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ADAPTIVE MULTILEVEL SOLUTION OF PARABOLIC EQUATIONS IN 3D

Folkmar A. Bornemann
Freie Universität Berlin and
Konrad-Zuse-Zentrum für Informationstechnik Berlin
Heilbronnerstr. 10, W-1000 Berlin 31, Germany
e-mail: bornemann@sc.ZIB-Berlin.de

Abstract

The mathematical simulation of physical problems with irregular space geometry often requires the solution of the fully 3D equations for significant results. The method of Rothe (discretization in time first) with time–step and order control is particularly well suited to allow each time–step an adaptive, highly nonuniform triangulation of the space domain. Applications of the thus developed software KASTIO3 to an example from the medical sciences in cancer therapy show the significant perspectives opened by the approach.

1 Introduction

In the presence of complicated space geometries, discontinuous coefficients, inconsistent initial data etc., the numerical solution of parabolic problems in *three* space dimensions requires a *sophisticated* reduction of the computational amount of work. Only then we can hope to break through the complexity barrier of many important problems of the natural sciences and technology. A nowadays increasingly important concept of such an amount of work reduction is *adaptivity*, i.e., the automatic choice of the degrees of freedom, such as the automatic distribution of nodes in a triangulation or the local order of a discretization. If we compute a *family* of approximations to an infinite dimensional problem with different local discretization parameters or orders instead of a single approximation, we speak of *multilevel* methods. Such a computation of simultaneous approximations allows to construct effective error estimates, which support the adaptation control. Moreover the construction of fast iterative solvers for the arising linear systems of very high dimension becomes possible by multilevel techniques.

We favor an approach which strictly separates time and space — *time is not just another dimension of space*, [4]. The method of Rothe, i.e., discretization in time first, is particularly well suited to allow adaptivity:

- The parabolic initial boundary value problem can be considered as an abstract Cauchy problem in an appropriate function space.
- A variable–step variable–order discretization in time applied in that function space gives rise to an approximation of the known standard for ordinary differential equations.
- Discretization of the elliptic subproblems is considered as a perturbation, which can be controlled independently of the time discretization.

The full advantage of our approach in the 2D and 3D case was achieved by the construction of a variable order discretization in time with an optimal amount of work, [4].

The multilevel adaptive finite element solver for the arising elliptic problems is constructed by using a preconditioned conjugate gradient method. A proper preconditioner allows to handle error estimation and the fast solver in an analogous way. Because of its use of orthogonal projections the BPX preconditioner, [8], is ideally suited as conceptual base for our purposes. Several authors have proven optimal convergency rates, e.g., [6, 14, 15, 17] and the literature given therein. An optimal implementation for highly nonuniform triangulations was investigated for the 2D case in [5], for the 3D case in [7].

All together the proposed algorithm has *multigrid complexity* over all time-steps.

In order to prove the applicability of our approach to real life problems we will present computations on the Bio–Heat–Transfer equation in 3D. This equation plays a prominent role in planning *hyperthermia*, a recent clinical method for the treatment of malignancies (cancer), which at this time is in an experimental status.

2 Outline of the Algorithm

2.1 The Problem

We are concerned with temporally homogeneous linear scalar parabolic equations on a polyhedral domain $\Omega \subset \mathbb{R}^3$, which can be written as an *abstract Cauchy problem* in $L^2(\Omega)$:

$$u_t + Au = f, \qquad u(0) = u_0.$$

Here $A : \mathcal{D}(A) \subset L^2(\Omega) \longrightarrow L^2(\Omega)$ is the linear, unbounded, positive selfadjoint operator induced by an selfadjoint strongly elliptic operator of second order and boundary conditions. Since $(-A)$ generates a holomorphic semigroup, we are provided with an appropriate scale of Hilbert spaces

$$\dot{H}^\alpha = \mathcal{D}(A^{\alpha/2}),$$

equipped with the corresponding graph norm. This scale allows us to describe smoothness and consistency of the initial data u_0.

