ADAPTIVE LINEARLY IMPLICIT METHODS IN DYNAMICAL PROCESS SIMULATION

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Abstract. *Dynamical process simulation of complex real–life problems often advises the use of modern algorithms, which automatically adapt both the time and space discretization in order to get error–controlled approximations of the solution. In this paper, a combination of linearly implicit time integrators of Rosenbrock type and multilevel finite elements based on a posteriori error estimates is presented. This approach has proven to work quite satisfactorily for a wide range of challenging industrial problems.*

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1 INTRODUCTION

Dynamical process simulation is nowadays the central tool to assess the modelling process for large scale physical problems arising in such fields as biology, chemistry, metallurgy, and medicine. Moreover, successful numerical methods are very attractive to design and control economical plants at low costs in a short time. Due to the great complexity of the established models, the development of fast and robust algorithms has been a topic of continuing investigations during the last years.

One of the important requirements that modern software must meet today is that it is able to judge the quality of their numerical approximations in order to assess safely the modelling process. Adaptive methods have proven to work efficiently providing a posteriori error estimates and appropriate strategies to improve the accuracy where needed. They are now entering into real–life applications and starting to become a standard feature in simulation programs. The present paper reports on one successful way to construct fully adaptive discretization methods, which are applicable to a wide range of industrially relevant problems.

We concentrate on nonlinear evolution problems which can be written in the form

$$B(x,t,u)\partial_t u = \nabla \cdot (D(x,t,u)\nabla u) + F(x,t,u,\nabla u) , \qquad (1)$$

supplemented with suitable boundary and initial conditions. The vector–valued solution $u = (u_1,\ldots,u_m)^T$ is supposed to be unique. This problem class includes the well–known reaction–diffusion equations and the Navier–Stokes equations as well. We first discretize in time and consider the spatial discretization afterwards as a perturbation, which has to be controlled within each time step. Combined with a posteriori error estimates this approach is known as adaptive Rothe method. First theoretical investigations have been made by BORNEMANN [3] for linear parabolic equations. LANG and WALTER [14] have generalized the adaptive Rothe approach to reaction–diffusion systems. A rigorous analysis for nonlinear parabolic systems is given in LANG [18]. For a comparative study of the most popular discretization technique, the method of lines (first space then time), and Rothe's approach, we refer to DEUFLHARD, LANG, and NOWAK [8].

Since differential operators give rise to infinite stiffness, often an implicit method is applied to discretize in time. We use linearly implicit methods of Rosenbrock type, which are constructed by working the Jacobian directly into the formula. These methods offer several advantages. They completely avoid the solution of nonlinear equations, that means no Newton iteration has to be controlled. There is no problem to construct Rosenbrock methods with optimal linear stability properties for stiff equations. According to their one–step nature, they allow a rapid change of step sizes and an efficient adaptation of the spatial discretization in each time step. Moreover, a simple embedding technique can be used to satisfactorily estimate the error in time. A description of the main idea of linearly implicit methods is given in Section 2.

Stabilized finite elements are used for the spatial discretization to prevent numerical

instabilities caused by advection–dominated terms. To estimate the error in space, the hierarchical basis technique has been extended to Rosenbrock schemes in LANG [18]. Hierarchical error estimators have been accepted to provide efficient and reliable assessment of spatial errors. They can be used to steer a multilevel process, which aims at getting a successively improved spatial discretization drastically reducing the size of the arising linear algebraic systems with respect to a prescribed tolerance (BORNEMANN, ERDMANN, and KORNHUBER [4], DEUFLHARD, LEINEN and YSERENTANT [9], BANK and SMITH [1]). A brief introduction to multilevel finite element methods is given in Section 3.

Section 4 is dedicated to three real–life applications that arise in today's chemical industry, semiconductor–device fabrication, and health care.

