EXPERIMENTAL RESULTS FOR MULTIGRID AND TRANSPORT PROBLEMS

by

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Abstract

An experimental study of the applicability of a multigrid algorithm to the solution of the neutron transport problem in a slab is described. Only the simplest choices are made for the components of the algorithm. Experimental results indicate that the coarse grid operator obtained from finite differences works better and is cheaper than the Galerkin choice.

1 Introduction

In this report the application of a multigrid algorithm to solving the neutron transport in a slab problem is discussed. The goal of this experimental study, simply put, is to observe whether such an algorithm is applicable to the neutron transport problem and to compare the multigrid algorithm to a classical algorithm, in this case damped Jacobi.

For the multigrid implementation only the simplest, and perhaps most naive, choises are made for the various components. This demonstrates that a 'quick and dirty' implementation is feasible. From a computational standpoint two coarse grid operators are compared, the usual Galerkin choice and the operator obtained from finite differences. Surprisingly, the finite difference operator works better and is cheaper than the Galerkin choice.

The report is organized as follows: Section 2 describes the particular problem that was solved. In Section 3 the discrete problem is described along with the Jacobi iterative scheme. The multigrid scheme is detailed in Section 4 and the experimental results are discussed in Section 5. Finally, Section 6 contains some concluding remarks. The derivation in Section 2 can be found in the book by Wing [Wing62a] while the books by Chandrasekhar [Chan60a] and by Lewis and Miller [Lewi84a] provide additional insight into the problem.

2 The Problem

Let the slab width a be chosen, then the goal in the general case is to determine the neutron density, $\psi(\mu; x)$, satisfying

$$\mu \frac{\partial \psi}{\partial x} + \sigma(x)\psi = \frac{1}{2}\gamma\sigma(x) \int_{-1}^{1} \psi(\mu; x)\, d\mu + S \tag{1}$$

with boundary conditions

$$\begin{aligned} \psi(\mu, 0) &= g_1(\mu), \qquad \mu > 0 \\ \psi(\mu, a) &= g_2(\mu) \qquad \mu < 0. \end{aligned}$$

Here $\sigma(x)$ is the cross section of the material. Define

$$H_\mu = \mu \frac{\partial}{\partial x} + \sigma(x) I$$

and

$$L\cdot = \frac{1}{2}\sigma(x)\int_{-1}^{1}\cdot\, d\mu.$$

Then (1) is equivalent to

$$H_\mu\psi = \gamma L\psi + S$$

or

$$\psi = H_\mu^{-1}\gamma L\psi + S_1. \tag{2}$$

Applying L to both sides of (2) and multiplying by γ gives

$$\gamma L\psi = \gamma L H_\mu^{-1}\gamma L\psi + \gamma L S_1.$$

Finally, define

$$K\cdot \equiv LH_\mu^{-1}\cdot = \frac{1}{2}\int_{-1}^{1} H_\mu^{-1}\cdot\, d\mu$$

and call

$$\phi = \gamma L\psi.$$

Then (1) is seen to be equivalent to

$$\phi = \gamma K\phi + \gamma L S_1$$

or

$$(I - \gamma K)\phi = \gamma L S_1 = S_2. \tag{3}$$

It is important to note that in the case $\sigma(x) \equiv 1$ that

$$K\phi(x) = \frac{1}{2}\int_0^a E_1(|x-y|)\phi dy$$

where E_1 is the exponential integral

$$E_n(x) = \int_0^\infty \frac{e^{-sx}}{s^n} ds.$$

The method of solution described here, however, does not use the relationship between K and E_1. In particular this allows the treatment of problems where $\sigma \not\equiv 1$.

Once $\phi(x)$ is determined, to obtain the density $\psi(x;\mu)$ note that

$$\phi(x) = \frac{1}{2}\gamma\sigma(x)\int_{-1}^{1}\psi(x;\mu)d\mu + S_2,$$

so

$$\mu \frac{\partial \psi}{\partial x} + \sigma(x)\psi(x;\mu) = \phi(x) + S.$$

For later use define

$$M = (I - \gamma K) \tag{4}$$

and problem (3) is written

$$M\phi = S_2. \tag{5}$$

It is problem (3) that is solved in the succeeding sections.

3 The Discrete Problem

The first step in computing the numerical solution of (3) is to discretize

$$\Omega = [0, a]$$

into $N - 1$ evenly spaced pieces each of width

$$h = \frac{1}{N-1}.$$

The discrete points are thus the points $x_i = ih$ with $0 \leq i \leq N$. A solution to (3) is desired at each of the unknowns $\phi(x_i)$, which are denoted ϕ_i.

The discrete analogue of (5) is written

$$M_h \phi = S_2 \tag{6}$$

where M_h is the discrete analogue of the operator M.

For both the Jacobi scheme and the multigrid algorithm it is necessary to approximate $K\phi$. Recall that

$$K\cdot = \frac{1}{2}\int_{-1}^{1} H_\mu^{-1} \cdot \, d\mu. \tag{7}$$

The integral in (7) is approximated by the six point Gauss-Legendre rule

$$\int_{-1}^{1} f \, dx \approx \sum_{j=1}^{6} \mu_j f(x_j).$$

In addition, the equation

$$H_\mu^{-1} V = \phi$$

is equivalent to solving

$$\mu \frac{\partial}{\partial x} V + V = \phi \tag{8}$$

for each of the μ_j used in the Gauss-Legendre rule. Again, the boundary conditions are

$$\begin{aligned} V(\mu, 0) &= g_1(\mu), \qquad \text{for } \mu > 0 \\ V(\mu, a) &= g_2(\mu) \qquad \text{for } \mu < 0. \end{aligned}$$

For this study the trapezoid rule is used to solve (8). This results in, for example for $\mu_j > 0$, evaluating

$$\int_x^{x+h} V(\mu_j, x) \approx \frac{h}{2}[\phi(x+h) - V(x+h) + \phi(x) - V(x)].$$

In other words, for $\mu_j > 0$,

$$V_i = \frac{2\mu_j - h}{2\mu_j + h} V_{i-1} + \frac{h}{2\mu_j + h}[\phi_i + \phi_{i-1}]$$

with $V_0 = g_1(\mu_j)$ given. Similarly for $\mu_j < 0$ the integration proceeds backwards starting at $x = a$. Given

$$V_{N+1} = V(a; \mu_j) = g_2(a),$$

set

$$V_i = \frac{2\mu_j + h}{2\mu_j - h} V_{i+1} - \frac{h}{2\mu_j - h}[\phi_i + \phi_{i+1}].$$

Finally, to compute $K\phi$, simply sum the V_i as in (7) and the Gauss-Legendre rule; set

$$[K\phi]_i = \frac{1}{2} \sum_{j=1}^{6} \mu_j V_i.$$

Of course during the computation it is not necessary to store the values of V_i — just form $[K\phi]_i$ as each V_i is calculated.

3.1 The Jacobi Iterative Scheme

The basic iterative scheme considered is the damped Jacobi scheme with parameter ω. Formally, given ϕ^0 set

$$\phi^{\nu+1} = \phi^{\nu} + \frac{1}{1+\omega}[S_2 - (I - \gamma K)\phi^{\nu}]. \tag{9}$$

For $\omega = 0$ this is simply the Jacobi scheme.

4 The Multigrid Implementation

As has been known for some time iterative improvement is one approach to obtaining an improved estimate to

$$M_h\phi = f \tag{10}$$

given an estimate ϕ^i. Formally, computing χ satisfying

$$(I - \gamma K)\chi = S_2 - (I - \gamma K)\phi^i \tag{11}$$

and setting

$$\phi^{i+1} = \phi^i + \chi$$

solves (10). Unfortunately the problem with this procedure is that solving (11) is as difficult as solving the original problem.