2.2 Adaptive Method of Rothe

As discussed in the introduction we want to discretize in time first and intend to construct a variable order, variable time-step single step procedure in the space $L^2(\Omega)$. However, we have to solve some elliptic subproblems. A finite element solver for them will introduce perturbations. These perturbations have to be controlled by some error estimator of the *spatial* error. A typical loop for a time-stepping procedure, which locally in time controls the computational error corresponding to a given tolerance TOL, would look like this:

ParabolicSolver(TOL, T_{stop}, τ_{start}):
  Initialize;
  while $(t < T_{\text{stop}})$
  begin
    for all allowed p **do**
      $\hat{u}_p$ = SingleStepMethod(EllipticSolver($\chi_p(1-\rho)$TOL));
      $[\epsilon_p]$ = estimated error of $\hat{u}_p$ (due to discretization in time)
    until convergence ($[\epsilon_p] < \rho$TOL)
    if convergence
    begin
      $t = t + \tau$;
      $\hat{u}(t) = \hat{u}_p$;

τ = NewTimeStep;
end else
τ = ReduceTimeStep;
end;

Note that the choice $\rho = 1$ corresponds to the exact solution of the elliptic subproblems. The choice $\rho = 0$ would not make sense. As shown in [4], it is always possible for $0 < \rho < 1$ to choose a χ_p, such that the error of $\hat{u}_p$ due to the finite element discretization in space is below $(1-\rho)$TOL and that in addition the estimate $[\epsilon_p]$ really reflects the error in time. Thus the condition ($[\epsilon_p] < \rho$TOL) is enough to ensure the local error control in time *and* space. The value of χ_p depends only on the single step method which is used. Optimizing the amount of work yields $\rho = 1/4$, cf. [4].

The applicability of certain single step methods to the abstract Cauchy problem is guaranteed by the following result due to [4].

THEOREM 2.1. *Given a strongly A_0-stable rational approximation $r(z)$ to $\exp(-z)$ of order p, the single step method*

$$\Phi_\tau(u,\tau) = r(\tau A)u + \Big(I - r(\tau A)\Big) A^{-1} f$$

is well defined for $\tau > 0$ and the sequence $u_{n+1} = \Phi(u_n, \tau)$, $n = 1, 2, \ldots$, approximates the solution of the abstract Cauchy problem at $t_n = n\tau$ with an error of

$$\|u_n - u(t_n)\|_{L^2(\Omega)} \leq C\tau^p t_n^{\min(1,\alpha-p)} \|u_0\|_{\dot{H}^{2\alpha}}.$$

This result extends estimates due to BRENNER/THOMÉE [9] and LEROUX [13].

In particular we can use the order and stepsize selecting procedure known for ODEs, which locally optimizes the amount of work needed for a unit time interval, cf. DEUFLHARD [10]:

NewTimeStep:
for all p with computed $\hat{u}$ **do**
$$\tau_p = \sqrt[p+1]{\frac{\rho\text{TOL}}{[\epsilon_p]}} \cdot \tau;$$
compute p^* such that
$$\frac{\text{amount of work for computing } \hat{u}_{p^*}}{\tau_{p^*}} = \min_p \frac{\text{work}_p}{\tau_p};$$
return τ_{p^*};

2.3 The Single Step Method

Extrapolation methods or related methods like deferred corrections lead to very small factors χ_p, which is not very desirable in view of computational effort. For instance yields the extrapolated implicit Euler scheme the value $\chi_5 = 1.3_{10} - 3$. The reason lies in the fact that the error estimation is built as a *difference* of two approximations of successive order:

$$[\epsilon_p] = \|\hat{u}_{p+1} - \hat{u}_p\|_{L^2(\Omega)}.$$

The spatial perturbations have to be very small in order that this difference reflects something of the time error — a problem which is very similar to the "cancellation effect".

On the contrary, we have constructed in [4] a method which *directly* computes a correcting function η_p such that $[\epsilon_p] = \|\eta_p\|_{L^2(\Omega)}$ and the higher order approximation is given thereafter as

$$u_{p+1} = u_p + \eta_p,$$

in order to avoid any cancellation.

