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PRECONDITIONING WAVEFORM RELAXATION ITERATIONS FOR DIFFERENTIAL SYSTEMS *

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Abstract.

We discuss preconditioning and overlapping of waveform relaxation methods for sparse linear differential systems. It is demonstrated that these techniques significantly improve the speed of convergence of the waveform relaxation iterations resulting from application of various modes of block Gauss-Jacobi and block Gauss-Seidel methods to differential systems. Numerical results are presented for linear systems resulting from semi-discretization of the heat equation in one and two space variables. It turns out that overlapping is very effective for the system corresponding to the one-dimensional heat equation and preconditioning is very effective for the system corresponding to the two-dimensional case.

AMS subject classification: 65L05.

Key words: Waveform relaxation, splittings, preconditioning, overlapping, error analysis, parallel computing.

1 Introduction.

Consider the linear system of differential equations

$$\begin{cases} y'(t) + Qy(t) = g(t), & t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{1.1}$$

where Q is a constant matrix of dimension n. Splitting this matrix Q as

$$Q = M - N$$

we can solve the problem (1.1) by the method of successive approximations

$$\begin{cases} \frac{d}{dt} y^{(k+1)}(t) + My^{(k+1)}(t) = Ny^{(k)}(t) + g(t), \\ y^{(k+1)}(t_0) = y_0, \end{cases} \tag{1.2}$$

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where $y^{(0)}$ is a given initial guess. Usually $y^{(0)}(t) = y_0$, $t \in [t_0, T]$. These approximations, also called dynamic iterations or (continuous) waveform relaxation (WR) iterations, were first proposed as computational techniques by Lelarasmee [12] and Lelarasmee et al. [13] for time domain analysis of large differential systems modelling electrical networks (metal oxide semiconductor digital circuits). They were further studied for ordinary differential equations by Nevanlinna [18, 19] and Miekkala and Nevanlinna [16, 17], Skeel [22], Lie and Skålin [14], Lubich [15], Bellen and Zennaro [1] and Bellen et al. [2]. We also refer to a survey paper with emphasis on simulation of large electrical circuits by White et al. [27], to the book by White and Sangiovanni-Vincentelli [26] and to the recent book by Burrage [3].

The choice $M = 0$ (zero matrix) corresponds to the classical Picard-Lindelöf iterations. Let

$$Q = L + \Gamma + U,$$

where L, Γ and U stand for the lower triangular, diagonal and upper triangular part of the matrix Q, respectively. Choosing $M = \Gamma$ or $M = L + \Gamma$ we obtain dynamic analogues of the Gauss-Jacobi and Gauss-Seidel iterations. As in the static case we can also define the block variants of these iterations.

Waveform relaxation methods can be very effective if they converge quickly. Unfortunately, this is not always the case and it is of practical interest to develop techniques for accelerating the convergence of these iterations. The possibility to accelerate the Picard-Lindelöf scheme by taking linear combinations of the iterates is discussed in [15], [20] and [22]. The acceleration of convergence by multigrid techniques was investigated by Vandewalle [25] in the context of waveform relaxation methods for parabolic partial differential equations.

It is the purpose of this paper to investigate the effect of preconditioning the differential system (1.1) on the speed of convergence of the resulting iterative process. This technique, which was also described in [3], will be developed in the next section. It will be demonstrated that if the preconditioning matrix is chosen properly then there is a substantial improvement in the speed of convergence of the resulting iterative scheme over the original one defined by (1.2). The effectiveness of this technique will be demonstrated for many waveform relaxation methods applied to systems of differential equations resulting from semi-discretization of the heat equation in one and two dimensions.

2 Preconditioning of dynamic iterations.

There are many techniques to improve the contractivity properties of the static iterations for large linear systems of equations. Some of these techniques include preconditioning on the left, on the right, or the combination of both. The hope is that the resulting iterative scheme converges faster than the original one. These concepts of preconditioning can be extended in a very general way to the case of dynamic iterations considered in this paper.

