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CWI/Shell colloquium adaptive grid techniques for time-dependent partial differential equations

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CWI/SHELL COLLOQUIUM ADAPTIVE GRID TECHNIQUES FOR TIME - DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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This report contains the summaries of all lectures presented at the CWI/Shell Colloquium 'Adaptive Grid Techniques for Time-Dependent Partial Differential Equations'. This colloquium was held at CWI and the Koninklijke/Shell-Laboratorium in Amsterdam during the year 1988.

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PREFACE

During recent years, a great deal of interest has emerged on the use of adaptive approaches and techniques in the field of numerical partial differential equations. Unlike the situation in the field of ordinary differential equations, where adaptive techniques are widely used and have been implemented in general purpose software, the state of the art in the field of partial differential equations is far less developed. This is not surprising since the latter field is much more complex and diverse. Recognizing the importance of adaptivity, the Numerical Mathematics Department at CWI and the Koninklijke/Shell-Laboratorium in Amsterdam organized a "Colloquium on Adaptive Grid Techniques for Time-Dependent Partial Differential Equations". The aim of this colloquium was to draw attention to the growing interest in adaptive techniques and to learn about recent developments. For this purpose a number of well-known specialists from the Netherlands and from abroad were invited to present lectures. The success of the colloquium was due principally to these speakers. To all of them we extend our sincere thanks and appreciation.

December 1988

R.M. Furzeland, J.G. Verwer

LIST OF LECTURES

Dr. M.J. Baines, The University of Reading, U.K.
Grid Adaptation via Residual Minimisation.

M. Berzins, School of Computer Studies, The University, Leeds, U.K.
Global Error Estimation in the Method of lines.

Adaptive Mesh Algorithms in the Method of Lines.

J.E. Flaherty, Rensselaer Polytechnic Institute, Troy, New York
Adaptive Methods for Time-Dependent Partial Differential Equations.

R.M. Furzeland, Koninklijke/Shell Laboratorium, Amsterdam
Adaptive Space and Time Gridding - A Lagrangian Finite-Difference Approach with the Method of Lines.

P. Michielse, TU Delft
Parallel Adaptive Reservoir Simulation

K. Miller, University of California, Berkeley, USA
Moving Node Finite Element Methods for Problems with Sharp Moving Fronts.

Recent Developments with the Moving Finite Element Method in Two Dimensions.

L.R. Petzold, Lawrence Livermore National Laboratory, Livermore, California
Observations on Some Adaptive Moving Mesh Methods for One-Dimensional Systems of Partial Differential Equations.

Adaptive Moving Grid Method for One-Dimensional Systems of Partial Differential Equations and its Numerical Solutions.

J.E. Romate, Waterloopkundig Laboratorium, Emmeloord
Time-dependent Grid Generation for a 3-D Panel Method.

G.H. Schmidt, Koninklijke/Shell Laboratorium, Rijswijk
Adaptive Local Mesh Refinement and Multi-Grid in Numerical Reservoir Simulation.

W. Schönauer, Rechenzentrum der Universität Karlsruhe, BRD
Principles of Error Control and Selfadaption for the Solution of Elliptic and Parabolic PDEs

J.G. Verwer, CWI
An Adaptive Moving Grid Method for One-Dimensional Systems of Partial Differential Equations.

P.A. Zegeling, CWI
A Numerical Method of Lines Study of the Moving Finite Element Method

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Grid Adaptation via Residual Minimisation

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In recent years there has been much interest in the quality of the computational grids needed to resolve the numerical solution of mathematical equations describing physical processes. Many workers are presently using finite element and finite difference methods on irregular grids in their calculations, and the construction (and reconstruction) of these grids together with the quality of the solutions obtained on them is becoming a major consideration. Whilst the original motivation for irregular grids was economy of gridpoints, particularly in regions of little physical interest, it is now realised that for some problems sufficient resolution may be unobtainable practically in any other way. At the same time it is clear that considerable care is required in the manipulation of grids to ensure that the intentions of the programmer are realised, in particular that the solution is not degraded by the character of the grid.

