

NO-A191 539

GRID ADAPTATION AND PARABOLIC EQUATIONS BY MULTIGRID
TECHNIQUES(U) WEIZMANN INST OF SCIENCE REMOVOTH
(ISRAEL) A BRANDT 31 OCT 87 DAJA45-85-C-0036

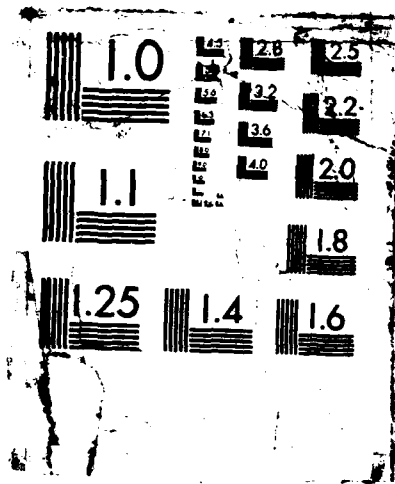
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SECURITY CLASSIFICATION OF THIS PAGE

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No 0704-0188
Exp Date Jun 30, 1986

REPORT SECURITY CLASSIFICATION

Unclassified

1b. RESTRICTIVE MARKINGS

3. DISTRIBUTION / AVAILABILITY OF REPORT

Approved for public release; distribution
unlimited

AD-A191 539

5. MONITORING ORGANIZATION REPORT NUMBER(S)

R&D 4305-MA-01

NAME OF PERFORMING ORGANIZATION

The Weizmann Institute of
Science6b. OFFICE SYMBOL
(If applicable)

7a. NAME OF MONITORING ORGANIZATION

USARDSG-UK

ADDRESS (City, State, and ZIP Code)

Rehovot 76100
Israel

7b. ADDRESS (City, State, and ZIP Code)

Box 65
FPO NY 09510NAME OF FUNDING / SPONSORING
ORGANIZATION

USARDSG-UK ARO-E

6b. OFFICE SYMBOL
(If applicable)

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER

DAJA45-84-C-0036

ADDRESS (City, State, and ZIP Code)

Box 65
FPO NY 09510-1500

10. SOURCE OF FUNDING NUMBERS

PROGRAM
ELEMENT NO.
61102APROJECT
NO.
1L161102BH57TASK
NO.
0WORK UNIT
ACCESSION NO.

TITLE (Include Security Classification)

Grid Adaptation and Parabolic Equations by Multigrid Techniques

PERSONAL AUTHOR(S)

Professor Achi Brandt

TYPE OF REPORT

Final

13b. TIME COVERED

FROM 1984 TO 1987

14. DATE OF REPORT (Year, Month, Day)

1987/10/31

15. PAGE COUNT

10

SUPPLEMENTARY NOTATION

COSATI CODES

FIELD GROUP SUB-GROUP

0 04

0 11

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)

ABSTRACT (Continue on reverse if necessary and identify by block number)

The long-term goal of research at the Weizmann Institute is the development of multi-level methods of solving all types of large-scale problems in science and engineering. In addition to an extensive and diverse development of multigrid solvers for differential and integral equations, completely new multilevel approaches have recently been introduced to the areas of large-scale global optimization, statistical physics and calculations of many-body interactions.

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FEB 19 1988
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DISTRIBUTION / AVAILABILITY OF ABSTRACT

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21. ABSTRACT SECURITY CLASSIFICATION

Unclassified

NAME OF RESPONSIBLE INDIVIDUAL

G.R. Andersen

22b. TELEPHONE (Include Area Code)

01-409 4423

22c. OFFICE SYMBOL

AMXSN-UK-RP

FORM 1473, 84 MAR

83 APR edition may be used until exhausted

All other editions are obsolete

SECURITY CLASSIFICATION OF THIS PAGE
Unclassified

United States Army Contract No.

DAJA 45-84-C-0036

**Grid Adaptation and Parabolic Equations by
Multigrid Techniques**

Final Technical Report

Covering November 1, 1984 — October 31, 1987

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DTIC TAB	☐
Unannounced	☐
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Availability Codes	
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1. General

→ The long-term goal of our research at the Weizmann Institute is the development of multi-level methods for solving all types of large-scale problems in science and engineering. In addition to an extensive and diverse development of multigrid solvers for differential and integral equations, completely new multilevel approaches have recently been introduced to the areas of large-scale global optimization, statistical physics and calculation of many-body interactions (see our review, [1]).

