The MOWIN concept in hydraulic and transport modeling in the Coastal Aquifer Test Field (CAT-Field) between Bremerhaven and Cuxhaven, Germany

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INTRODUCTION

For many areas with intense use of groundwater resources it is desirable to build up a high resolution groundwater data base for management and quality prediction. These data bases should be updated continuously by model calculations. Models for this purpose will typically be very large and need more random access memory (RAM) than available on PCs. Therefore the Moving Window (MOWIN) technique was developed to reduce the RAM requirements of high resolution flow and transport models on a regional scale. For this purpose MOWIN utilizes domain decomposition methods on PCs. Similar techniques are widely used for parallel computing since a number of years [e.g. Byrde et al., 1999; Dou & Phan-Thien, 1998; Farhat, 2000].

The region of the CAT-Field [Kessels et al., 2001] between Bremerhaven and Cuxhaven, Germany, extending over an area of approximately 1800 km², is the first area to be simulated with MOWIN. Simulation of the groundwater regime should be performed with a lateral grid spacing of 50 m, which is normally used for geological data processing. For a sufficient vertical resolution (50 layers) about 3.6·10⁷ cells are therefore necessary. For the coastal aquifer also salt transport and density driven flow processes have to be included into the model.

Since reduction of RAM requirements usually is realized under the disadvantage of increasing calculation times optimization of calculation speed is an important aim of the project. Several techniques like overrelaxation, optimized calculation sequences, hierarchical grid coarsening (a multigrid algorithm), optimized window sizes and stepwise improvement of the convergence criteria were implemented into the model. Extensive tests with a 2D-MovingWindow were carried out for the CAT-field to quantify the benefits of these methods.

THE PRINCIPLE OF MOWIN

The principle of MOWIN is an overlapping domain decomposition method: To solve an initial and boundary condition problem on a large model region will be performed by iteratively solving the problem on a number of smaller regions (“windows”). All these regions together have to cover the complete model region and they must overlap each other (Fig. 1). For all window boundaries arising inside the original model region Dirichlet type boundary conditions are assumed. The window is moved over the model region until a criterion for convergence is met. MOWIN is designed for structured meshes.

Structurally, this method is a kind of generalized relaxation algorithm and for a window size of 3 nodes in any grid direction it is in fact identical with the normal relaxation method. Therefore, it is not unexpected that the convergence behavior of the MOWIN shows a similar exponential decrease of the residual with increasing
number of iterations as the relaxation method does. This means that the MOWIN method does not cause any numerical errors additional to those caused by the used discretisation and solver inside the windows, except termination errors which can be minimized to any desired level by increasing the number of iterations.

The reduction in RAM requirements is mainly done through the fact, that all arrays needed for the solution of the differential equations (especially the coefficient matrix of the nodal equation set) are necessary only for the window. The RAM requirements can be reduced further at the cost of increasing calculation time by
saving the actual values of the status variables for the complete model region in a file instead of keeping them in RAM.

**OPTIMIZATION OF CONVERGENCE SPEED**

Besides the problem of huge RAM-requirements the possibilities of calculating high resolution regional groundwater models are limited by the amount of calculation time needed for very large models. Therefore, a number of methods for enhancement of convergence speed were implemented and tested. For this purpose a simplified, stationary, homogeneous 2D-flow-model of the CAT-field was used. It consists of about $7.5 \cdot 10^5$ nodes and was calculated on a PC (600 MHz, 256 MB) utilizing a simple relaxation solver inside the window. For any method a number of calculations was carried out which was sufficient to analyze the dependency of calculation time from the optimization parameters and from calculation accuracy.

**Overrelaxation**

Since a relaxation solver was used in these tests the well known overrelaxation method was applied. Fig. 2 shows that overrelaxation strongly reduces calculation time with a pronounced optimum at an overrelaxation factor of about 1.95. The increase in convergence speed is approximately one decade. Unfortunately, the opti-

![Figure 2: The influence of overrelaxation on the calculation time depending on calculation accuracy.](image)

Fixed calculation parameters: Regular calculation sequence, grid coarsening factor 4 in two levels, 10197 nodes per window, accuracy improvement factor 0.316.
mum overrelaxation factor is very close to the critical value of 2 above which the method diverges, and therefore a value even slightly above the optimum results in a very poor convergence behavior. As the optimum value depends on the model problem and cannot be predicted reliably overrelaxation factors between 1.8 and 1.9 should be a cautious and reasonable guess for this optimization parameter.

The utilization of an overrelaxation solver is not essential for the MOWIN method and for practical use more efficient solvers like gradient methods will replace it.

**Optimization of the calculation sequence**

The regular calculation sequence where the window is moved over the model region in rows or columns with alternating directions is similar to the traditional IADI-scheme [Peaceman & Rachford, 1955]. The idea of the optimization of the calculation sequence is to concentrate the calculation effort at any time to those areas where it is really needed, this means where the state of the calculation is far from fulfilling the chosen convergence criteria. This approach always chooses that window for calculation that shows the largest changes in its Dirichlet boundary conditions since its last calculation (Fig. 3). To initialize this method, all windows have to be calculated once in a regular sequence before changing to the optimized process. The optimization of the calculation sequence usually improves convergence speed by 50 to 100%.

**Hierarchical grid coarsening**

Another approach to reduce calculation time is the implementation of multigrid techniques, which were developed in a great variety during the last decades [e.g. LeBorne, 1999; Dahmen et al., 1999; Hackbusch, 1998; Kornhuber, 1997]. The technique used here is a hierarchical coarsening of the grid to generate an improved “initial condition” for the time consuming iterative calculation on the fine grid by a relatively fast precalculation on a coarsened and therefore much smaller grid. This is
especially useful for the distribution of effects of long-wave information, e.g. originating from boundary conditions.