One approach to exploiting the iterative improvement idea is to solve (11) in a lower dimensional space, where less work is required to compute χ. Choose

$$\Omega_{2h} = \left\{ih | i = 1, 2, \ldots, \frac{N+1}{2}\right\}$$

for the lower dimensional space (called Ω_{2h}). In order to communicate (transfer information) between grid functions S_h defined on Ω_h and grid functions S_{2h} defined on Ω_{2h}, interpolation (I_h^{2h}) and restriction (I_h^{2h}) operators are needed.

For the interpolation operator piecewise linear interpolation is used, and for the restriction operator take

$$I_h^{2h} = \frac{1}{2}(I_{2h}^h)^T.$$

Then given ϕ^i, to compute ϕ^{i+1} using the two grid multigrid algorithm

1. Apply m applications of the damped Jacobi scheme to ϕ^i, store the result in $\tilde{\phi}^i$.

2. Restrict the residual to Ω_{2h}: Set

$$R_{2h} = I_h^{2h}[S_2 - (I - \gamma K)\tilde{\phi}^i].$$

3. Solve

$$M_{2h}\chi_{2h} = R_{2h}$$

where M_{2h} is defined later.

4. Correct $\tilde{\phi}^i$ by setting

$$\phi^{i+1} = \tilde{\phi}^i + I_{2h}^h \chi_{2h}.$$

Of coarse the same multigrid procedure can be used recursively (starting with initial guess 0) to compute the solution in step 3; this is called a true multigrid.

Two choices for M_{2h} are considered. In the multigrid literature the usual choice is to take

$$M_{2h} = \hat{M}_{2h} \equiv I_h^{2h} M_h I_{2h}^h.$$

This choice is referred to as the *Galerkin* choice. Unfortunately, unlike in the usual case where M_h is a matrix, it is impossible to form $\hat{M}_{2h}$ directly. Rather only $\hat{M}_{2h}$ acting on a vector can be computed. For the true multigrid cases, where more than two grids are used, the Galerkin choice will still be denoted $\hat{M}_{2h}$, with the understanding that the subscript is related to the size of the coarsest grid.

The second choice for M_{2h} is to take the natural finite difference analogue of M_h on the $2h$ grid Ω_{2h}. This choice of M_{2h} is denoted M_{2h}^{fd}. From a finite difference point of view this is the *natural* choice for M_{2h}.

5 Experimental Results

Both the multigrid algorithm of Section 4 and the Jacobi algorithm of Section 3.1 were implemented and tested. The goals of the experiments were to determine

1. How well the simple damped Jacobi scheme worked at solving problem (3);

2. Whether the multigrid algorithm is applicable to the solution of the transport equation;

3. How does the multigrid algorithm compete with the damped Jacobi algorithm in terms of rate of convergence and work?

4. What rate of convergence is obtained from the multigrid algorithm?

5. Is there any practical difference between using $\hat{M}_{2h}$ and M_{2h}?

5.1 General Remarks About the Experiments

The right hand side was computed by choosing the solution ϕ_{true} and setting

$$S_2 \equiv (I - \gamma K)\phi_{true}.$$

For testing purposes ϕ_{true} was chosen to be

$$\phi_{true}(x_i) = \frac{1}{x_i^2 + 1}.$$

Unfortunately from the standpoint of testing the algorithm there are a myriad of choices of parameters. Among the parameters that can be varied are: the number of points on the finest grid, N; the number of grid layers, g; the value of γ; the slab width a; and the value of the damped Jacobi parameter ω. For the experiments discussed here, N was fixed at 129 and γ was set to .999. All the experiments were run on a CRAY 1 at the Los Alamos National Laboratory.

To determine the rate of convergence the program was allowed to run until

$$\|r^k\|_{l_1} = \|S_2 - (I - \gamma K)\phi^k\|_{l_1}$$

was less than .0005. Then the final observed rate of convergence is

$$\rho_{final} = \frac{\|r^{final}\|_{l_1}}{\|r^{final-1}\|_{l_1}}.$$

Three choices for the slab width, a, were tested; $a = 1$, 10 and 100. The damped Jacobi parameter, ω, was set to run from .1 to 1.9 in increments of .1. For the $\hat{M}_{2h}$ case ω ran

from .1 to .9. So far no heuristic has been found for choosing the optimal ω. In general some form of an adaptive procedure might be used to find the optimal ω.

For the multigrid implementation, to solve the coarse grid equation directly, the same damped Jacobi iteration that appears in Section 3.1 was allowed to run until it convergenced. In a better developed implementation the solver for the coarse grid equations can be optimized. In any case, to compare the rates of convergence of the algorithm the coarse grid solver should be viewed as a 'black box.'

5.2 Numerical Results

The figures in Section 7 display the observed rate of convergence for the various experimental runs that were performed. The dotted line corresponds to $a = 1$, the dashed line corresponds to $a = 10$ and the solid line corresponds to $a = 100$. Note that for some graphs the $a = 1$ and $a = 10$ results overlap. Two situations where the algorithm diverged are noted. In one case the convergence rate tended towards one and eventually became one. This phenomenon happened slowly as the algorithm proceeded. At other times the algorithm diverged dramatically, with a residual on the order of 10^{20}. This would happen quickly, usually after just one iteration. These cases are displayed in the figures by plotting the observed rate as 1.05. The plots labelled 'Galerkin rate' correspond to using $\hat{M}_{2h}$. These runs are very expensive and unfortunately only the runs for ω less than one could be made due to limitations on computer resources.

6 General Conclusions

A number of general conclusions can be made about the experiments. The first is that for large a, $a = 100$, the damped Jacobi algorithm was not a viable solution technique. The algorithm converged too slowly. However, even this naive multigrid implementation worked well for this particular problem. Even when 7 grids were used (1 point on the coarsest grid) the algorithm converged (for $\omega = 1.6$).

From the standpoint of applying the multigrid algorithm it is very important to note that using M_{2h}^{fd} worked at least as well as the usual choice $\hat{M}_{2h}$. Applying $\hat{M}_{2h}$ on the coarser grids is necessary at each stage of the algorithm and is expensive. In particular, computing the coarse grid correction with the damped Jacobi algorithm on grid 3 (33

unknowns), means that

$$\hat{M}_3 = I_{4h}^{8h} I_{2h}^{4h} I_h^{2h} M_h I_{2h}^h I_{4h}^{2h} I_{8h}^{4h}$$

needs to be applied.

During the computation of the coarse grid correction a limit of 5,000 iterations was placed on how many damped Jacobi iterations were performed. For some of the runs this limit was reached. For these cases the 'best' estimate obtained so far was used for the coarse grid correction. This did not seem to affect the rate of convergence of the algorithm. Understandably as the multigrid algorithm proceeded fewer damped Jacobi iterations were required to compute the coarse grid correction. The reason being that as the error tends towards zero, the initial guess, zero, was a better estimate of the eventual solution.

For the *easy* problem, $a = 1$, it appeared that 1.0 was the optimal choice of ω. Unfortunately for *harder* problems, $a = 100$, the choice of the optimal value for ω appears to be related to the number of grids in use.