2 LINEARLY IMPLICIT METHODS

In this section a short description of the linearly implicit discretization idea is given. More details can be found in the books of HAIRER and WANNER [13], DEUFLHARD and BORNEMANN [7], STREHMEL and WEINER [23]. For ease of presentation, we set $B = I$ in (1) and consider the autonomous case. Then we can look at (1) as an abstract Cauchy problem of the form

$$u_t = f(u), \quad u(t_0) = u_0, \quad t > t_0, \tag{2}$$

where the differential operators and the boundary conditions are incorporated into the nonlinear function $f(u)$. Since differential operators give rise to infinite stiffness, often an implicit discretization method is applied to integrate in time. The simplest scheme is the implicit (backward) Euler method

$$u_{n+1} = u_n + \tau f(u_{n+1}), \tag{3}$$

where $\tau = t_{n+1} - t_n$ is the step size and u_n denotes an approximation of $u(t_n)$ at $t = n\tau$. This equation is implicit in u_{n+1} and thus usually a Newton–like iteration method has to be used to approximate the numerical solution itself. The implementation of an efficient nonlinear solver is the main problem for a fully implicit method.

Investigating the convergence of Newton's method in function space, DEUFLHARD [5] pointed out that one calculation of the Jacobian or an approximation of it per time step is sufficient to integrate stiff problems efficiently. Using u_n as an initial iterate in a Newton method applied to (3), we find

$$\begin{aligned} (I - \tau J_n) K_n &= \tau f(u_n), \\ u_{n+1} &= u_n + K_n, \end{aligned} \tag{4}$$

where J_n stands for the Jacobian matrix $\partial_u f(u_n)$. The arising scheme is known as *linearly implicit* Euler method. The numerical solution is now effectively computed by

solving the system of linear equations that defines the increment K_n. Among the methods which are capable of integrating stiff equations efficiently, linearly implicit methods are the easiest to program, since they completely avoid the numerical solution of nonlinear systems.

One important class of higher–order linearly implicit methods are extrapolation methods that are very effective in reducing the error (see DEUFLHARD [6]). Another generalization of the linearly implicit approach we will follow here are Rosenbrock methods (ROSENBROCK [22]). They have found widespread use in the ODE context. Applied to (2) a so–called s–stage Rosenbrock method has the recursive form

$$(I - \tau\gamma_{ii} J_n) K_{ni} = \tau f(u_n + \sum_{j=1}^{i-1} \alpha_{ij} K_{nj}) + \tau J_n \sum_{j=1}^{i-1} \gamma_{ij} K_{nj} , \tag{5}$$

$$u_{n+1} = u_n + \sum_{i=1}^{s} b_i K_{ni} ,$$

where the step number s and the defining formula coefficients b_i, α_{ij}, and γ_{ij} are chosen to obtain a desired order of consistency and good stability properties for stiff equations (see e.g. HAIRER and WANNER [13]). We assume $\gamma_{ii} = \gamma > 0$ for all i, which is the standard simplification to derive Rosenbrock methods with one and the same operator on the left–hand side of (5).

The linearly implicit Euler method mentioned above is recovered for $s = 1$ and $\gamma = 1$. For the general system

$$B(t, u)u_t = f(t, u) , \quad u(t_0) = u_0 , \quad t > t_0 , \tag{6}$$

an efficient implementation that avoids matrix–vector multiplications with the Jacobian was given by LUBICH and ROCHE [21].

Usually, one wishes to adapt the step size in order to control the temporal error. For linearly implicit methods of Rosenbrock type a second solution of inferior order, say $\hat{p}$, can be computed by a so–called embedded formula

$$\hat{u}_{n+1} = u_n + \sum_{i=1}^{s} \hat{b}_i K_{ni} , \tag{7}$$

where the original weights b_i are simply replaced by $\hat{b}_i$. If p is the order of u_{n+1}, we call such a pair of formulas to be of order $p(\hat{p})$. Introducing an appropriate scaled norm $\| \cdot \|$, the local error estimator

$$r_{n+1} = \|u_{n+1} - \hat{u}_{n+1}\| \tag{8}$$

can be used to propose a new time step by

$$\tau_{n+1} = \frac{\tau_n}{\tau_{n-1}} \left(\frac{TOL_t \, r_n}{r_{n+1} \, r_{n+1}} \right)^{\frac{1}{\hat{p}+1}} \tau_n \,. \tag{9}$$

Here, TOL_t is a desired tolerance prescribed by the user. This formula is related to a discrete PI–controller first established by GUSTAFFSON, LUNDH, and SÖDERLIND [11]. A more standard step size selection strategy can be found in HAIRER, NØRSETT, and WANNER [12], Chapter II.4.