One approach is automatic deformation of the grid, either during evolution of the physical processes or as part of an iteration towards an optimal grid. A mechanism for adapting the grids is necessary, two examples being equidistribution and residual minimisation. Here we concentrate on residual minimisation, which exhibits a remarkable structure and can be analysed in detail to predict the consequences of its use as a grid adapter. Penalty functions can be added to the mechanism if desired.

For time dependent problems the residual minimisation technique using finite elements is known as the Moving Finite Element method, while for steady problems a Jacobian iteration may be constructed which as the same structure.

Results are presented in which the Jacobian method is used to find finite element solutions of a quasi one-dimensional flow in a nozzle where both the solution and the grid are determined simultaneously.

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Adaptive Mesh Algorithms and Global Error Control in the Method of lines.

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The talk is concerned with the development of efficient and accurate integration algorithms in the method of lines . Three essential features of such an algorithm are a means of controlling the spatial discretisation error by remeshing, a variable order/variable step time integration algorithm and a means for automatically balancing the space and time discretisation errors. In the talk it is hoped to show how the ideas of the adaptive space remeshing scheme of Babuska and Bietermann [1] can be combined with the global error estimator of Berzins [2] in an algorithm which is adaptive in both space and time and which attempts to monitor (and hopefully control) the global error.

The starting point for the error balancing algorithm is the efficient global error indicator of Berzins [2]. The time integration strategy is considered in the light of this indicator and it is shown how to develop a technique which maintains the temporal error below the level of ths space error. This is achieved by requiring that the local time error per unit step is balanced against a fraction of the term which consists of the local contribution of the existing space errors and of the local contribution of the p.d.e. space truncation error. The implementation of the new technique in a stiff solver, is described and the approach is compared to two other techniques for balancing space and time errors, [4], [5] on a number of test problems.

This work will then be linked with the algorithm which adapts the space mesh locally in order to control the energy norm of a given error estimate. The new algorithm is applied to test problems and the results compared with the more straightforward remeshing algorithm inside the SPRINT software [3] .

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Adaptive Methods for Time-Dependent Partial Differential Equations

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We discuss adaptive mesh moving and local refinement procedures for solving vector systems of time-dependent partial differential equations in one and two space dimensions. Each adaptive algorithm contains a basic finite element or finite volume procedure to compute approximate solutions of the differential system on a given mesh, an error indication procedure to decide which regions of the problem domain require greater solution resolution, and an adaptive feedback strategy to generate a finer mesh when accuracy is not sufficient. Finite element and finite volume procedures utilizing piecewise polynomial approximations in space and either explicit or implicit finite difference methods in time will be discussed.

Temporal mesh refinement strategies can either be local or global. Global temporal refinement strategies lead to adaptive methods of lines. Such schemes can fully utilize the power of existing software for solving initial value problems for ordinary differential equations. Local temporal refinement strategies, on the other hand, offer the promise of greater efficiency by using different time steps on different portions of the problem domain.

Spatial refinement strategies are grouped into three categories: h-refinement where a mesh is refined, but the order of the finite volume or finite element method is unchanged; p-refinement where the same mesh is used for methods of increasing order of accuracy; and r-refinement where the structure of a mesh is changed without either increasing the number of cells or the order of the method. Mesh refinement can further be classified as being cellular or noncellular. With cellular refinement, the computational cells of finer meshes are properly nested within the boundaries of cells of coarser meshes; thus, simplifying the transfer of solutions between meshes having different spacings. With noncellular refinement, the cells of finer meshes can overlap those of coarser ones. Mesh structures can be kept uniform and this may offer improved performance on computers having vector processors. In either case, a tree structure, with finer grids regarded as offspring of coarser ones, is used to manage the data associated with the refinement process. Several specific cellular and noncellular refinement techniques will be presented. The use of these procedures in combination with r-refinement and p-refinement techniques and with mesh generation codes will also be discussed.

Error indicators based on estimates of the local discretization error are used to control the adaptive refinement process. Several error estimates for finite element methods that utilize a hierarchic p-refinement approach will be presented. There is an interesting dichotomy between the errors in odd- and even-order finite elements. In particular norms, errors in odd-order finite element solutions are concentrated near element edges, whereas the errors in even-order methods are principally in element interiors. These results are used to improve the computational efficiency of the error estimates.