7 Figures

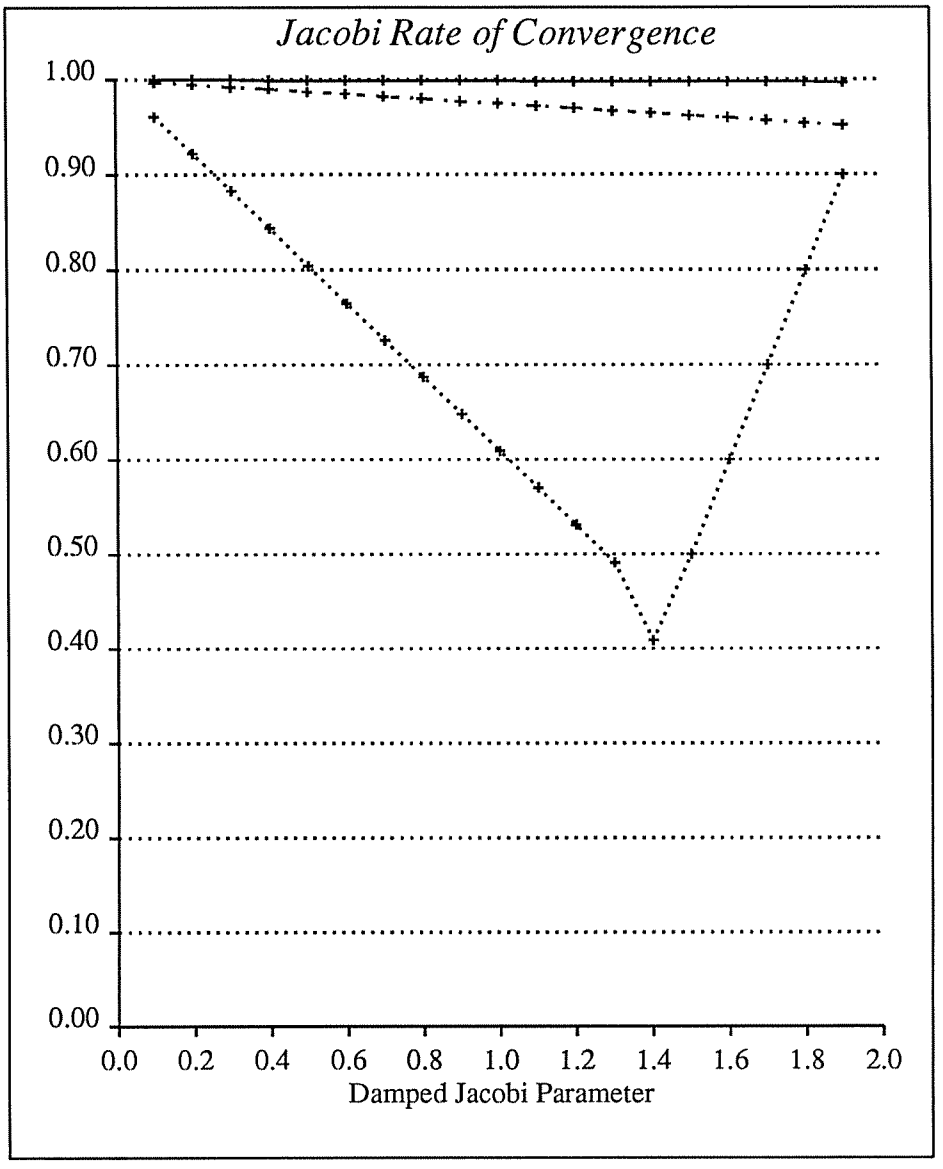

Figure 1: Jacobi Rate of Convergence

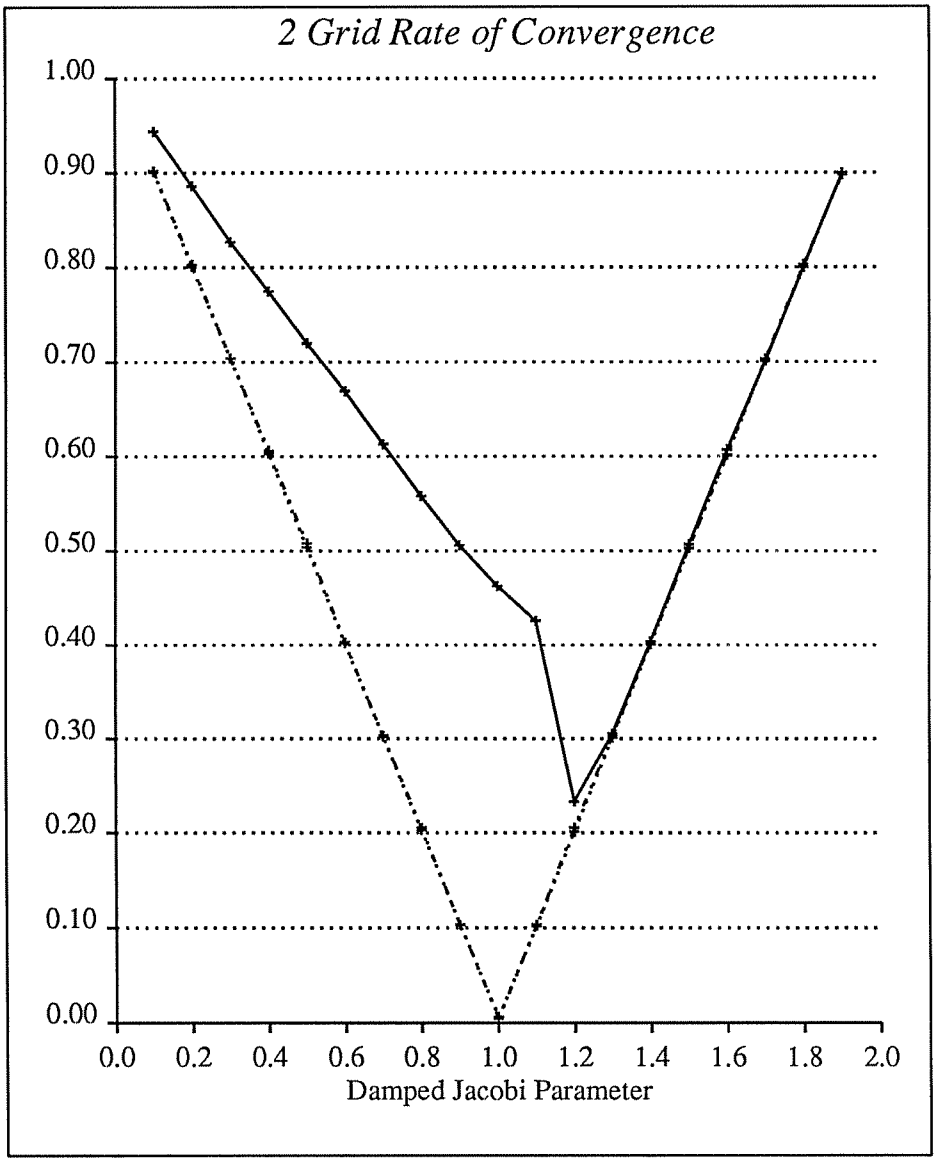

Figure 2: Rate using M_{2h}, 2 grids

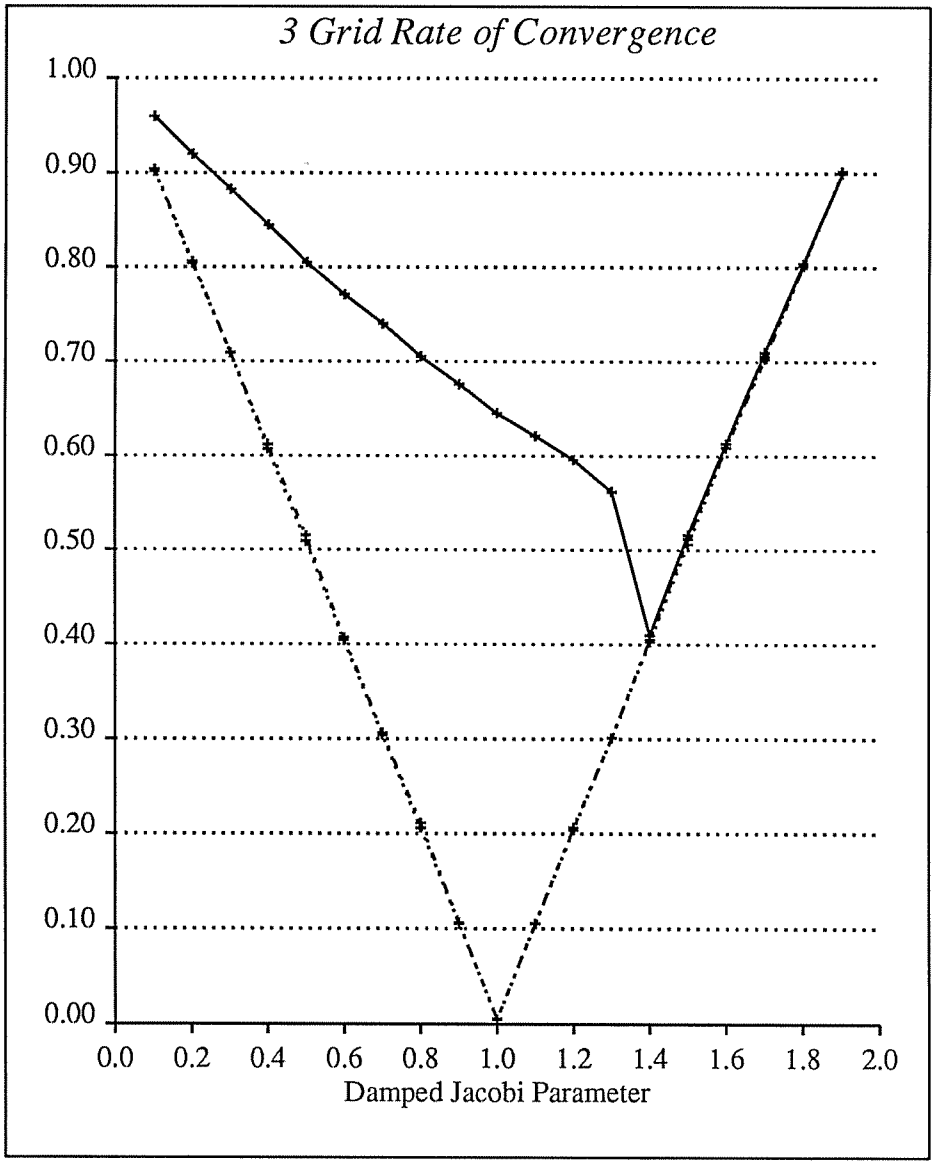