The grid coarsening is performed by merging a chosen number (the “grid coarsening factor”) of cells per grid direction in one coarser cell with averaged state variables, material properties and boundary conditions. This can be done in a hierarchical way, that means a coarsened grid can be coarsened once again. Usually it is not useful to employ more than two levels of grid coarsening since higher levels only result in negligible additional changes of convergence speed.

The influence of this technique on calculation time strongly depends on the importance of long-wave phenomena in the model problem. For groundwater modeling on a regional scale boundary conditions like groundwater recharge or the influence of topography typically include relevant long-wave characteristics. Therefore, the results of the test calculations for the influence of multigrid technique on calculation time carried out for the CAT-field can be regarded as representative for many regional models. It was found that the dependency of calculation time from the grid coarsening factor shows a typical optimum characteristic, which is nearly independent from the chosen accuracy (Fig. 4). The calculation time could be reduced by a factor of 2.5 compared to calculations without multigrid algorithm.

Figure 4: The influence of hierarchical grid coarsening on the calculation time depending on calculation accuracy. A grid coarsening factor 1 denotes no use of multigrid technique. Fixed calculation parameters: Overrelaxation factor 1.8, optimized calculation sequence, two levels of grid coarsening, 10197 nodes per window, accuracy improvement factor 0.316.
Optimization of window size

Obviously the size of the windows will strongly effect the calculation time necessary for the solution of a model problem. Since the use of a domain decomposition technique like MOWIN increases the complexity of the problem, one might expect that a calculation without domain decomposition (which is equivalent to a window size equal to the size of the complete model) will be the fastest. Nevertheless the tests carried out reveal a different behavior: Calculation time shows a broad minimum for an intermediate window size and increases three to four times for very small or very large windows (Fig. 5). This means that MOWIN is not only a tool to reduce RAM requirements of very large models but can also be used as a means of convergence enhancement.

Note, that the influence of window size on calculation time strongly depends on the equation solver used inside the window, because any solver has a different time requirement versus window size characteristic. Furthermore the hardware and settings of the operating system can have great effect on the analyzed behavior, since the necessity to use virtual memory by swapping will reduce calculation speed significantly, when the window size exceeds a machine-dependent upper limit.

Figure 5: The influence of window size on the calculation time depending on calculation accuracy. The maximum window size used is 745841 nodes and represents a calculation without MOWIN.
Fixed calculation parameters: Overrelaxation factor 1.95, optimized calculation sequence, grid coarsening factor 4 in two levels, 10197 nodes per window, accuracy improvement factor 0.316.
Stepwise improvement of the convergence criteria

For nonlinear differential equations like the density-dependent flow and transport equation the solution for any window will be calculated by using iterative methods. Even in case of linear differential equations iterative solvers are preferable, because the performance and the numeric behavior of direct methods is very poor for larger matrices. Therefore, in virtually all applications of the MOWIN concept two iterative processes will interact, namely the equation solving inside any window and the MOWIN procedure itself. In this case calculation time not only depends on the intended accuracy of the solution but is also effected by a stepwise improvement of the convergence criteria for these two processes.

Test simulations have shown that it is not useful to apply the convergence criteria, which are intended for the final result, inside any window just from the beginning of the calculation process. Starting with less strict convergence criteria and improving them stepwise by a chosen “accuracy improvement factor” turned out to be a reasonable approach for saving calculation time (Fig. 6). The observed benefit of this method was a reduction of calculation time to approximately a half.

Figure 6: The influence of stepwise improvement of the convergence criteria on the calculation time depending on calculation accuracy. An accuracy improvement factor 0 denotes no stepwise improvement of the convergence criteria.
Fixed calculation parameters: Overrelaxation factor 1.95, optimized calculation sequence, grid coarsening factor 4 in two levels, 10197 nodes per window.
Summary of methods for convergence improvement

All methods discussed here could be proved to be useful for an acceleration of convergence speed. Whereas the overrelaxation is specific for the utilization of a relaxation solver inside the windows, the other four methods can be employed in any MOWIN application. Tab. 1 gives an overview of their efficiency and the optimum parameter values found for the CAT-field 2D-simulation. Since the effects of these methods interact the maximum enhancement of convergence speed is less than the product of the maximum acceleration factors found for these five techniques. Nevertheless, the cumulative acceleration is approximately 100.

<table>
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<th>method</th>
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<td>optimization of calculation sequence</td>
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<tr>
<td>stepwise improvement of convergence criteria</td>
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</table>

Table 1: Comparison of the tested techniques for the reduction of calculation time of MovingWindow applications.

SUMMARY

MOWIN is an overlapping domain decomposition technique which was developed to reduce the RAM requirements for the solution of very large, high resolution regional scale flow and transport models. It represents a type of generalized relaxation method and shows a robust convergence behavior.

Five methods to accelerate convergence were implemented, namely overrelaxation, optimization of the calculation sequence, a multigrid-type hierarchical grid coarsening, optimized window sizes and the stepwise improvement of the convergence criteria. All five methods were found to be useful to enhance the performance of the MOWIN. They are fully compatible among each other and make it possible to reduce the calculation times by two orders of magnitude.

A three-dimensional multi-component flow and transport model MOWIN_3D is under development. It uses a gradient type solver and permits to control the extent of overlap between neighboring windows flexibly for further enhancement of convergence speed.

References


**Keywords**: Numerical modeling, domain decomposition, multigrid, convergence acceleration, groundwater model.

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