The technique of preconditioning on the left in the dynamic case consists of

applying an iterative scheme to the linear system

$$Py'(t) + \overline{Q}y(t) = Pg(t), \quad t \in [t_0, T], \tag{2.1}$$

$\overline{Q} = PQ$, obtained by multiplying (1.1) by some matrix P. Assuming that P and $\overline{Q}$ are split as

$$P = M_p - N_p, \qquad \overline{Q} = M_q - N_q,$$

$\det(M_p) \neq 0$, leads to the dynamic iterations of the form

$$\begin{cases} M_p \frac{d}{dt} y^{(k+1)}(t) + M_q y^{(k+1)}(t) = N_p \frac{d}{dt} y^{(k)}(t) + N_q y^{(k)}(t) + Pg(t), \\ y^{(k+1)}(t_0) = y_0, \end{cases} \tag{2.2}$$

$k = 1, 2, \ldots$, where $y^{(0)}$ is a given initial guess. Putting

$$\begin{aligned} \mathcal{K}y(t) &= A_1 y(t) + \int_{t_0}^{t} e^{M_p^{-1} M_q (s-t)} A_2 y(s)\, ds, \\ \phi(t) &= e^{M_p^{-1} M_q (t_0 - t)} (I - A_1) y_0 \\ &\quad + \int_{t_0}^{t} e^{M_p^{-1} M_q (s-t)} M_p^{-1} P g(s)\, ds, \end{aligned}$$

where

$$A_1 = M_p^{-1} N_p, \qquad A_2 = M_p^{-1}(N_q - M_q M_p^{-1} N_p),$$

the scheme (2.2) can be written as a fixed point iteration process of the form

$$y^{(k+1)}(t) = \mathcal{K} y^{(k)}(t) + \phi(t),$$

$k = 0, 1, \ldots$, compare [3].

The technique described above was used by Spilling [23] to accelerate the convergence of dynamic iterations of differential systems resulting from the application of pseudospectral methods to the one-dimensional hyperbolic partial differential equation of the form

$$y_t + f(x, t, y) y_x = 0.$$

Spilling [23] describes how to construct a specific preconditioner P in the case of Chebyshev polynomial basis functions and collocation points based on the extrema of Chebyshev polynomials, and examines various splittings of P and $\overline{Q}$.

We will now describe the technique of preconditioning on the right which is the main focus of this paper. Assuming that Q is split as

$$Q = C + D \tag{2.3}$$

and making the transformation

$$z(t) = e^{D(t-t_0)} y(t)$$

the system (1.1) can be written in the form

$$\begin{cases} z'(t) + B(t-t_0)z(t) = e^{D(t-t_0)}g(t), & t \in [t_0, T], \\ z(t_0) = y_0, \end{cases} \tag{2.4}$$

where the matrix $B(t)$ is defined by

$$B(t) = e^{Dt}Ce^{-Dt}. \tag{2.5}$$

Choosing the splitting of the matrix $B(t)$

$$B(t) = M - N(t) \tag{2.6}$$

where M is a constant matrix determined by the desired iteration scheme (Gauss-Jacobi, Gauss-Seidel, etc.) leads to the process

$$\begin{cases} \frac{d}{dt}z^{(k+1)}(t) + Mz^{(k+1)}(t) = N(t-t_0)z^{(k)}(t) + e^{D(t-t_0)}g(t), \\ z^{(k+1)}(t_0) = z_0, \end{cases} \tag{2.7}$$

$z_0 = y_0$, $k = 0, 1, \ldots$, with given initial guess $z^{(0)}$, which, hopefully, converges faster than the original one defined by (1.2). Intuitively, this will be the case if we can choose the matrix D in (2.3) in such a way that it absorbs most of the stiffness of the matrix Q leaving a nonstiff part C. Then the speed of convergence of (2.7) will be governed by the size of the Lipschitz constant for C rather than Q.

Putting

$$\mathcal{K}z(t) = e^{-Mt}\int_{t_0}^{t} e^{Ms}N(s-t_0)z(s)\,ds,$$

$$\phi(t) = e^{M(t_0-t)}z_0 + e^{-Mt}\int_{t_0}^{t} e^{Ms}e^{D(s-t_0)}g(s)\,ds,$$

the formula (2.7) can be rewritten as

$$\begin{cases} z^{(k+1)}(t) = \mathcal{K}z^{(k)}(t) + \phi(t), \\ z^{(k+1)}(t_0) = z_0, \end{cases} \tag{2.8}$$

$k = 0, 1, \ldots$.