Figure 3: Rate using M_{2h}, 3 grids

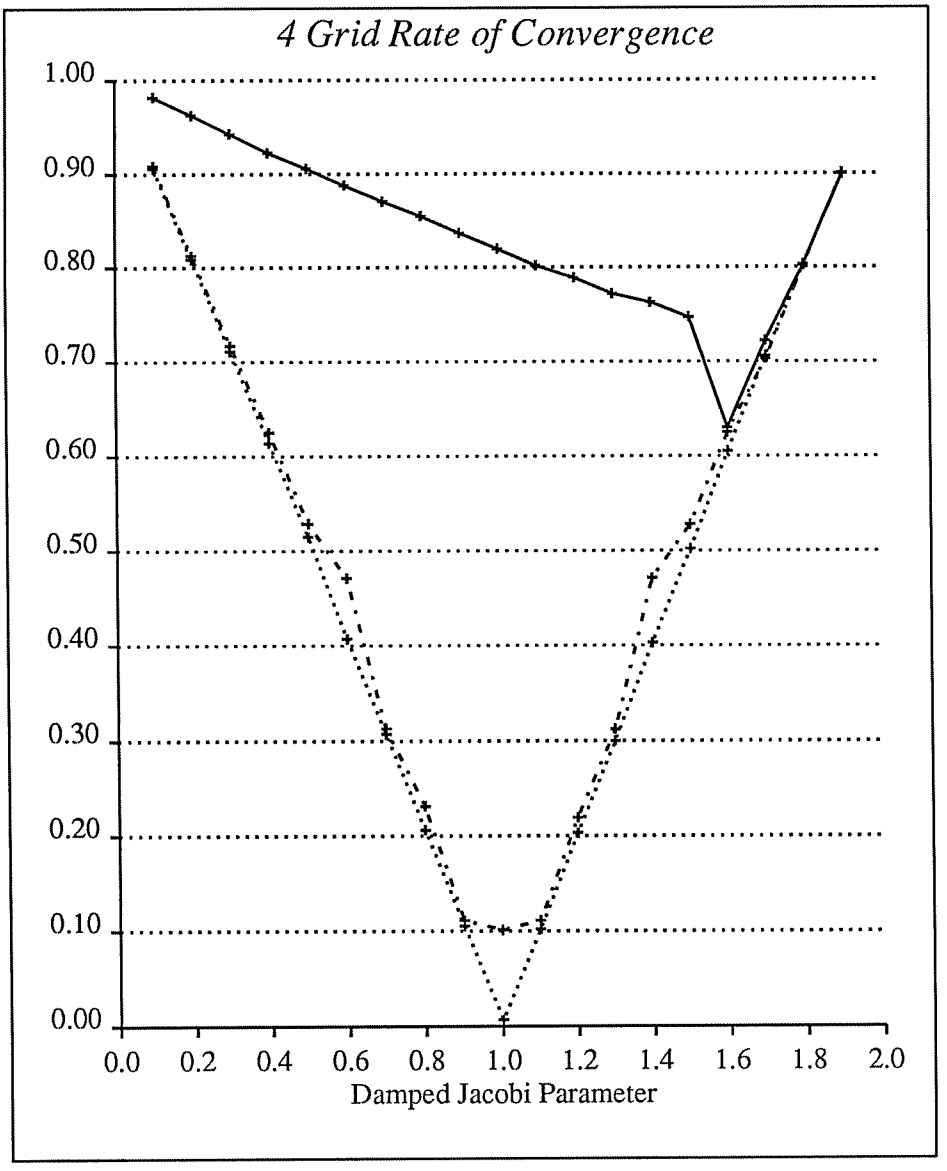

Figure 4: Rate using M_{2h}, 4 grids

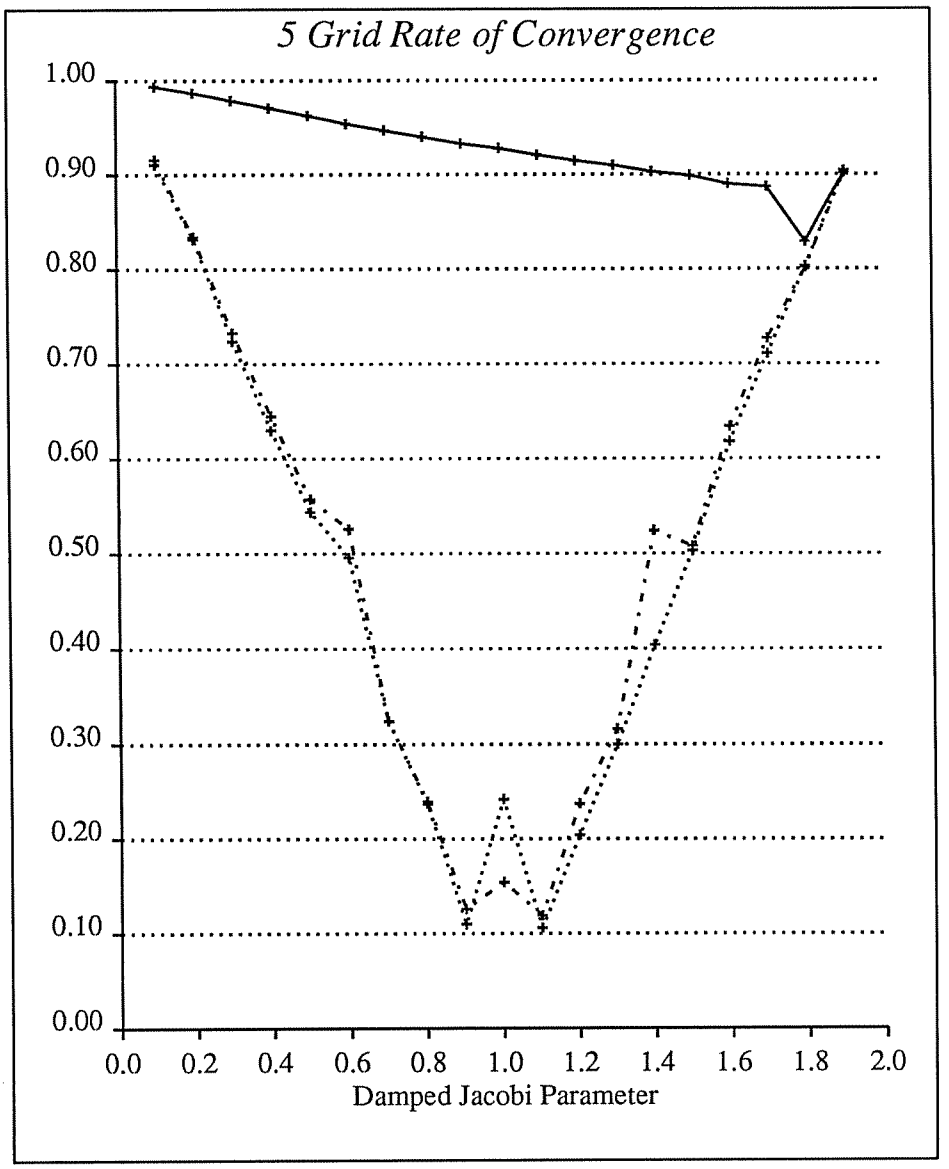