Rosenbrock methods offer several structural advantages. They preserve conservation properties like fully implicit methods. There is no problem to construct Rosenbrock methods with optimal linear stability properties for stiff equations. Because of their one–step nature, they allow a rapid change of step sizes and an efficient adaptation of the underlying spatial discretizations as will be seen in the next section. Thus, they are attractive for solving real world problems.

3 MULTILEVEL FINITE ELEMENTS

In the context of PDEs, system (5) consists of linear elliptic boundary value problems possibly advection–dominated. In the spirit of full adaptivity a multilevel finite element method is used to solve this system. The main idea of the multilevel technique consists of replacing the solution space by a sequence of discrete spaces with successively increasing dimension to improve their approximation property. A posteriori error estimates provide the appropriate framework to determine where a mesh refinement is necessary and where degrees of freedom are no longer needed. Multilevel methods have proven to be a useful tool for drastically reducing the size of the arising linear algebraic systems and to achieve high and controlled accuracy of the spatial discretization (see e.g. DEUFLHARD, LEINEN, and YSERENTANT [9], LANG [16]).

Let T_h be an admissible finite element mesh at $t = t_n$ and S_h^q be the associated finite dimensional space consisting of all continuous functions which are polynomials of order q on each finite element $T \in T_h$. Then the standard Galerkin finite element approximation $K_{ni}^h \in S_h^q$ of the intermediate values K_{ni} satisfies the equation

$$(L_n \, K_{ni}^h, \phi) = (r_{ni}, \phi) \quad \text{for all } \phi \in S_h^q, \tag{10}$$

where L_n is the weak representation of the differential operator at the left–hand side in (5) and r_{ni} stands for the entire right–hand side in (5). Since the operator L_n is independent of i its calculation is required only once within each time step.

It is a well–known inconvenience that the solutions K_{ni}^h may suffer from numerical oscillations caused by dominated convective and reactive terms as well. An attractive way to overcome this drawback is to add locally weighted residuals to get a stabilized discretization of the form

$$(L_n K_{ni}^h, \phi) + \sum_{T \in T_h} (L_n K_{ni}^h, w(\phi))_T = (r_{ni}, \phi) + \sum_{T \in T_h} (r_{ni}, w(\phi))_T , \tag{11}$$

where $w(\phi)$ has to be defined with respect to the operator L_n (see e.g. FRANCA and FREY [10], LUBE and WEISS [20], TOBISKA and VERFÜRTH [24]). Two important classes of stabilized methods are the streamline diffusion and the more general Galerkin/Least–squares finite element method.

After computing the approximate intermediate values K_{ni}^h a posteriori error estimates can be used to give specific assessment of the error distribution. Considering a hierarchical decomposition

$$S_h^{q+1} = S_h^q \oplus Z_h^{q+1} , \tag{12}$$

where Z_h^{q+1} is the subspace that corresponds to the span of all additional basis functions needed to enrich the space S_h^q to higher order, an attractive idea of an efficient error estimation is to bound the spatial error by evaluating its components in the space Z_h^{q+1} only. This technique is known as hierarchical error estimation and has been accepted to provide efficient and reliable assessment of spatial errors (BORNEMANN, ERDMANN, and KORNHUBER [4], DEUFLHARD, LEINEN and YSERENTANT [9], BANK and SMITH [1]). In LANG [18], the hierarchical basis technique has been carried over to time–dependent nonlinear problems. Defining an a posteriori error estimator $E_{n+1}^h \in Z_h^{q+1}$ by