Computational results will be presented for a variety of academic and practical problems involving compressible flow and combustion.

Adaptive Space and Time Gridding

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The Method of Lines is a powerful tool for the solution of coupled, non-linear partial differential equations (p.d.e.s). It gives efficient and accurate time integration based on proven time integrators such as the variable-step, variable-order Gear's method. The choice of space grid is left to the user and is the main source of error and inefficiencies. An adaptive space grid will give a more efficient solution as long as the regridding scheme does not force the time integrator to use much smaller time steps or too many extra Jacobian evaluations. A Lagrangian type scheme has these benefits and, further, does not require interpolation from old to new grids.

In the Lagrangian approach the governing p.d.e.s are rewritten to integrate in time along trajectories $x_i(t)$. For hyperbolic problems the aim is to make these trajectories follow the characteristic directions. Subsidiary differential equations for $x_i(t)$ have to be constructed and solved. Two related methods to produce smooth $x_i(t)$ movement are those of Flaherty & Petzold and Dorfi & Drury. The Lagrangian idea can be augmented with occasional 'rezoning' i.e. at certain time values one requests a complete change of the grid spacing and number of points. However, this is expensive since it necessitates a complete integrator restart and solution interpolation.

In this talk, the Lagrangian method will be applied to diffusion-convection-reaction problems such as flame propagation and the interaction of two pulses. Further, solutions will be given for the classic shock-tube problem where the Euler hyperbolic equations have to be solved.

PARALLEL ADAPTIVE RESERVOIR SIMULATION

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In oil–industry, it is common use to simulate the exploitation of oil–reservoirs by means of a numerical method. In many cases, such a numerical method is simulating the so–called injection – production – mechanism: somewhere in the reservoir water is injected, while somewhere else oil is produced. After some period of time, however, oil together with water will be produced.

The most simple modelproblem for such a simulation consists of a two–dimensional square oil–reservoir, with injection of water in one corner and production of oil in the opposing corner. An important property in reservoir simulation is the permeability of the porous medium, which may be different for oil and water.

After the injection there will be a moving front of water towards the production–well. To mark this front, the numerical method may use a local grid–refinement technique. Since the front is moving, this grid–refinement (and grid–unrefinement, when the front has passed) should be dynamical: the grid–update should be done adaptively.

In [1], a mixed finite element method is used to discretize the underlying partial differential equations. The elements are squares: blocks. The local grid refinement, as described in [1], is based on the computation of saturation–gradients for neighbouring blocks. If these gradients are too large, then they cause refinement; if they are small enough, then they cause unrefinement.

In this talk, we will focus on parallel aspects of the numerical reservoir simulation problem. After a brief introduction and description of the underlying equations and discretization, we first consider the sequential reservoir simulation algorithm. Afterwards, we discuss our parallellization method, which is based on the use of a small number of quite powerful processors. The computational domain is split into a number of subdomains, which equals the number of processors. Each subdomain is assigned to one processor.

This domain decomposition method introduces internal boundaries between the subdomains. These internal boundaries may be described by a datastructure, which is as local as possible (i.e. restricted to subdomains). The definition of a well–suited data-structure is complicated by the adaptive grid–refinement technique.

Furthermore, we will discuss the parallel algorithm. In this parallel algorithm, we have

to make a distinction between computational and communicational work. Since the waterfront is moving through the complete domain, there has to be some interaction between neighbouring subdomains.

We have implemented the parallel algorithm on an NCube, a parallel local memory computer based on the hypercube architecture. We first describe some characteristic features of the hypercube architecture, whereafter some timing results of the parallel algorithm on the NCube are given.