Figure 5: Rate using M_{2h}, 5 grids

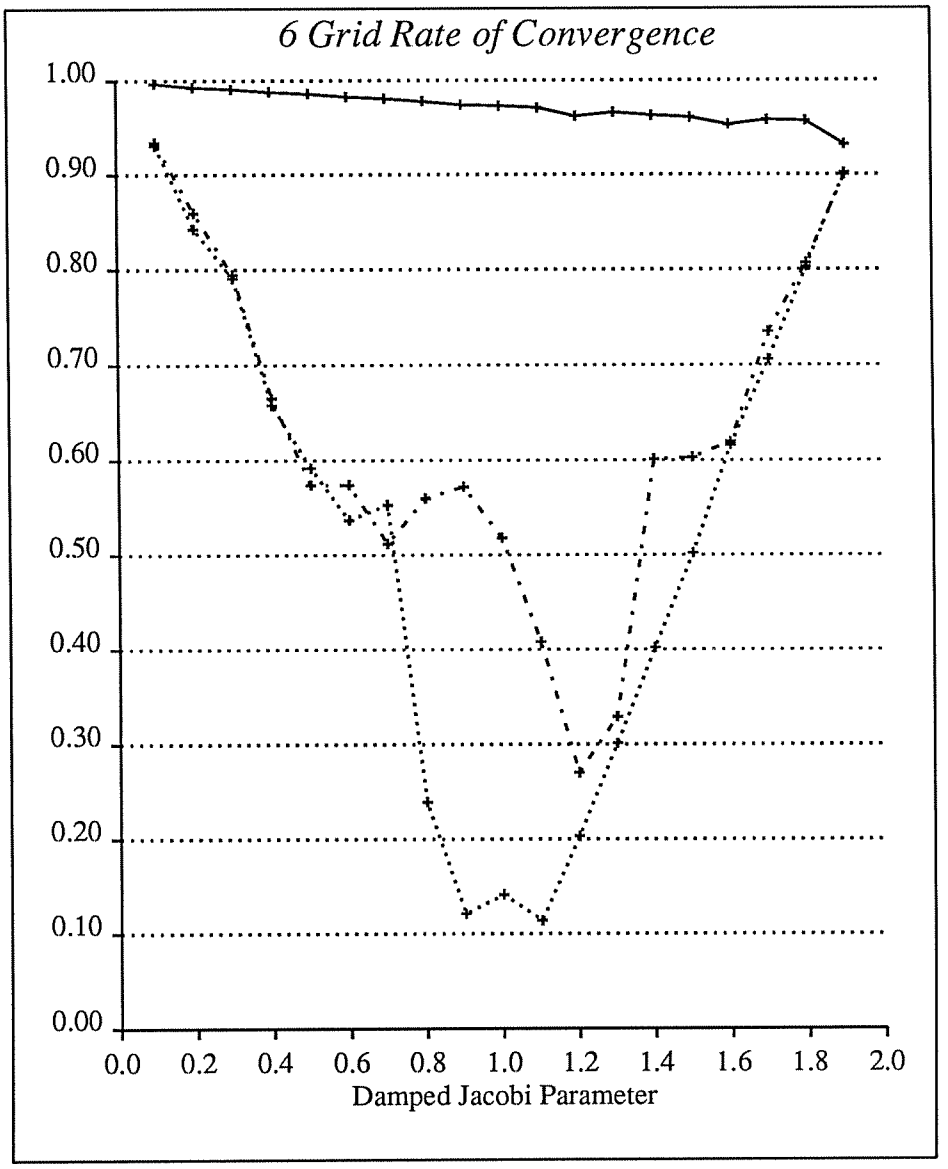

Figure 6: Rate using M_{2h}, 6 grids

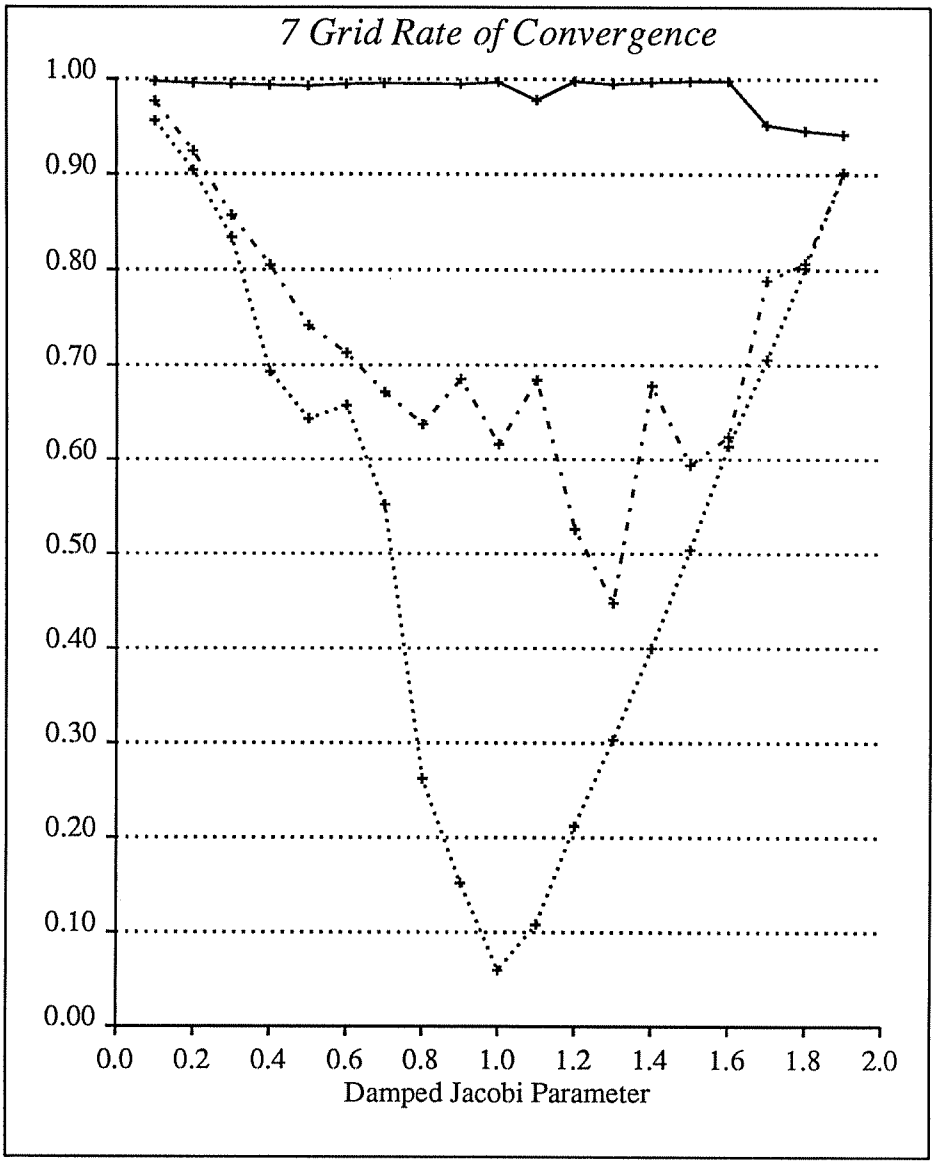

Figure 7: Rate using M_{2h}, 7 grids