This correction function is obtained *multiplicatively* as an update of the former one:

$$\eta_p = \gamma_p \tau A(I + \tau A)^{-1}\eta_{p-1}, \qquad p = 2, \ldots,$$

cf. [4]. Advantages of the approach:

- reasonable size of χ_p, e.g., $\chi_8 = 1/4$
- minimal storage requirement: just *two* finite element functions
- $(u_p, \eta_{p-1}) \to (u_{p+1}, \eta_p)$ needs the solution of just *one* elliptic subproblem — always with the same operator $(I + \tau A)$.

The following Theorem, proven in [4] and [5], shows that we have constructed in this way approximations with the desired properties.

THEOREM 2.2. *Given u_1 as the implicit Euler discretization and the first correction as*

$$\eta_1 = -\frac{1}{2}\tau A(I + \tau A)^{-1}(u_1 - u_0).$$

Then the factors $\gamma_p = \frac{p}{p+1}\frac{L'_{p+1}(1)}{L'_p(1)}$, where L_p denotes the pth Laguerre polynomial, yield strongly A_0-stable approximations u_p of order p to the abstract Cauchy problem.

2.4 Algorithmic Details of Order and Stepsize Selection

A lot of subtle heuristics is necessary for an algorithmically effective and robust order and stepsize control. A quite systematic approach was offered in DEUFLHARD [10] for ODEs and extended in [3] for parabolic equations. It consists in comparing the actual computational behavior of the device with a *standard model* based on Shannon's information theory. This standard model allows to predict maximal orders in time — depending on the given tolerance TOL, cf. [5, 10]. For our 3D problem one gets a maximal order of 2 for TOL $> 10^{-3}$.

3 The Elliptic Solver

In order to construct a nearly optimal algorithm we use as elliptic solver an *adaptive* finite element code with *nested multigrid* or *multilevel* iteration. Such algorithms have been described for the 2D case by BANK [1] (program: PLTMG) and DEUFLHARD/LEINEN/YSERENTANT [11] (program: KASKADE). They typically look like this:

```
EllipticSolver(accuracy):
  create starttriangulation T;
  u = direct FEM–solution on T;
  estimate error;
  while (error > accuracy)
  begin
    T = refine(T);
    u = IterativeFEMSolver(T, predicted discretization error on T, u);
    estimate error;
  end;
```

The procedure "IterativeFEMSolver(triangulation, break accuracy, startvalue)" consists of a multigrid like iteration. We use a conjugate gradient method with multilevel *preconditioner*.

An effective preconditioner provides an elegant tool for the construction of *cheap error estimators*, as explained in detail in [5].

3.1 The Preconditioner

When handling the elliptic subproblems $(I + \tau A)u = \cdots$ arising by discretization in time of parabolic equations, a problem occurs:

A straightforward generalization of purely elliptic multilevel preconditioners by just taking $(I + \tau A)$ instead of A is not possible since for $\tau \downarrow 0$ the ellipticity constant of the problem, which seriously enters the condition number estimates, vanishes. On the other hand for $\tau = 0$ there is no need of preconditioning at all, since then $(I + \tau A) = I$.

This problem can be solved by a modification [5] of the recently presented elliptic preconditioner of BRAMBLE/PASCIAK/XU [8] (called BPX–preconditioner). The modification is possible due to the use of *orthogonal* L^2–projections in the BPX–preconditioner. Besides this preconditioner has two major advantages:

- it works well in every space dimension
- one can use highly nonuniform meshes

More precisely one can prove that the condition number of the preconditioned system can be bounded by a constant for each space dimension. This constant is independent of the quasi–uniformity of the triangulation and of the depth of triangulation, i.e., any mesh–size parameter. It depends only on the shape–regularity, i.e., the smallest angle. Moreover, no elliptic regularity assumptions are made. Many people were busy to prove this optimal result, [14, 6, 15, 17].

As shown in [5] this result extends to our elliptic subproblems and gives rise to a condition number estimate which is in addition *independent of the time–step* τ.