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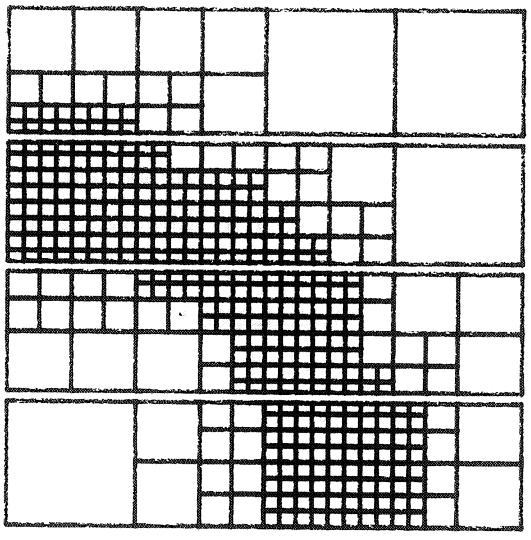

Moving node finite element methods for problems with sharp moving fronts

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Abstract: The Moving Finite Element method gives one very general and robust recipe for moving the nodes continuously in a time evolving problem. It is designed especially for those problems which develop shocks and other sharp moving fronts. By allowing the nodes to concentrate and move automatically, one can often solve such problems with greater accuracy, far fewer nodes, and far larger time steps than would otherwise be the case. We will introduce the method in 1 and 2 dimensions, tell of some generalizations (such as gradient-weighting) which greatly increase robustness, and show graphics of applications to a wide variety of systems of PDE's.

Recent developments with the moving finite element method in two dimensions.

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Abstract: We will discuss recent computational experience and plans for the future in the development of general purpose moving grid MFE methods in two dimensions. Applications to be discussed include the semiconductor equations (the system of transient PDEs for the voltage and the electron density in semiconductor devices), the Buckley-Leverett equations (the system of saturation and pressure equations for water flooding in oil reservoirs), and the equations for highly nonlinear diffusion of arsenic ions in the manufacture of semiconductor chips. We will also discuss the prospect for explicit versions of MFE for certain purely hyperbolic problems, based on the "local" MFE results of Walthen and Baines.

Observations on Some Adaptive Moving Mesh Methods for One-Dimensional Systems of Partial Differential Equations

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In this lecture we outline several moving grid strategies for the solution of one-dimensional systems of partial differential equations, along with some of their strengths and limitations. We concentrate on moving mesh methods arising from two distinct philosophies. One class of methods is designed to minimize a function of the PDE solution which is derived from spatial error estimates or geometrical considerations. The second class of methods is designed to choose the moving mesh based on minimizing the time rate of change of the solution in the moving coordinates. We examine some of the regularizations which have been suggested to increase the robustness and efficiency of these moving mesh methods. We discuss the solution by the code DASSL of the systems of differential algebraic equations which result when moving mesh systems are discretized in space. We compare the methods and show by example the effects of the different strategies.

An Adaptive Moving Grid Method for One-Dimensional Systems of Partial Differential Equations and its Numerical Solution

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In this lecture we examine a scheme for choosing a moving mesh based on minimizing the time rate of change of the solution in the moving coordinates. We show how to apply this method to systems where the time derivatives cannot be solved for explicitly, writing the moving mesh equations in an implicit form. We give a geometrical interpretation of the moving mesh equation which exposes some of its weaknesses, and suggest some modifications based on this interpretation which increase the efficiency of the scheme.

Upon discretization of the original PDE system coupled with the moving mesh equations, a system of differential/algebraic equations (DAEs) is generated. We discuss the solution of this system using the code DASSL, and show how changing the error estimate for time step selection from the usual strategy can significantly reduce the computation time. We introduce a new DAE code, DASPK, which combines the time integration methods of DASSL with the preconditioned GMRES method for solving large sparse linear systems. We discuss the possibilities for preconditioners and the implications for the linear system solution of various formulations of penalty functions in the moving mesh equation. Finally, we present the results of some numerical experiments on reaction-diffusion equations which illustrate how well the resulting methods work.