Observe that the computation of the iterations (2.8), as compared with the corresponding integral form of (1.2), involves the extra cost of evaluating $e^{D(t_\mu - t_0)} \times Ce^{-D(t_\mu - t_0)}$ for the discrete set of points

$$t_0 < t_1 < \cdots < t_N = T$$

which correspond to the discretization of the integral appearing in $\mathcal{K}$ on the given window $[t_0, T]$. However, at the expense of extra storage space, this need only be computed once and reused for all iterations assuming that subsequent discretization grids are a subset of the discretization grid for the first sweep.

Moreover, at the completion of the iteration process, we are faced with the computation of the quantities

$$e^{-D(t_\mu - t_0)} z^{(\nu)}(t_\mu),$$

where ν is the index which corresponds to the accepted iterate $z^{(\nu)}$. Efficient techniques for doing this based on Krylov techniques are described in Sidje [21] and Gallopoulos and Saad [7]. As will be explained later, for some iterative schemes (block Gauss-Jacobi for example), the matrix D will have such a form that if Q has a block tridiagonal structure, the computation of e^{Dt_μ} and e^{-Dt_μ} will be trivial.

In the case that C and D commute (equivalently, Q and D commute), then (2.5) and (2.6) imply

$$B(t) = Q - D.$$

Hence, the solution to (1.1) (with $g(t) \equiv 0$) can be written as

$$e^{-(Q-D)(t-t_0)} e^{-D(t-t_0)} y_0 \tag{2.9}$$

and waveform relaxation applied to (2.4) represents the computation of the first factor in (2.9). This effect bears some relation to the concept of operator splitting which will be discussed in Section 3.4.

3 Convergence of preconditioned dynamic iterations.

3.1 An error bound.

For any continuous function y from $[t_0, T]$ into R^n let $||y||_T$ be defined by

$$||y||_T := \sup\{||y(t)|| : t \in [t_0, T]\},$$

where $||\cdot||$ is some norm on R^n. It is well known (see [18] for example) that the iterates $\{y^{(k)}\}_{k=0}^{\infty}$ defined by (1.2) converge superlinearly for any window $[t_0, T]$ and the error of the iterate $y^{(\nu)}$ can be bounded by

$$||y - y^{(\nu)}||_T \leq \frac{(A(T-t_0))^\nu}{\nu!} ||y - y^{(0)}||_T, \tag{3.1}$$

where y is the solution to (1.1) and A is a constant such that

$$||e^{-Mt} N||_T \leq A.$$

It is the purpose of this section to study the convergence of the iterations defined by (2.8) which are obtained from (1.2) by preconditioning on the right. Putting

$$\epsilon^{(k)}(t) = z(t) - z^{(k)}(t)$$

and subtracting (2.8) from

$$\begin{cases} z(t) = \mathcal{K} z(t) + \phi(t), \\ z(t_0) = z_0 \end{cases}$$

we obtain the error equation

$$\epsilon^{(k+1)}(t) = e^{-Mt} \int_{t_0}^{t} e^{Ms} N(s - t_0) \epsilon^{(k)}(s)\, ds, \tag{3.2}$$

$k = 0, 1, \ldots$. Recall that

$$N(t) = M - e^{Dt} C e^{-Dt}.$$

To study the behavior of $\epsilon^{(k)}$ we will need the following lemmas.

LEMMA 3.1. *We have the following expansion*

$$e^{D(t-t_0)} C e^{-D(t-t_0)} = \sum_{i=0}^{\infty} \Delta_i \frac{(t - t_0)^i}{i!}, \tag{3.3}$$

where the matrices Δ_i are defined by

$$\Delta_i = \sum_{j=0}^{i} \binom{i}{j} D^{i-j} C (-D)^j. \tag{3.4}$$

PROOF. Expanding $e^{D(t-t_0)}$ and $e^{-D(t-t_0)}$ into Taylor series around $t = t_0$ and comparing the corresponding terms in (3.3) yields (3.4). □

LEMMA 3.2. *The matrices Δ_i, $i = 0, 1, \ldots$, satisfy the recurrence relation*

$$\Delta_{i+1} = D\Delta_i - \Delta_i D,$$

with $\Delta_0 = C$.