An implementation for highly nonuniform triangulations in 3D which needs $\mathcal{O}(\#$ of nodes) operations is discussed in [7].

All together this preconditioner yields, when used in the nested multigrid iteration, an optimal order of complexity, cf. [5]. In particular our algorithm has multigrid complexity over all time–steps.

3.2 The Refinement of Tetrahedra

The local refinement of tetrahedra is somewhat more subtle than refinement of triangles, for the following reasons:

- bisection of the edges of a tetrahedron does *not* decompose uniquely the tetrahedron into eight new ones: there are precisely *three different* possibilities
- the question of *stability* arises, i.e., whether or not the angles distort during successive refinement of a tetrahedron into eight new ones
- in order to create nested triangulations there are much more combinatorial possibilities for the so called geometrical closure of the refinement than in the 2D case

We follow the ideas of GO ONG, ZHANG, BEY [12, 16, 2], who extended the red/green refinement of triangles due to BANK [1]. The question of stability was positively answered by BEY [2], who constructed an algorithm for choosing one of the above mentioned three possibilities, which guarantees that there occurs only a finite number of (quasi)–similarity classes of tetrahedra during refinement. More details may be found in [7], where a 3D extension of the 2D elliptic solver KASKADE is described.

4 An Application: Hyperthermia

In order to prove the applicability of our method to real life problems, which *combine* the difficulties of complex problem geometry, discontinuous coefficients etc., we will present the solution of the so–called *bioheat–transfer equation* (BHT equation) in the framework of *hyperthermia.* Hyperthermia, i.e., the heating of tissue

to temperatures approximately above 42 °C, is a recently developed clinical method for cancer therapy. It allows *in combination with radiotherapy* an improvement of the local control of the tumor. The deep heating of tissue is obtained by an electric field (E–field), which is generated by the radio waves of four antenna pairs. Their parameters (frequency 60 – 120 MHz, phase and amplitude) have to be selected appropriately. It is essential to solve effectively and robust the BHT equation, which models the temperature distribution for a given E–field.

The detailed equation and further information may be found in [5].

A typical geometry is shown in Fig. 1. The mesh was automatically generated from the CT–data of a hip of a female patient, who has been treated for a rectum malignancy at the Klinikum Rudolf Virchow, Freie Universität Berlin. For reasons of presentation we only show the bone.

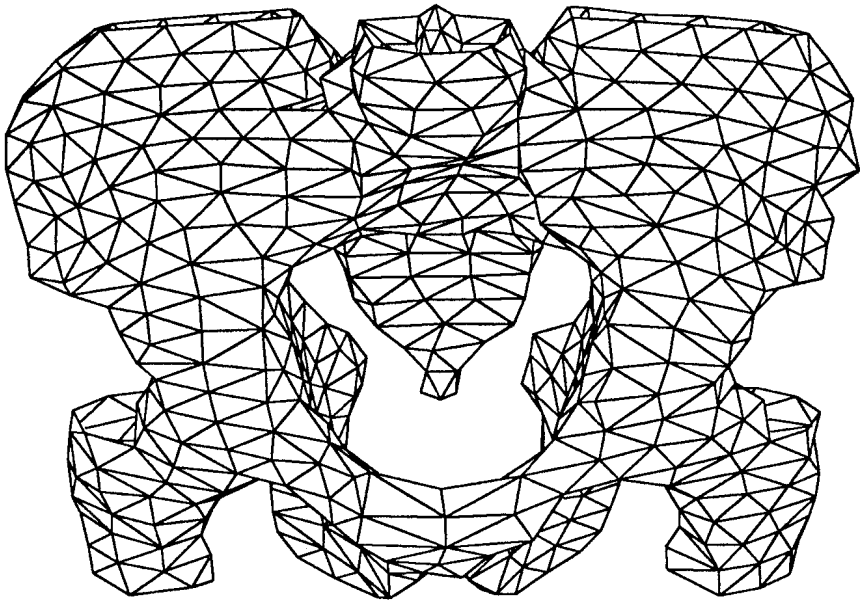

Figure 1: Initial (unrefined) mesh for a human hip

The advantages of our approach can be particularly well read off from the distribution of the computational time for a typical run. Table I shows that the bulk of the computational time is spend in the local integrations for the mass matrix and the stiffness matrix, i.e., for providing the necessary problem information.