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AN ADAPTIVE MOVING GRID METHOD FOR ONE-DIMENSIONAL SYSTEMS OF PARTIAL DIFFERENTIAL EQUATIONS

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This lecture deals with a general method for the numerical solution of initial-boundary value problems for systems of PDEs in one space dimension. The class of problems considered have the form

$$u_t = L(u), \quad x_L < x < x_R, \quad t > t_0,$$

$$u(x,0) = u^0(x), \quad x_L < x < x_R,$$

$$g_L(x, t, u(x), u_x(x)) = 0, \quad x = x_L, \quad t > t_0,$$

$$g_R(x, t, u(x), u_x(x)) = 0, \quad x = x_R, \quad t > t_0,$$

where the spatial operator L is supposed to be of second order. Many problems from physics can be reduced to the solution of such coupled systems. Since most of these cannot be solved with analytical tools, numerical methods are indispensable. In recent years, several sophisticated MOL (Method of Lines) packages have been developed for one-space dimensional PDE systems. These packages greatly benefit from the very successful developments of automatic ODE solvers for stiff systems. MOL packages integrate in a semi-automatic way in the sense that they automatically adjust the time stepsizes, but use a fixed, a priori chosen space grid for the entire calculation. Depending on the degree of spatial activity, such an a priori chosen space grid is usually equispaced or mildly nonuniform. In many cases this semi-automatic approach works very satisfactorily. Notably for problems in which the solution does not exhibit a high degree of spatial activity, but also for problems where regions of rapid variation in space do not move when time evolves (stationary layers). However, for solutions possessing sharp moving spatial transitions, like travelling wavefronts or emerging boundary and interior layers, a grid held fixed for the entire calculation can be computationally inefficient, since this grid readily must a large amount of nodes. In such cases, methods which adjust automatically both the space and the time stepsizes are usually more efficient in resolving critical regions of high spatial and temporal activity. Methods and codes which operate this way, belong to the realm of adaptive or moving grid methods.

The moving grid method we discuss is of the finite difference, Lagrangian type. The method has been designed for the efficient computation of solutions containing sharp spatial and temporal transitions, e.g. typical solutions of problems arising in combustion modelling. Of course, the method can be applied to compute less difficult solutions. However, in these cases it is likely that it will operate less efficiently than the above mentioned MOL codes. It is assumed that any initial-boundary value problem under consideration is meaningful in the sense that it does possess a unique solution. However, since we suppose that the spatial operator L is of second order, truly discontinuous solutions (shocks), as arising in purely hyperbolic systems, are excluded.

The work presented is a continuation of that of our two earlier contributions [1,2] in which we have studied various finite difference, Lagrangian type moving grid schemes. These schemes are 'intermediate' to the so-called static regridding methods, where nodes remain fixed for intervals of time, and continuously moving grid methods, where the space node movement and the PDE integration are fully coupled (as in the moving finite element method). In our approach, the computation of the moving grids and the solution on these moving grids are carried out separately, while the nodes are moved at each time step. We here report on our first attempt [3] to supply the most successful one with full adaptivity capabilities (variable stepsizes both in time and space) and, ultimately, to implement the resulting algorithms into a user oriented automatic code. Apart from the obvious efficiency requirement, such a code should be easy to use and applicable to a wide variety of problems, like current MOL codes, so that comparisons with algorithms and codes based on other approaches are possible. In recent years the interest in adaptive grid techniques has increased enormously. However, despite the fact that we are dealing with the relatively simple 1D-case, one observes at the same time that in the literature hardly any comparisons are made and that easy-to-use automatic codes are, as yet, hard to find. The availability of codes is important for a proper assessment of promising developments.

At each integration step two error monitors are computed. These errors monitors are rather simple and can be implemented in a fairly straightforward manner. One of these governs the time step selection and the other the location and, eventually, the number of space nodes. Thus the method not only automatically adjusts the space grid to regions of high spatial activity, but also provides a facility to adapt the number of nodes in order to meet a user specified tolerance. This adaptation is embedded in the generation of new space nodes at the forward time level, which is based on equidistribution of the second space derivative. We should remark that we give the variable time step selection a higher priority, since already in the case of a fixed number of nodes the space mesh is automatically adapted. Further, a change in the number of nodes normally disrupts the Lagrangian time stepping process a bit. Another facility of our algorithm is that one has the possibility to select for each different PDE component a different space grid. Herewith one can avoid the use of finely meshed zones in regions where, componentwise, a fine mesh is not needed. The price to be paid for this facility are additional overhead costs originating from somewhat more complicated linear algebra (sparse matrix solver) and extra interpolation tasks. It should be mentioned that the need for interpolation imposes a restriction on the use of different, moving space grids, and that, in this connection, some care should be exersised in using this facility in order not to loose the anticipated advantages.