$$E_{n+1}^h = E_{n0}^h + \sum_{i=1}^{s} b_i E_{ni}^h \tag{13}$$

with E_{n0}^h approximating the projection error of the initial value u_n in Z_h^{q+1} and E_{ni}^h estimating the spatial error of the intermediate value K_{ni}^h, the local spatial error for a finite element $T \in T_h$ can be estimated by $\eta_T := \|E_{n+1}^h\|_T$. The error estimator E_{n+1}^h is computed by linear systems which can be derived from (11). For practical computations the spatially global calculation of E_{n+1}^h is normally approximated by a small element–by–element calculation. This leads to an efficient algorithm for computing a posteriori error estimates which can be used to determine an adaptive strategy to improve the accuracy of the numerical approximation where needed. A rigorous a posteriori error analysis for a Rosenbrock–Galerkin finite element method applied to nonlinear parabolic systems is given in LANG [18].

In order to produce a nearly optimal mesh, those finite elements T having an error η_T larger than a certain threshold are refined. After the refinement improved finite element solutions K_{ni}^h defined by (11) are computed. The whole procedure solve–estimate–refine is applied several times until a prescribed spatial tolerance $\|E_{n+1}^h\| \le TOL_x$ is reached. To maintain the nested property of the finite element subspaces coarsening takes place only after an accepted time step before starting the multilevel process at a new time. Regions of small errors are identified by their η–values.

The numerical algorithm described was coded in a fully adaptive package KARDOS developed at the Konrad–Zuse–Centre in Berlin. Several types of Rosenbrock solvers and Finite Elements are implemented. Nowadays it is an efficient and flexible working horse to solve a wide range of practically relevant problems in 1D–3D. To demonstrate the efficiency and reliability of this code, we will present some practical examples in the next section.

4   APPLICATIONS

Two–Phase Bubble Reactor [15]. Bubble reactors are special chemical plants for carrying out synthesis processes of different gaseous chemicals. The bubbles stream in at the bottom of the reactor and rise to the top dissolving and reacting with each other (see Fig. 1). The right proportions of such reactors, which depend mainly on the rising behaviour of the bubbles and specific reaction velocities are of great importance for chemical engineers in order to construct economical plants.
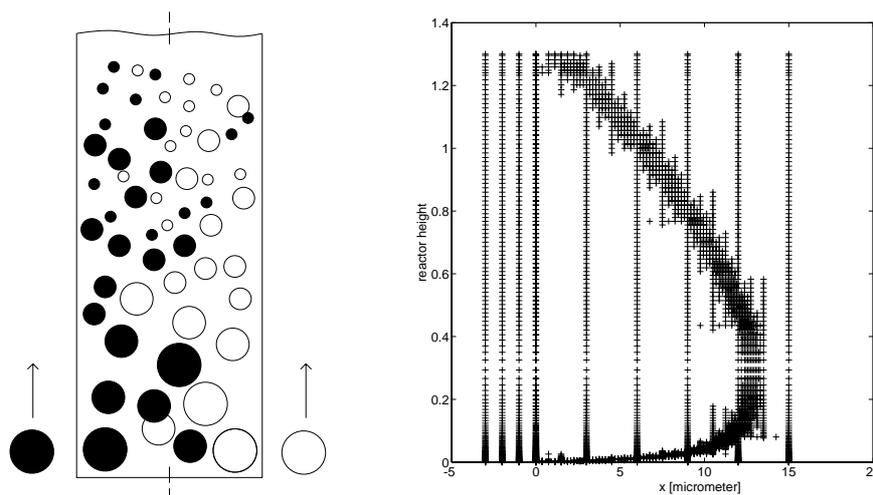
Figure 1: Bubble reactor in section (left) and evolution of the grid (right) where the reactor height is taken as time axis.