Table 1:
AMOUNT OF CPU TIME FOR THE COMPUTATIONAL TASKS

task	amount of CPU–time
direct solver on coarse grid	0.5%
PCG iterations for implicit Euler u_1	6.4 %
PCG iter. time error corrections η_1	4.2 %
refinement	5.1 %
local error indicators	4.4%
local integration	79.4%

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References

1. Bank, R.E.: *PLTMG: A Software Package for Solving Elliptic Partial Differential Equations*, SIAM, Philadelphia, 1990.

2. Bey, J.: "Analyse und Simulation eines Konjugierte–Gradienten–Verfahrens mit einem Multilevel Präkonditionierer zur Lösung dreidimensionaler, elliptischer Randwertprobleme für massiv parallele Rechner", Diplomarbeit, RWTH Aachen, Germany, 1991.

3. Bornemann, F.A.: "An Adaptive Multilevel Approach to Parabolic Equations I. General Theory and 1D–Implementation", *IMPACT Comput. Sci. Engrg.*, Vol. 2, pp. 279–317, 1990.

4. Bornemann, F.A.: "An Adaptive Multilevel Approach to Parabolic Equations II. Variable–Order Time Discretization Based on a Multiplicative Error Correction", *IMPACT Comput. Sci. Engrg.*, Vol. 3, pp. 93–122, 1991.

5. Bornemann, F.A.: "An Adaptive Multilevel Approach to Parabolic Equations III. 2D Error Estimation and Multilevel Preconditioning", *IMPACT Comput. Sci. Engrg.*, Vol. 4, pp. 1–45, 1992.

6. Bornemann, F.A., Yserentant, H.: "A Basic Norm Equivalence for the Theory of Multilevel Methods", *Numer. Math.*, to appear, 1992.

7. Bornemann, F.A., Erdmann, B., Kornhuber, R.: "Adaptive Multilevel Methods in 3 Space Dimensions", Konrad-Zuse-Zentrum, Berlin, Germany, Preprint 92.XX, 1992.

8. Bramble, J.H., Pasciak, J.E., Xu, J.: "Parallel Multilevel Preconditioners", *Math. Comp.*, Vol. 55, pp. 1–22, 1990.

9. Brenner, P., Thomée, V.: "On Rational Approximations of Semigroups", *SIAM J. Numer. Anal.*, Vol. 16, pp. 683–694, 1979.

10. Deuflhard, P.: "Order and Stepsize Control in Extrapolation Methods", *Numer. Math*, Vol. 41, pp. 399–422, 1983.

11. Deuflhard, P., Leinen, P., Yserentant, H.: "Concepts of an Adaptive Hierarchical Finite Element Code", *IMPACT Comput. Sci. Engrg.*, Vol. 1, pp. 3–35, 1989.

12. Go Ong, M.E.: "Hierarchical Basis Preconditioners For Second Order Elliptic Problems in Three Dimensions", Ph.D. Thesis, University of California, Los Angeles, 1989.

13. LeRoux, M.-N.: "Semidiscretization in Time for Parabolic Problems", *Math. Comp.*, Vol. 33, pp. 919–931, 1979.

14. Oswald, P.: "On Discrete Norm Estimates Related to Multilevel Preconditioners in the Finite Element Method", *Proceedings Int. Conf. Constr. Theory of Functions, Varna 1991*, 1992.

15. Xu, J.: "Iterative Methods by Space Decomposition and Subspace Correction", *SIAM Review*, to appear, 1992.

16. Zhang, S.: "Successive Subdivision of Tetrahedra and Multigrid Methods on Tetrahedral Meshes", Report No. AM 21, Pennsylvania State University, 1988.

17. Zhang, X.: "Multilevel Schwarz Methods", *Numer. Math.*, to appear, 1992.