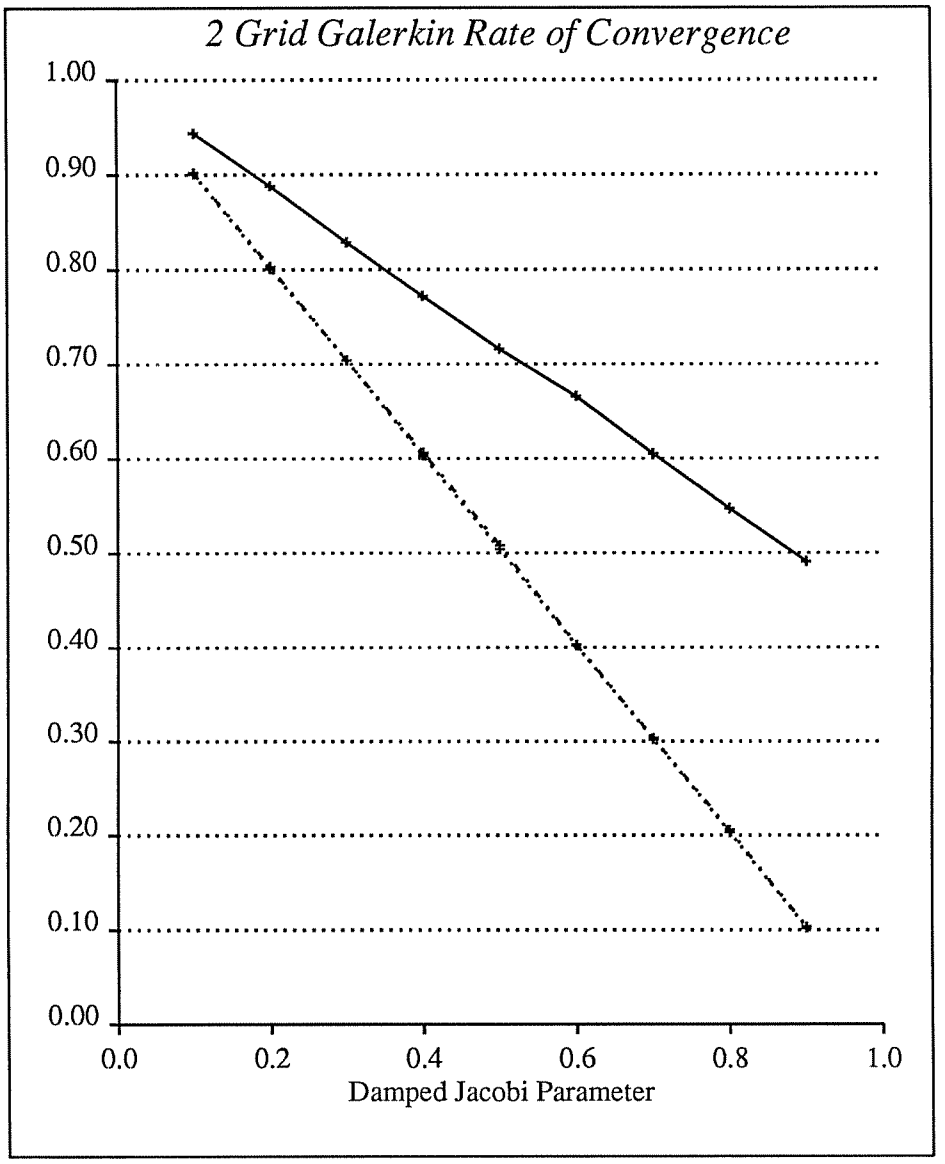

Figure 8: Rate using $\hat{M}_{2h}$, 2 grids

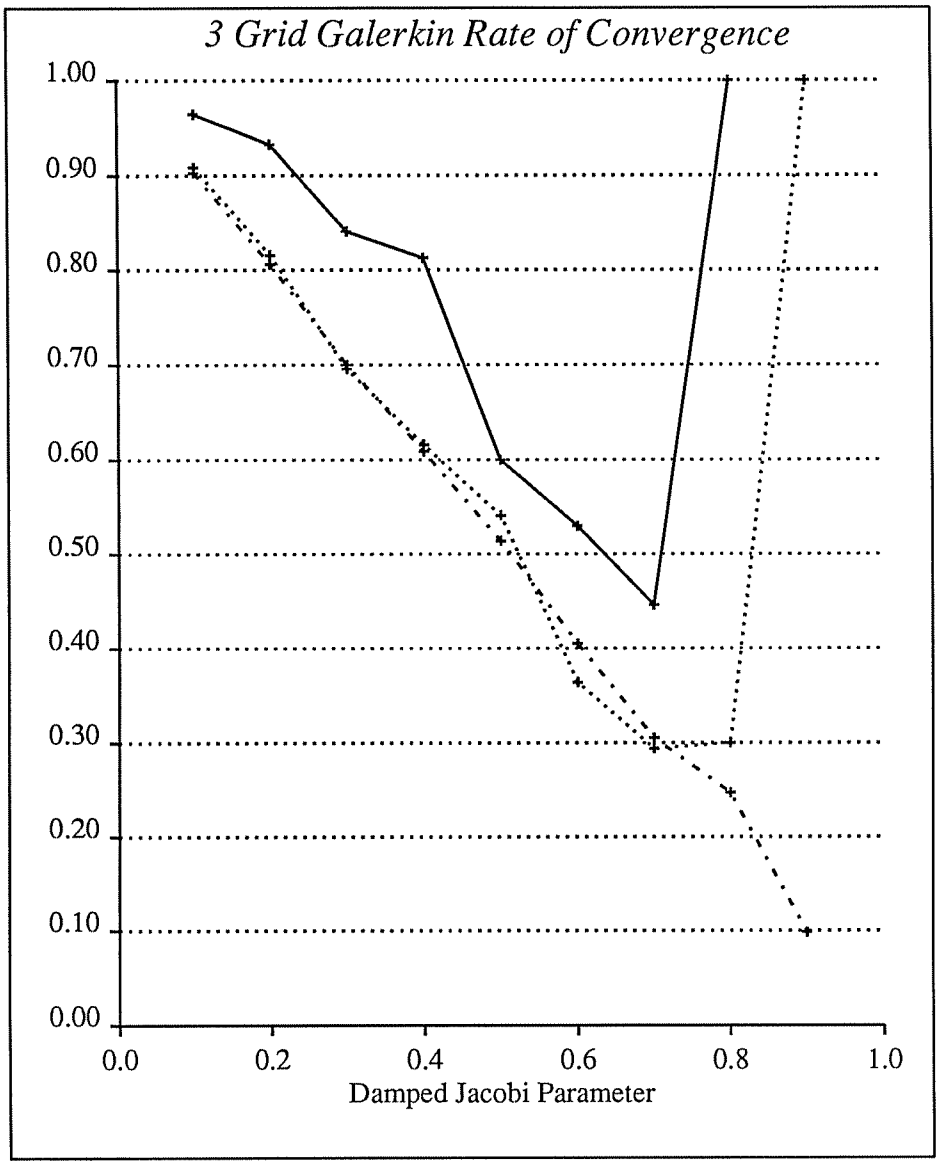

Figure 9: Rate using $\hat{M}_{2h}$, 3 grids

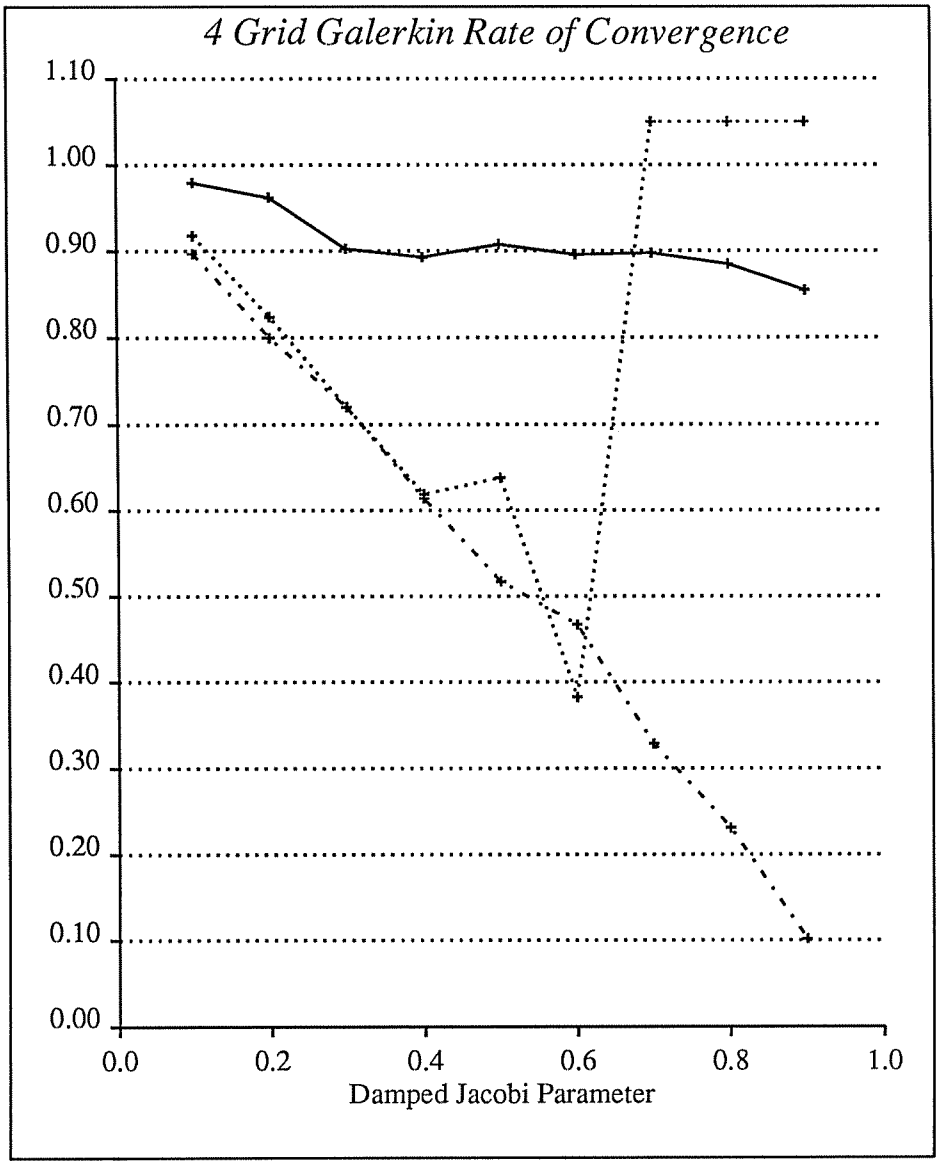