The three-year contract summarized below has undertaken two multigrid themes: grid adaptation and time-dependent problems. Due to some personnel reasons, it turned out that during the first year and part of the second the main advance had been in the first theme, while in the second phase effort has been concentrated in the latter. The paper summarizing our work on grid adaptation has already appeared [2], while the final paper on time-dependent problems is still in preparation, and will be sent later. For scientific reports attached herein — see the list of references.

2. Grid adaptation

Another work. ←

Since our research on multigrid mesh refinement techniques is fully reported in [2], we confine the present description to a brief summary.

→ The purpose of our study was to provide criteria for optimizing mesh sizes near singularities and to develop fast and flexible multigrid methods for creating the nonuniform grids, their difference equations and their solutions. For simplicity, the Poisson problem was studied, with singularities introduced either in the forcing terms (algebraic singularities or sources) or in the shape of the boundaries (reentrant corners). Local refinements were created by multigrid structures in which some extra finer levels cover increasingly narrower neighborhoods of the singularity, as proposed in [3]. The main innovations developed under the present contract are described below.

2.1 Local relaxation sweeps

Structural singularities, such as reentrant corners or discontinuities in coefficients (of the interior or boundary differential operators) result in degraded multigrid performance for the following two reasons: 1) Error components slow to converge in relaxation are approximate solutions of the homogeneous differential equation. Near a structural singularity components of this type can have large derivatives and hence large errors in their interpolation from any coarse-grid

approximation. 2) When transferring residuals from a fine grid to a coarse one, unusual weighting should be given to residuals near the singularity.

Experiments show that the asymptotic convergence degrades only when V cycles (not when W cycles) are used, and especially when the number of levels is large. Which is why this trouble particularly bothers us when local refinements (needed near structural singularities for accuracy purposes) are used: With local refinements many levels are usually introduced, and W cycles are prohibitively expensive (since the number of points on coarse levels is not necessarily small compared to that on fine levels).

We have therefore developed a general approach to obtain the full efficiency of multigrid V cycles despite structural singularities. The technique is to make special local relaxation passes over a small number of points near the singularity. This eliminates the large interpolation errors (which are large only locally there) and reduces large local residuals, hence making their correct weighting immaterial.

Experiments with this approach were conducted on the Poisson problem with Dirichlet boundary conditions in a domain with a 2π re-entrant boundary. They showed that the same asymptotic convergence rates as in regular problems (i.e., as in the Poisson problem on regular domains) can be obtained by applying, on each grid at its turn, one local relaxation pass over a few points near the singularity before each usual relaxation sweep over the entire grid. The number of points where the local relaxation should be performed is a small fraction of the entire grid, hence the amount of extra computations involved in the special passes is negligible compared to the usual multigrid work.

Incidentally, the technique of extra relaxation sweeps over a small region near the boundary was later incorporated into a general rigorous theory of multigrid solvers. It is used even in some cases without structural singularities, to ensure that the "interior convergence factor" is always attained (see [4]).

2.2 The λ -FMG algorithm

A general technique for treating singularities is by local mesh refinement. As mentioned above, a method for creating local refinements as a natural part of multigrid fast solvers had been suggested in [3, §8] and [5, §9], and was further studied by us as part of this contract.

The main question we first treated is how to modify the FMG algorithm [5, §7] for the situation where many levels of local refinements are created. In that situation, when finer levels cover much smaller subdomains, the number of gridpoints on coarser levels is not necessarily small in comparison to their number on finer levels, hence the work expended on coarser levels by the usual FMG algorithm is much too large.

A modified algorithm, called λ -FMG, has been devised. It is based on the same exchange rate (the Lagrange multiplier λ) used in the grid-adaptation equations (see [3, §8]). For each value of λ these equations determine a set of local-refinement grids on which the problem should be discretized. The λ -FMG algorithm uses a sequence $\lambda_0 > \lambda_1 > \lambda_2 > \dots$ of exchange-rate values, where λ_0 is large so that its set of local-refinement grids is relatively coarse, giving a crude solution for a small amount of work, and $\lambda_i = \alpha \lambda_{i-1}$, with constant factor $\alpha < 1$. For each λ_i ($i \geq 1$), the first approximation is obtained by interpolating the λ_{i-1} solution from the λ_{i-1} set of grids into the λ_i set. Assuming λ_{i-1} to be close enough to λ_i , this first approximation is such that a multigrid cycle with only a small number of relaxation sweeps on each grid of λ_i is required to obtain the λ_i solution to within truncation errors.