PROOF.

$$\begin{aligned}
\Delta_{i+1} &= \sum_{j=0}^{i+1} \binom{i+1}{j} D^{i+1-j} C (-D)^j \\
&= D^{i+1} C + \sum_{j=1}^{i} \left(\binom{i}{j} + \binom{i}{j-1} \right) D^{i+1-j} C (-D)^j + C(-D)^{i+1} \\
&= D^{i+1} C + \sum_{j=1}^{i} \binom{i}{j} D^{i+1-j} C (-D)^j \\
&\quad + \sum_{j=0}^{i-1} \binom{i}{j} D^{i-j} C (-D)^{j+1} + C(-D)^{i+1} \\
&= D \sum_{j=0}^{i} \binom{i}{j} D^{i-j} C (-D)^j - \sum_{j=0}^{i} \binom{i}{j} D^{i-j} C (-D)^j D \\
&= D\Delta_i - \Delta_i D.
\end{aligned}$$

REMARK 3.1. Observe that if C and D commute then $\Delta_i = 0$ for $i \geq 1$.

Using (3.3) the equation (3.2) can be rewritten in the form

$$\epsilon^{(k+1)}(t) = e^{-Mt} \int_{t_0}^{t} e^{Ms} \left(M - Q + D + \sum_{i=1}^{\infty} \Delta_i \frac{(s-t_0)^i}{i!} \right) \epsilon^{(k)}(s)\, ds, \tag{3.5}$$

$k = 0, 1, \ldots$. We will choose D to annihilate the constant term $M - Q + D$ hoping that this will speed up the convergence to zero of the error $\epsilon^{(k)}$ as $k \to \infty$. That this is indeed the case follows from the theorem given below.

THEOREM 3.3. *Assume that* $M - Q + D = 0$, $||e^{-Mt}\Delta_i|| \leq A_i$ *and that* $||\epsilon^{(0)}||_T \leq 1$. *Then*

$$||\epsilon^{(\nu)}||_T \leq \sum_{i=1}^{\infty} \frac{A_i^{\nu} (T-t_0)^{\nu(i+1)}}{((i+1)!)^{\nu} \nu!}, \tag{3.6}$$

$\nu = 0, 1, \ldots$.

PROOF. Define $\epsilon_i^{(\nu)}(t)$ by

$$\epsilon_i^{(\nu+1)}(t) = -\frac{1}{i!} \int_{t_0}^{t} e^{-M(t-s)} \Delta_i (s-t_0)^i \epsilon_i^{(\nu)}(s)\, ds,$$

$i = 1, 2, \ldots$. We have

$$||\epsilon_i^{(\nu+1)}(t)|| \leq \frac{1}{i!} \int_{t_0}^{t} A_i (s-t_0)^i ||\epsilon_i^{(\nu)}(s)||\, ds,$$

and since $||\epsilon_i^{(0)}(s)|| \leq 1$ an easy induction argument leads to

$$||\epsilon_i^{(\nu)}(t)|| \leq \frac{A_i^{\nu} (t-t_0)^{\nu(i+1)}}{((i+1)!)^{\nu} \nu!}.$$

It follows from the superposition principle that

$$\epsilon^{(\nu)}(t) = \sum_{i=1}^{\infty} \epsilon_i^{(\nu)}(t)$$

which leads to (3.6). □

In the case that there is no preconditioning the bound on the right hand side of (3.6) can be written as, see (3.1),

$$\psi_N(T, \nu) = \frac{A_0^{\nu} (T-t_0)^{\nu}}{\nu!}, \tag{3.7}$$

$\nu = 0, 1, \ldots$. On the other hand, preconditioning gives a bound which consists of an infinite number of terms. However, if the A_i's do not grow (as is the case for waveform relaxation block Gauss-Jacobi scheme) then a reasonable approximation to this bound is

$$\psi_P(T, \nu) = \frac{A_1^{\nu} (T-t_0)^{2\nu}}{2^{\nu} \nu!}, \tag{3.8}$$

$\nu = 0, 1, \ldots$, as long as $T - t_0$ is not too large. For the test problem given by (4.1) the waveform relaxation block Jacobi method leads to the same bound for A_0 and A_1, which in the case of the infinity norm is $A_0 = A_1 = ||\Delta_0||_\infty = ||\Delta_1||_\infty = 1$. Furthermore, for this problem (3.8) is an accurate bound if $T - t_0 \leq 1$. We computed below the number of iterations required to attain an accuracy of 10^{-4} and 10^{-8} for (3.7) and (3.8) when $T - t_0$ is, respectively, 0.25, 0.5, 1, and 2 and $||\Delta_0||_\infty = ||\Delta_1||_\infty = 1$.