Figure 10: Rate using $\hat{M}_{2h}$, 4 grids

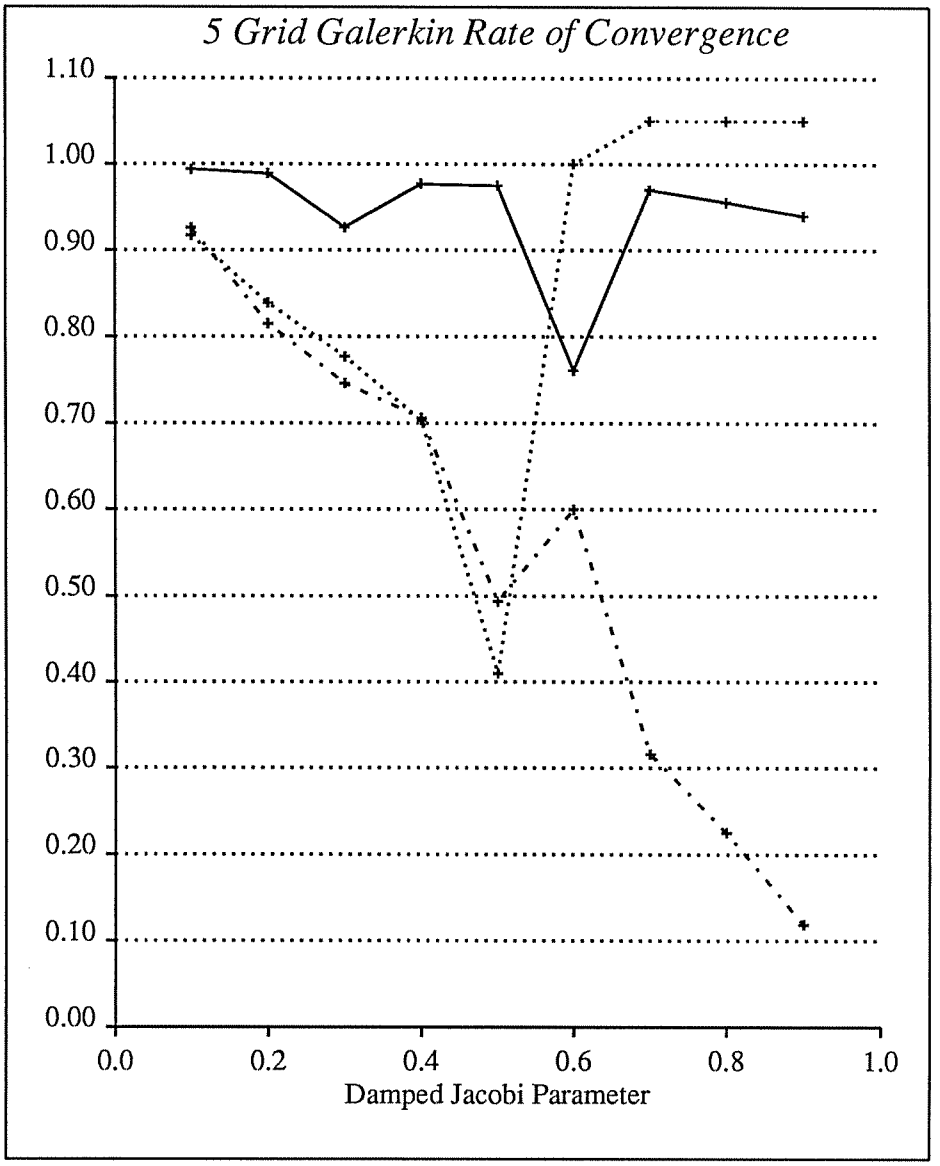

Figure 11: Rate using $\hat{M}_{2h}$, 5 grids

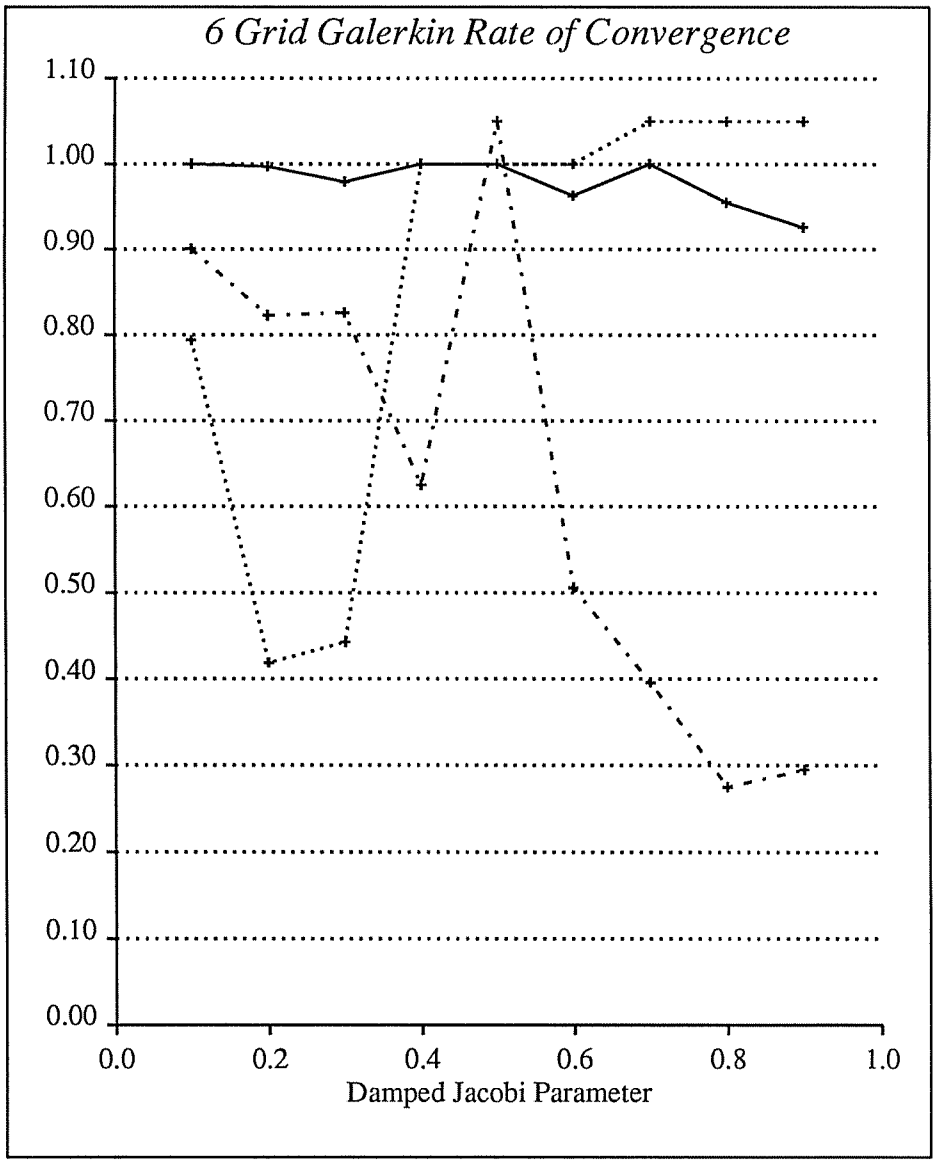