A detailed analysis shows that the efficiency of the algorithms is not sensitive to the exact value of $\alpha = \lambda_i / \lambda_{i-1}$. For example, for second-order problems in two dimensions, any value of α roughly in the range $.02 \leq \alpha \leq .25$ will give results close to optimal. In our numerical experiments $\alpha = 1/16 = .0625$ was taken.

The numerical experiments were first carried out for a problem with right-hand side singularity, in order to separate the above question (the efficiency of FMG) from other questions (specific to structural singularities; see §2.1). Namely, we have solved the equation $\Delta u = \gamma^2 r^{\gamma-2}$ on the square $\{0 \leq x \leq R_0, 0 \leq y \leq R_0\}$ where r is the distance from the corner $(0,0)$. The Dirichlet boundary conditions were such that the exact solution is $u = r^\gamma$. The known solution allows us to make precise comparisons of algebraic errors with truncation errors.

We then experimented also with the problem with 2π reentrant corner, aided by local relaxation sweeps as described above (§2.1). The boundary conditions were chosen so that the exact solution of the differential equations was $u = r^{1/2} \sin \varphi/2$, where (r, φ) are radial coordinates such that the re-entrant corner is at $r = 0$ and the re-entrant boundary is at $\varphi = 0$ and $\varphi = 2\pi$. This solution exhibits the typical singularity at such a corner.

The grid-adaptation equations [3, §8] yield for each of these problems a set of grids where the finest meshsize h at distance r from the singularity is given by a known rule $h = h(r, \lambda)$. For example, for the right-hand singularity problem $h = O(\lambda^{1/4} r^{(2-\gamma)/4})$. We have used for each λ a set of grids approximately satisfying this rule, and applied the λ -FMG algorithm described above. Two important results were established:

1. The λ -FMG algorithm solves the equations in linear times; i.e., for each problem, the solution time is proportional to the total number of gridpoints on all levels. (The usual FMG algorithm falls far behind such linear dependence in the case under study, because of the many levels of local refinements).
2. Due to the optimal choice of h as a function of r and the above efficiency of the λ -FMG, each problem was solved in the same over-all accuracy-to-

work convergence rate as a regular problem. Namely, despite the singularity, the error E in approximating the true differential solution decreases as W^{-1} , where W is the over-all computational work; this rate $E = O(W^{-1})$ is the best possible for any second-order approximation to any two-dimensional problem.

2.3 Interior singularity. Conservative local refinement

Source singularities and other interior singularities appear in many applications. As a model we took the equation $\Delta u(x, y) = 4\pi\delta$, where δ is the Dirac's distribution, with boundary conditions that yield the solution $u = \log(x^2 + y^2)$. The singularity is at $(0, 0)$, which was placed at the center of the square domain. We tested local refinement techniques on this model. This led to some modifications of those techniques.

First we found that *no* local refinement is really needed to obtain regular accuracy *far* from the source: if the second-order differencing is in conservation form, and if the correct source strength is represented, then solution errors are always $O(h^2/r^2)$ at distance r from the source. Furthermore, adding *non-conservative* local refinements very substantially *increases* these errors — proportionately in fact to the spurious (numerically created) fluxes. It is therefore important to use *conservative local refinements*.

We have developed a general approach to maintain conservation where local refinements are introduced. The FAS coarse grid equations near the refinement boundary are suitably modified for this purpose: a special term is added to the fine-to-coarse defect correction τ .

Using such conservative refinements for the above model problem gave the accuracy one should expect. That is, the solution error at distance r from the source is $O(h(r)^2/r^2)$, where $h(r)$ is the largest meshsize at distances up to r from the source.

It was also realized that the general criteria for grid refinement [5, §9.5] should be modified in case of interior singularities, so as to take into account the large cancellations among the large contributions to the error functional from the local truncation errors (τ) near the singularity. Such cancellations are typically achieved if conservative discretization is used.

3. Multigrid for time-dependent problems

A preliminary description of the results of our contract work on time-dependent (primarily parabolic) problems is contained in [6]. Two detailed papers are under preparation, containing results from more extensive numerical studies. It has taken

longer than expected, since a student who worked on this project (E. Gendler) could not stay with us, and his ad-hoc programs needed major re-writing. In fact, we are still busy calculating results and producing graphs needed to present a comprehensive and convincing account of the new techniques. We will send this account to the U.S. Army as soon as it is completed. Here we summarize the main points; for detailed formulae and sample tests see [6].

