performance for wide fractures than our method ('···') but does not converge for smaller fracture widths. This might be due to roundoff errors or to the method itself. Another algebraic multigrid method by *Braess* [5] only converged in combination with a Krylov–method, e. g. BCGS. On the right picture we depict the convergence rates over the hydraulic conductivity in the matrix. Obviously neither the algebraic multigrid method nor our two–level multigrid has any difficulties with the jump in the hydraulic coefficients at the fracture–matrix interface.

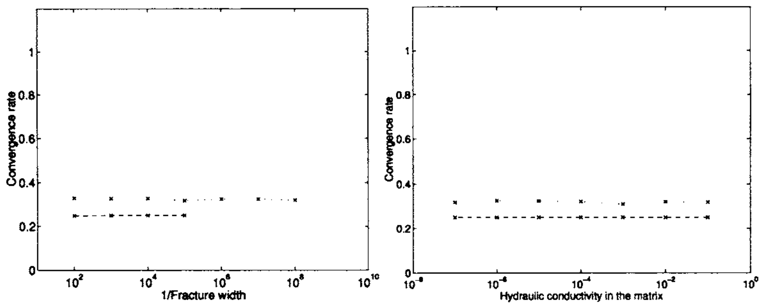

Figure 5. Convergence rates for small ε and large jumps in the hydraulic conductivity k_f in fracture and matrix

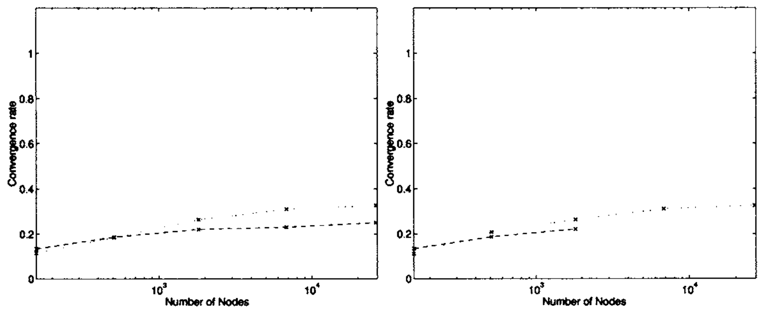

Figure 6. Convergence rates for varrying refinement depth, $\varepsilon = 10^{-5}$ left, $\varepsilon = 10^{-6}$ right

Figure 6 shows the convergence rates for an increasing number of unknowns. On the left the fracture width ε is slightly bigger (10^{-5}) than on the right (10^{-6}). It turns out that the algebraic multigrid method is not independent of the refinement depth inasmuch the smaller the fracture width, the earlier the algebraic multigrid method diverges. The convergence rates of our two–level multigrid method seem to saturate with increasing refinement.
All computations in this paper were done with the software toolbox MUFTE–UG (*Bastian et al.* [3] and *Helmig et al.* [7]).

5. CONCLUSIONS

We have seen in the numerical examples that usual multigrid methods do not work well for the extreme conditions in fractured porous media with equidimensional fractures. For example, the convergence rates of straightforward Gauß–Seidel multigrid rapidly tend to 1 with decreasing fracture width ε. Algebraic multigrid method, though faster for moderate ε, did not converge at all for small values of ε.
Our method turned out to be robust with respect to vanishing fracture width ε, strongly varying coefficients and vanishing mesh size. Mathematical justification is the subject of current work.
Future research will concentrate on extensions of our approach to mixed methods.

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REFERENCES

1. T. Apel und J. Schöberl. Multigrid methods for anisotropic edge refinement. Forschungsbericht SFB–Report No.00–19, Universität Linz, SFB F013 Numerical and Symbolic Scientific Computing, Juli 2000.
2. C. Barlag. Adaptive Methoden zur Modellierung von Stofftransport im Kluftgestein. Bericht Nr. 52, Institut für Strömungsmechanik und Elektronisches Rechnen im Bauwesen, Universität Hannover, 1997.
3. P. Bastian, K. Birken, K. Johannsen, S. Lang, K. Eckstein, N. Neuss, H. Rentz Reichert and C. Wieners. UG – A Flexible Software Toolbox for Solving Partial Differential Equations. Computing and Visualization in Science (1997) 1(1):27 – 40.
4. D. Braess. Finite Elemente. Springer, 1997.
5. D. Braess. Towards Algebraic Multigrid for Elliptic Problems of Second Order Computing (1995) 55:379–393.
6. R. Helmig. Multiphase Flow and Transport Processes in the Subsurface. Springer – Verlag, Heidelberg, 1997.
7. R. Helmig, P. Bastian, H. Class, J. Ewing, R. Hinkelmann, R. Huber, H. Jakobs and H. Sheta. Architecture of the modular program system MUFTE–UG for simulating multiphase flow and transport processes in heterogeneous porous media. In H. Thiergärtner, Hrsg., Mathematische Grundwassermodellierung – unkonventionelle Lösungen und Randbedingungen, Band 2 von Mathematische Geologie. CPress Verlag, Dresden, 1998.
8. P. Jamet. Estimation d'erreur pour des éléments finis droits presque dégénérés. R. A. I. R. O. , Série Analyse Numérique, 10, No. 3, p. 43–61 (1976).
9. L. Neunhäuserer, S. Gebauer, S. Ochs, R. Hinkelmann, R. Kornhuber and R. Helmig. Mehrgittermethoden und adaptive Euler–Lagrange–Verfahren zur Simulation von Strömungs- und Transportvorgängen in Kluftaquifersystemen. Report 01.11.1999 – 30.10.2001, DFG–Projekte Nr. Ko1806/2–1 und Nr. Hi640/1–1, Universität Stuttgart, Institut für Wasserbau, Lehrstuhl für Hydromechanik und Hydrosystemmodellierung and Freie Universität Berlin, Fachbereich Mathematik und Informatik, Institut für Mathematik II (2001).
10. J. W. Stüben, K. Ruge. Algebraische Mehrgittermethoden In S. McCormick, ed., Multigrid methods. Frontiers in Applied Mathematics, 3. Philadelphia: Society for Industrial and Applied Mathematics (SIAM), XVII, 282p.,1987.
11. G. Wittum. On the Robustness of ILU-Smoothing. SIAM J. Stat. Comput, 10:699 – 717, 1989.
12. J. Xu. Iterative methods by space decomposition and subspace correction. SIAM Review, 34:581–613, 1992.
13. H. Yserentant. On the multi-level splitting of finite element spaces. Numer. Math., 49:379–412, 1986.