Figure 12: Rate using $\hat{M}_{2h}$, 6 grids

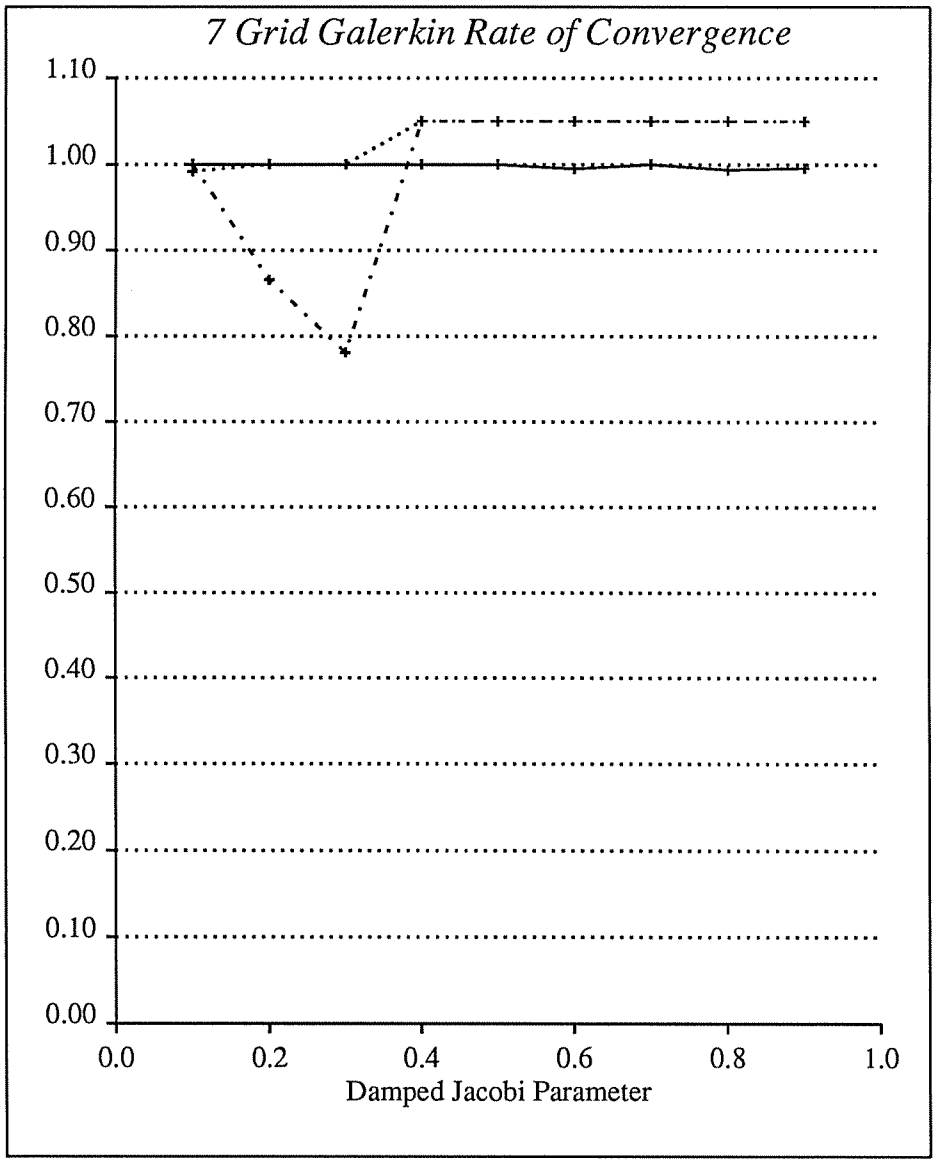

Figure 13: Rate using $\hat{M}_{2h}$, 7 grids

8 References

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