3.1 Multigrid solvers for implicit systems

Some time-dependent problems may need no multileveling. These are hyperbolic schemes where all the characteristic velocities are comparable to each other, and their explicit discretization on one grid is therefore fully effective: the amount of processing is essentially equal to the amount of physical information. However, as soon as any stiffness enters, implicit discretization and multigrid techniques become important.

The multigrid algorithm can first simply be used at each time step as a fast solver for the system of equations arising from the implicit discretization. This use could be considered quite straightforward, but it did produce some confusion among several investigators, mainly with regard to the following two questions:

(i) In the usual full-multigrid (FMG) algorithm for steady-state problems, the first approximation to the solution on a fine grid is obtained by interpolating from a coarse-grid approximation (see [1, §4] or details in [5, §7]). In case of evolution problems, should the first approximation still be taken from the coarser grid, or should it simply be the solution at the previous time step?

(ii) The FMG algorithm in case of steady-state problems usually solves the problem in one cycle; i.e., starting from the above first approximation, *one* multigrid correction cycle (usually a *V* cycle; for some problems a *W* cycle) is all one needs to obtain algebraic errors small compared with the truncation (discretization) errors. Hence the algorithm is called *1-FMG (op.cit.)*. In case of time-dependent problems, at each time step one needs to solve to the level of the *incremental* truncation error, i.e., the (much smaller) discretization error added at that time step, not to the level of the *accumulated* truncation error. Is the 1-FMG powerful enough to do that?

The simultaneous answer to these two questions is that *the 1-FMG algorithm should be consistently applied to the incremental problem*, and then it will easily obtain algebraic errors small compared to the *incremental* truncation error. In case of linear problems this can be done by writing the system of equations as equations for the *increment* (the difference between the solution and the solution at the previous time step), and applying the 1-FMG algorithm for this new system. As a result, for example, the first approximation on the fine grid will effectively be the *sum* of the previous-time solution and an interpolated-from-the-coarser-grid

first approximation to the *increment*. In case of nonlinear problems, the same can be done by using the FAS-type multigrid formulation ([1, §7] or [5, §8]).

To demonstrate the above, we have conducted detailed tests with second-order Crank-Nicolson discretization of the heat equations, with various types of initial conditions: smooth, highly oscillatory, and discontinuous. In all cases a 1-FMG algorithm, employing $V(1, 1)$ (i.e., a V cycle with one pre-relaxation and one post-relaxation; cf. [1, §4] or [5, Fig. 1.1]) or $V(2, 0)$ cycles, was used at each time step. We tested cases where the errors can be exactly calculated, and showed that the remaining algebraic errors were indeed negligible compared to the truncation errors. We have also showed that some wrong multigrid approaches produce far worse results.

The computational cost of the 1-FMG solver at each time step is several (typically 6) "work units", independently of h and k (the meshsize and the time-step-size), where the work unit is the computational work of one explicit time step. For many types of problems, advanced multigrid techniques, discussed next, even reduce the required work much further, to a fraction of a work unit per time step, while other multigrid procedures (discussed in Secs. 3.3 and 3.4) inexpensively enhance accuracy and cure some possible bad features of the usual discretization.

3.2 Frozen τ techniques

In many problems, notably in parabolic ones, at most locations during most of the time the increment function is very smooth, hence seldom requires fine-grid processing. In the heat equation $u_t = \Delta u + F$, for example, the increment can be *non-smooth* only near non-smooth initial or boundary conditions or near non-smooth *changes* in F , where "near" means distance $O(h)$ in space and $O(h^2)$ in time.

The frozen- τ technique is a method to avoid unnecessary fine-grid processing. It was described in [7, §3.9]. It is based on the FAS multigrid formulation [5 §8]. The finest grid is employed only once per many times steps. When it is not employed, its τ corrections to the next-coarser-grid equations (see [5, §8.2]) are calculated from previous times (assuming their decay in time is proportional to the decay shown in the coarser-grid solution norm). The next coarser grid is similarly skipped: It is employed only twice as often as the finest; and so on. Returning to a grid after an unemployment interval, its values are first calculated from its former values (assuming again a decay proportional to the decay in the coarser-grid solution norm), and then corrected from the coarser grid values by FAS interpolation (Eq. (8.6) in [5]).

Automatic criteria to decide at what time a return should be made to a finer level have been described in [7, §3.9]. Since the criteria can be employed *locally*, finer levels can be activated only *when* and *where* needed.