Above we have used the term error monitor instead of error estimator in order to emphasize that the quantities involved are not estimates of genuine local errors. The error monitors are thus heuristic. However, they provide cheap means for efficiently computing rapidly varying solutions of a widely different nature by keeping both the number of

space nodes and the number of time steps at a fairly acceptable level.

During the lecture we first outline the underlying Lagrangian method of solution of our fully adaptive moving grid procedure. Next we discuss the actual regridding technique and the two error monitors which govern the time step and number of space nodes selection. If time permits, we shall also discuss the possibility of using different moving grids for different PDE components. Further we shall present results of extensive numerical testing on a set of known sample problems from existing moving grid literature, including two problems from combustion theory. We conclude the lecture with some final comments and conclusions.

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Time-dependent grid generation for A 3-D panel method

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In the past ten years integral equation techniques have been applied with considerable success to the simulation of nonlinear water waves in two dimensional models. After Longuet-Higgins and Cokelet's paper [1], in which wave deformation on water of infinite depth was considered, this numerical technique obtained much attention, and several extensions and alternative integral equation methods have been developed.
The free surface model is defined by the following set of equations:

$$\nabla^2 \phi = 0 \qquad \text{in } \Omega \tag{1}$$

$$\frac{D\underline{x}}{Dt} = \nabla\phi \qquad \text{at } S_f \tag{2}$$

$$\frac{D\phi}{Dt} = \frac{1}{2}(\nabla\phi)^2 - gz \qquad \text{at } S_f \tag{3}$$

where the fluid motion is described by the velocity potential ϕ throughout the domain Ω, and the free surface is denoted by S_f.

The aim of this presentation is to show some aspects of the extension of the integral equation technique to the simulation of time-dependent nonlinear waves in three dimensions.
The 3-D panel method which is used for solving the Laplace equation with appropriate boundary conditions, is based on Green's third identity:

$$\phi(\underline{x}) = \iint_S \frac{\partial\phi}{\partial n} G - \phi \frac{\partial G}{\partial n} \, dS \tag{4}$$

Higher order approximations are used for the singularities and the panel geometry, resulting in an efficient and accurate panel method. See [2] for more details.

Here we focus on some of the specific problems related to the numerical generation of the computational grid, needed for the solution of (1)-(3).

Geometric modelling

For integral equation methods only the boundary S of the fluid domain has to be discretized. Here, in analogy to field discretization methods the boundary S is decomposed into subsurfaces, which can be mapped one-to-one onto a rectangular computational domain.
It is assumed that each subsurface is given by a set of points in space, ordered in an (m x n) network. These points then serve as input data for a surface approximation routine, e.g. a standard bicubic spline interpolation routine.
However, in the model considered a time-dependent boundary is involved. A part of that boundary, such as the bottom and solid walls, is treated Eulerian, whereas another part, the free surface, is treated using a Langrangian description. On a new time-level the boundary is known only in a disrete set of points, and because of the mixed Eulerian-Lagrangian treatment, the surface representations cannot be recovered from this discrete set on the new time level in a straightforward manner, but special procedures are needed instead.

Numerical grid generation

In this case the grid generation problem is restricted to the generation of a surface grid (instead of a volume grid), but the time-dependency of the geometry, and therefore of the grid, leads to the necessity of constructing a fully automatic, adaptive grid generator.
Also, despite the fact that the computer program runs on a Cray X-MP, the 3-D simulation does require special attention with respect to the use of core and computing time, also for the grid generation part.
A short outline is given of some possible grid generation systems. This includes algebraic and elliptic grid generation systems for regular grids. Also some problems connected with the implementation of an adaptive method are discussed.
Numerical results will be presented of the present work on both the geometric modelling part and the grid generation system.

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ADAPTIVE LOCAL MESH REFINEMENT AND MULTI-GRID IN NUMERICAL RESERVOIR SIMULATION

by

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Improvements of the accuracy of the mathematical methods in numerical reservoir simulation is the aim of many research topics, among which adaptive local mesh refinement is a promising one. The approach envisaged here brings within reach the gain in accuracy associated with complete refinement over the whole reservoir, but without the tremendous increase in computational costs linked with complete refinement.