Since a fully three–dimensional description of the synthesis process would become to complicated, a simplified one–dimensional model is used in the simulations presented in LANG [15]. Fig. 1 shows the evolution of the computational mesh adapted to a travelling reaction front. At the beginning, the front moves very fast from the outer (left) to the inner (right) boundary of a thin bubble surface layer. In order to resolve this process, small time steps and a grid with local refinement within the front arise automatically. After keeping nearly unchanged during the time period $t \in [0.1, 0.5]$, the reaction front
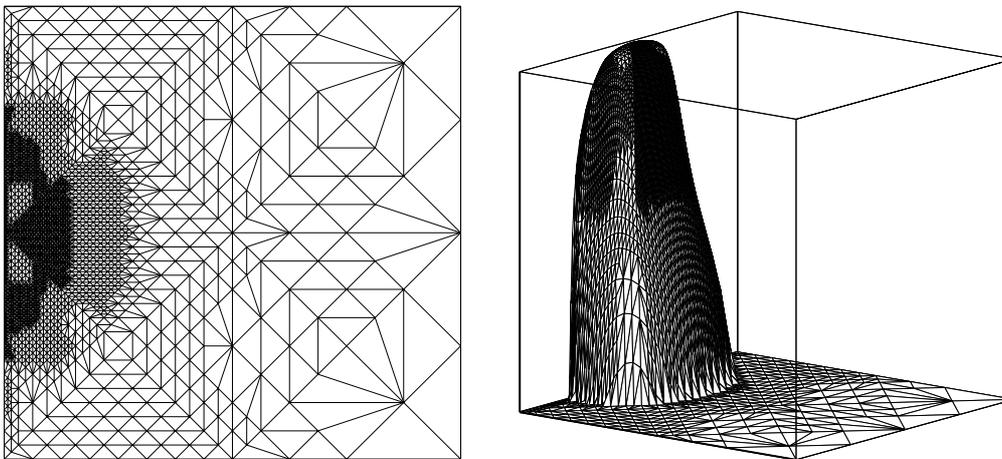
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Figure 2: Refined mesh and the phosphorus concentration near the wafer surface.

travels back, but now with moderate speed which allows larger time steps.

Phosphorus Diffusion in Silicon [19]. Semiconductor device simulations which utilize sound physical models are nowadays an attractive tool to create new generations of devices. One important step in the fabrication of silicon–based integrated circuits is the creation of semiconducting areas by diffusion of dopant impurities such as arsenic, boron, or phosphorus into silicon. Complex models have been developed to investigate the redistribution of dopants and point defects.

The two–dimensional model used in LANG and MERZ [19] to study phosphorus diffusion in silicon comprises the following system of reaction–drift–diffusion equations

$$\partial_t C_j + \operatorname{div} J_j(\mathbf{C}, \psi) + R_j(\mathbf{C}, \psi) \; = \; 0 \,, \quad j = I, V, A, AI, AV, \qquad (14)$$

$$-\frac{\epsilon}{e} \triangle \psi + 2 n_i \sinh\left(\frac{\psi}{U_T}\right) - \sum_{j=1}^{5} Q_j(\psi) C_j \; = \; 0 \,,$$

wherein the six state variables are: interstitials (I), vacancies (V), phosphorus (A), mobile species (AI and AV), and the chemical potential ψ. Here, J_j denote the drift–diffusion terms vanishing for phosphorus, R_j are the generation–recombination rates, and Q_j are the total charges.

The principle difficulties in solving this system numerically are the strong nonlinearities and the differential–algebraic structure. Fig. 2 shows a typical snap shot of a phosphorus concentration near the wafer surface. The profile shows a characteristic "kink and tail" behaviour, a phenomenon which is known as anomalous diffusion of phosphorus at

temperatures around $900°C$. The corresponding mesh reveals that step gradients are well resolved, not wasting degrees of freedom.

Heat Transfer in Regional Hyperthermia [17]. Hyperthermia, i.e., heating tissue to $42°C - 43°C$, is a method of cancer therapy. It is usually applied as an additive therapy to enhance the effect of conventional radio– or chemotherapy. The standard way to locally heat up a human body is the use of electromagnetic waves produced by a so–called Hyperthermia applicator (e.g. Sigma 60 Applicator of the BSD 2000 Hyperthermia System). Within a medical planning system (BECK, DEUFLHARD, HEGE, SEEBASS, and STALLING [2]), a sequence of nonlinear heat transfer equations has to be solved in order to optimize the temperature distribution in the human body. High temperatures have to be avoided in healthy tissue, whereas they are desirable in the tumor region.