In the present research the automatic criteria were not implemented. Our primary aim was to demonstrate, through a simple example, the huge reduction obtainable in the computational effort by a uniform use of frozen- τ techniques for uniform problems. For this purpose we chose the above heat equation in a square domain with periodic boundary conditions and with arbitrary initial conditions. Since we want to solve to the level of fine-grid truncation errors, the more difficult case is $F = 0$, where the solution, and hence also the truncation errors, tend to zero as $t \rightarrow \infty$. We thus examined this case in particular. In this case exact solutions to the differential and discrete equations based on Fourier series can be calculated. They have been incorporated into our programs for comparison purposes.

We defined as our target truncation errors the *spatial* truncation error; i.e., the difference between the true differential solution and the solution obtained when our space discretization (the usual 5-point $O(h^2)$ discretization) is used with vanishing time step (the "method of lines"). This is the error level below which we wanted to solve, by applying the Crank-Nicolson discretization together with the frozen τ approach.

Simple order-of-magnitude analysis shows that, if our finest meshsize is h , any grid with meshsize H should be visited once per time interval $\delta t = O(tH/h^3)$, where t is the time from the (potentially non-smooth) initial conditions. Implementing this rule in our algorithm, we have indeed confirmed that our differential error (the difference between our solution and the differential solution) was always comparable to the spatial truncation error. This has been demonstrated for both smooth and non-smooth initial conditions.

From the rule we implemented, it is readily seen that the total work in solving (to the level of spatial truncation error) our evolution problem from $t = 0$ to $t = T$ requires only $O(\log(T/h^2))$ work units.

3.3 Double discretization technique

The Crank-Nicolson (CN) discretization is the least expensive and most convenient stable scheme with second order accuracy in both the meshsize h and the time step k . It has, however, one serious flaw for $k \gg h^2$: Transient highest spatial frequencies (transient Fourier components with wavelength close to $2h$), which in the differential solution decay almost completely in time k , hardly decay at all at each time step (only their sign is flipped). In another simple stable discretization, the Fully-Implicit (FI) scheme, such components properly decay in one time step, but accuracy is only first order in k (hence $k \gg h^2$ does not really make sense).

This situation can be described as a conflict between low frequencies (for which CN is better) and high ones (for which FI is better; accuracy order is irrelevant for non-smooth components). In multigrid processing the latter are treated only at fine-grid relaxation, while the former are effectively determined by the coarse-

grid corrections. It is therefore possible to resolve the conflict by using the two discretization schemes at different parts of the algorithm (similar to the "double discretization" schemes in steady-state multigrid solvers; see [5, §10.2]): CN is used in most places, but it is replaced by FI at relaxation on the finest grids during the first time steps. CN is still used, even on each of those finest grids even during the first time steps, for calculating the residuals transferred to the next coarser grid.

We have tested this approach on our model heat problem, and found the expected behavior: while slowly decaying high frequencies were completely eliminated, the CN accuracy was always maintained, both for smooth and discontinuous initial data.

Not concluded yet are tests which combine this double discretization approach with frozen τ (Sec. 3.2). We expect this to be a powerful combination.

3.4 τ extrapolation

In multigrid solvers for *steady-state* problems, " τ extrapolation" [5, §8.4] is a local h extrapolation based on the fine-to-coarse correction τ_h^H appearing in the FAS formulation. It is used to obtain a higher order approximation for little extra work, without employing higher order discretization formulae. It is more useful than the Richardson extrapolation since it is local (extrapolating the equation, not the solution), hence it can be used even when global extrapolation is not available. It can be used for example together with any procedure of local refinements.

We have developed and tested a similar method for time dependent problems. The FAS multigrid formulation is used as in the frozen τ technique, so its fine-to-coarse defect correction $\tau_{h,k}^{H,K}$ is calculated, where $H = 2h$ is the coarse-grid meshsize and K is the time step for which the correction is calculated. Choosing $K = 2k$ in case of CN discretization, and replacing $\tau_{h,k}^{H,K}$ by $\frac{4}{3}\tau_{h,k}^{H,K}$, can be shown to formally raise the approximation order from $O(h^2 + k^2)$ to $O(h^4 + k^4)$.

We have tried doing this for the model heat problem described above. It was found that this τ extrapolation indeed considerably reduced truncation errors, but to obtain real fourth order approximation we had to use fourth-order restriction (fine-to-coarse transfer).

The reduced truncation errors of course makes the task of solving to the level of these errors more difficult, hence requires modification in how often a finer grid should be visited in a frozen- τ method (see Sec. 3.2). This question, as well as the combination of τ extrapolations with the CN-FI double discretization technique, require further investigations.

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