The specific numerical problems in reservoir simulation all stem from the occurrence of both elliptic and hyperbolic equations; both types are equally important and they are intensely coupled.

The need for dynamic local refinement mainly emerges from the hyperbolic equations, since these equations dominate the travelling (saturation-) shock waves. Among the broad class of flexible gridding methods for hyperbolic equations, the choice has been made for the method, which (dynamically) refines a block in an (initially regular) grid by splitting it into 4 (2-D) or 8 (3-D) identical smaller ones. Only for this relatively uninvolved method there is good hope to cope with the computational intricacies introduced by the refinements in the elliptic equations. The basic notion for efficient solution of elliptic equations on locally refined grids is multi-grid.

The different demands on accuracy imposed by the elliptic and hyperbolic equations suggest the use of different grids for the two types of equations in the same simulation study. The just mentioned uninvolved refinement can readily be used to create different grids which simply match to each other. Provisional experiments for model equations show that with these separate grids for the two parts of reservoir simulation, the accuracy can possibly be improved by orders of magnitude. However, extension to more general equations introduces many problems still to be investigated.

The lecture will give an overview of the development of this flexible gridding approach to reservoir simulation at KSEPL. A substantial part of the lecture will be devoted to multi-grid, since on that topic the most manifest results can be reported.

Principles of Error Control and Selfadaptation for the Solution of Elliptic and Parabolic PDEs

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Abstract: The requirements for a "black box" solver for PDEs are discussed. The decisions for the black box solver FIDISOL for the numerical solution of nonlinear systems of elliptic and parabolic PDEs in a rectangular domain are justified. The basic ideas for a variable order/variable step size finite difference method are presented. The access to the truncation error is obtained by the difference of difference formulas, using members of a whole family of formulas. In a Newton-difference method the linearization and discretization (including estimates for the truncation errors) of the PDEs leads to the error equation which is the key to the whole error control. The discussion of the error equation reveals the propagation of and the relationship between the different errors and shows the strategy of the optimal balancing of the errors.

The control of a robust Newton-Raphson method is presented. The determination of the optimal (consistency) orders in the space directions for a prescribed relative tolerance tol is discussed. The goal is to minimize the total computational amount, including the iterative solution of the linear system for the computation of the Newton-correction. The local application of the error law leads to an optimal (smoothed) step size distribution in the space directions. In the initial value (usually time) direction the order is optimized by minimizing the corresponding error term, and the step size is determined by adapting the time discretization error to the space discretization error.

A brief remark will be made to the iterative polyalgorithmic linear solver part LINSOL (that uses generalized CG-type methods) and to its stopping criterion. Further remarks concern the testing techniques. Some examples of PDEs, solved on different vector computers, are presented, followed by a critical discussion of FIDISOL.

Presently an experimental version is under investigation to extend the ideas of FIDISOL to more geometrical flexibility on body-oriented grids. The basic ideas are presented. The concept of "dividing lines" allows for multiply connected domain. The problem of corner singularities will be discussed. Some examples will be presented.

Some remarks to the references: In section 17 in /1/ a survey of the FIDISOL project is presented. The basic principles are reported in /2/. Reference /3/ is the user's guide for the customers of the FIDISOL program package. The details of the selfadaptation are presented in /4/. In /5/ recent developments are discussed.

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A NUMERICAL METHOD OF LINES STUDY OF THE MOVING FINITE ELEMENT METHOD

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It is well known that many discretizations of time dependent problems in partial differential equations (PDEs) can be derived by means of the following two-stage procedure. First the space variables are discretized on a selected space mesh, mainly using finite difference or finite element approximations, so as to convert the PDE problem into a system of, usually stiff, ordinary differential equations (ODEs) with time as independent variable. Then, the discretization in time of this stiff ODE system yields the sought fully discrete scheme. In the literature this two-stage approach is often referred to as the method of lines (MOL). With this approach in mind, several sophisticated PDE packages (e.g. the SPRINT package [1]) have been developed in recent years, notably for one-space dimensional problems. These MOL based packages, including SPRINT, greatly benefit from the very successful developments of automatic stiff ODE solvers. Needless to say that the development of implicit BDF codes, initiated by Gear and further improved by Hindmarsh, Petzold, and others, is a key factor here. Indeed, certainly for intelligent users who know their problem, Gear type solvers have proved to be highly efficient, robust and reliable, in that these solvers work for broad classes of problems and almost always solve the stiff ODE system under consideration in an accurate and efficient way. The experiences with MOL packages has clearly revealed that this is also true of semi-discrete PDE problems.