The basic model used in LANG, ERDMANN, and SEEBASS [17] is the instationary bio–heat–transfer equation

$$\rho c \, \partial_t T = \text{div}(\kappa \, \text{grad} T) - c_b W(T)(T - T_b) + Q_e \,, \tag{15}$$

which has to be solved for complex geometries involving discontinuous coefficients due to the different physical properties of the tissues. Here, $W(T)$ is the temperature–dependent mass flow rate of blood per unit volume of tissue. The temperature distribution is mainly determined by the power Q_e deposited by the electric field.

Fig. 3 shows two cuts through the computational domain which corresponds to a patient's abdomen. The coarse grid contains 7140 vertices, while the refined mesh which guarantees an accuracy of 2% has 35936 vertices. The corresponding uniform mesh would have about 500000 vertices. Comparing the coarse and fine mesh, the attained change of the temperature increment taken with respect to room temperature ranges in the order of 10%. The local refinement controlled by a posteriori error estimates leads to a better resolution in regions with high temperature gradients and material transitions.

5 CONCLUSION

Dynamical process simulation of complex real–life problems advises the use of modern algorithms, which are able to judge the quality of their numerical approximations and to determine an adaptation strategy to improve their accuracy in both the time and the space discretization. The paper presented a combination of efficient linearly implicit time integrators of Rosenbrock type and error–controlled grid improvement based on a multilevel finite element method. This approach leads to a minimization of the degrees of freedom necessary to reach a prescribed error tolerance. The savings in computational time are substantial and allow the solution of even complex problems in a moderate range of time.
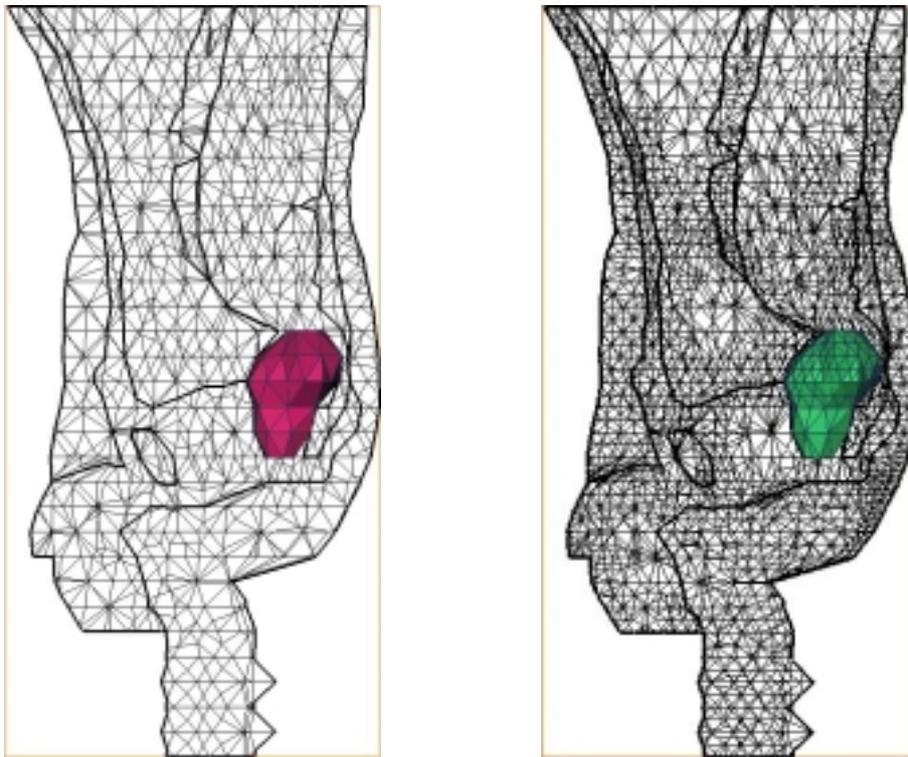
Figure 3: Coarse (left) and refined (right) grid with tumor boundary used for the computation of the optimized temperature distribution.

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