	$t = 0.25$		$t = 0.5$		$t = 1$		$t = 2$	
	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}
ν_N	6	9	7	11	10	14	14	14
ν_P	3	5	5	7	7	11	19	19

These numbers predicted by our theory are in good agreement with the experimental numbers obtained in Section 5.

Recently, Jackiewicz and Owren [8] investigated the rate of convergence of dynamic iterations using pseudospectra of the finite dimensional operator approximating (3.2).

3.2 Errors by Laplace transforms.

We can get further insight into the convergence behavior of the iterates $\epsilon^{(k)}(t)$ by using Laplace transform techniques. We will illustrate this approach assuming that $\Delta_0 = M$ and considering only linear terms in the expansion (3.3) for the function

$$e^{D(t-t_0)}Ce^{-D(t-t_0)}.$$

In such a case the error equation of the preconditioned iterations reads

$$\begin{cases} \frac{d}{dt}\epsilon^{(k+1)}(t) + Me^{(k+1)}(t) = \Delta_1 t\epsilon^{(k)}(t), \\ \epsilon^{(k)}(0) = 0, \end{cases}$$

$t_0 = 0$, or

$$(sI + M)\hat{\epsilon}^{(k+1)}(s) = -\Delta_1 \frac{d}{ds}\hat{\epsilon}^{(k)}(s),$$

where $\hat{\epsilon}^{(k)}(s)$ is the Laplace transform of $\epsilon^{(k)}(t)$. Assuming further that $k = 0$ and $\epsilon^{(0)}(t) = t$, the above equation can be written in the form

$$\hat{\epsilon}^{(1)}(s) = \frac{2(sI + M)^{-1}\Delta_1}{s}\hat{\epsilon}^{(0)}(s).$$

Let $\rho_\xi(\cdot)$ be the spectral radius in $L_{\xi,\infty}$, the ξ-weighted L_∞ space, $\xi > 0$, with the norm

$$||y||_{\xi,\infty} = \sup_{t\in[0,\infty)} ||e^{-\xi t}y(t)||.$$

Then it follows from the results by Miekkala and Nevanlinna [16] that

$$\rho_\xi(\mathcal{K}) = \sup_{\mathrm{Re}\,(s)>\xi} \rho(K_P(s)),$$

where

$$K_P(s) = \frac{2(sI+M)^{-1}\Delta_1}{s}$$

can be interpreted as the Laplace transform of

$$2\int_0^t e^{-M(t-\eta)}\Delta_1\, d\eta.$$

We recall that in the case when there is no preconditioning

$$\rho_\xi(\mathcal{K}) = \sup_{\mathrm{Re}\,(s)>\xi} \rho(K_N(s)),$$

where

$$K_N(s) = (sI+M)^{-1}N,$$

$Q = M - N$, compare [16, 18]. Leimkuhler [10] defines the abscissa of ω-convergence of waveform relaxation iterations as

$$\xi_\omega = \inf\{\xi : \rho_\xi(K_N(s)) < \omega\},$$

and demonstrates that

$$||\mathcal{K}^n\epsilon^{(0)}||_{T_\omega} \tilde{<} e\omega^n||\epsilon^{(0)}||_{T_\omega},$$

where $T_\omega = 1/\xi_\omega$ is the window of ω-convergence and the symbol "$\tilde{<}$" means "approximately bounded by." Plotting spectral radii of $\rho(K_N(s))$ and $\rho(K_P(s))$ versus s we can get rough estimates of ξ_ω and T_ω. These estimates, especially in the preconditioned case, should be treated with great caution since the above analysis neglects quadratic and higher order terms in the expansion (3.3) and examines only the influence of the linear starting error on the error of the first iteration. This analysis captures, nevertheless, the important point that for any ω there exist ξ_ω and T_ω such that the convergence of the preconditioned iterations $z^{(k)}$ defined by (2.7) is faster than the convergence of the iterations without preconditioning $y^{(k)}$ defined by (1.2).