However, from the PDE point of view, conventional MOL packages integrate in a semi-automatic way in the sense that they automatically adjust the time stepsizes, but use a fixed, a priori chosen space grid for the entire calculation. Depending on the degree of spatial activity, such an a priori chosen space grid is usually equispaced or mildly nonuniform. In many cases this semi-automatic approach works very satisfactorily. Notably for problems in which the solution does not exhibit a high degree of spatial activity, but also for problems where regions of rapid variation in space do not move when time evolves (stationary layers). However, for solutions possessing sharp moving spatial transitions, like travelling wavefronts or emerging boundary and interior layers, a grid held fixed for the entire calculation can be computationally inefficient, since this grid readily must contain a very large number of nodes. In such cases methods which attemp to adjust automatically both the space and the time stepsizes, are likely to be more successful in efficiently resolving critical regions of high spatial and temporal activity. Methods and codes which operate this way belong to the realm of adaptive or moving grid methods.

Over the past several years the interest in moving grid methods has rapidly increased. Unfortunately, very little, if any, moving grid software packages, generally applicable up to nearly the same level of efficiency, robustness and reliability as conventional packages, are available yet, not even for the relatively simple 1D case. Admittedly, for an interesting variety of difficult example problems, various adaptive techniques have been shown to be potentially very efficient, a prominent example being the moving finite element method [4]. However, most of the techniques, including the moving finite element method, require some form of tuning to safely govern the automatic choice of made clear that in general the automatic space node selection is intrinsically difficult, in the sense that the tuning is rather problem dependent and not so amenable to automize. Hence, the use of algorithms employing moving grid techniques, usually require considerably more expertise from the user than most of the common fixed grid algorithms,

in order to obtain the best possible results in terms of efficiency, robustness and reliability. Noteworthy, in this connection, is that the moving grid construction with the accompanied tuning, is often a determining factor for the computational effort spent in the time integration. Traditionally, this point has been neglected in most of the work on time dependent problems, probably because the greater part of the development effort is spent in doing a good job in the spatial direction.

Following the philosophy of the MOL approach, our current research is devoted to an evaluation and comparison, mainly based on extensive numerical tests, of three moving grid techniques for 1D problems, viz., the finite element technique of Miller et al. [4], the algorithm published by Petzold [5], and a method based on ideas adopted from Dorfi & Drury [2]. The two latter ones are finite difference methods. All three methods are of Lagrangian type. Concerning the time integration, each of these moving grid techniques can be straightforwardly combined with a stiff solver, just as in the conventional MOL approach. In [4,5] interesting results have been shown already using such a type of time integrator. Our examination of the three methods is principally aimed at assessing which of the three methods is most suitable for retaining the acknowledged features of reliability, robustness and efficiency of the conventional MOL approach. As already indicated by the remark made above, in such an examination the moving grid determination should be considered not only in relation to spatial solvability properties, but also in relation to the time stepping process. Hence we shall pay considerable attention to the question of efficiency of the time stepping process.

In this lecture we shall present some first results of our investigations. These results have been obtained using the Gear solver of the SPRINT package for the numerical time integration and concern a test set of three example problems, viz. a reaction-diffusion equation which models a problem from combustion theory, the well-known Burgers' equation which is the nonlinear prototype of a convection-diffusion equation, and a system of two quasi-nonlinear hyperbolic equations which may be considered as a prototype of an opposite travelling waves problem. Because of the limited time available, we shall restrict ourselves to presenting results only for the moving finite element method. Results for the other two methods will be reported in [3].

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