The spectral radii corresponding to waveform relaxation block Jacobi schemes for linear differential systems of dimension 64 which approximate the one-dimensional and two-dimensional heat equation considered in Section 5 are plotted in Figures 3.1 and 3.2, respectively. On these graphs the solid lines correspond to $\rho(K_N(s))$ and dashed lines to $\rho(K_P(s))$ for the indicated block sizes.

By comparing Figures 3.1 and 3.2, we can expect preconditioning to be more effective for the two-dimensional problem than the one-dimensional problem. This conclusion is borne out from numerical results presented in Section 5 (Figures 5.1 and 5.2).

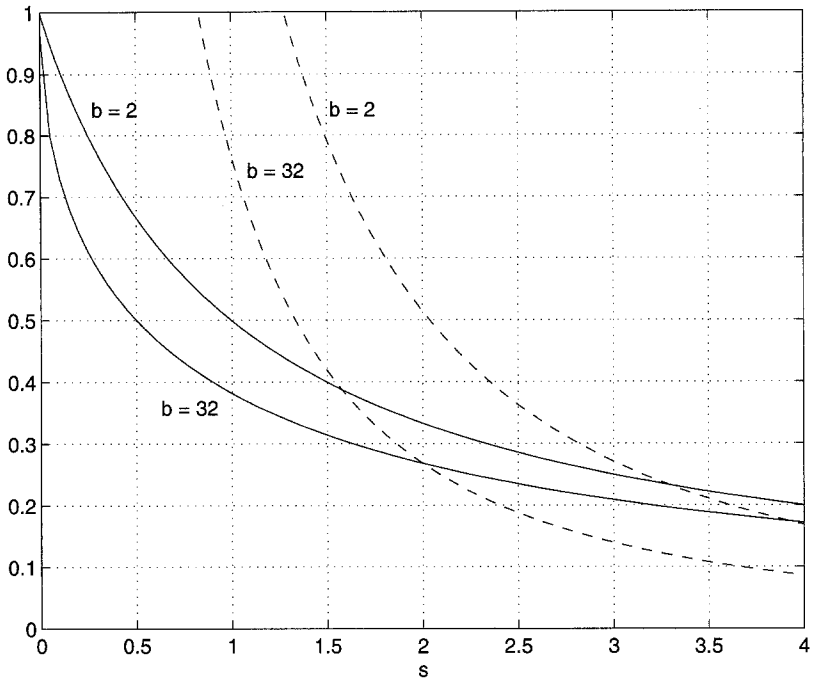

Figure 3.1: Spectral radii $\rho(K_N(s))$ and $\rho(K_P(s))$ for BJ scheme corresponding to one-dimensional heat equation.

3.3 More general preconditioners.

The choice $\Delta_0 = M$ means that we are preconditioning with the matrix $e^{D(t-t_0)}$, where $D = Q - M$ is the complement of the matrix M which defines the desired iteration scheme (block Jacobi, block Seidel, etc.). As mentioned above, this preconditioning involves the extra cost of computing $e^{D(t_\mu - t_0)} M e^{-D(t-t_0)}$ and $e^{-D(t_\mu - t_0)} z^{(\nu)}(t_\mu)$. This can be done in a very efficient way if the matrix Q has a special structure (for example tridiagonal or block tridiagonal with off diagonal blocks being identity matrices of appropriate dimensions). However, in many applications the matrix Q may be dense and the cost of computing the matrix exponentials may be significant. Such problems arise, for example, in application of pseudospectral methods to problems of hyperbolic type (compare [4]). In such cases it may be advantageous from the point of view of parallel processing to consider more general preconditioning with the function $R(t)$, where $R(t)$ is a polynomial or rational approximation to the matrix exponential e^{Dt}. This process is briefly outlined below.

Putting $z(t) = R(t)y(t)$ the system (1.1) can be rewritten in the form

$$z'(t) + Mz(t) = P(t)z(t) + Rg(t),$$

where

$$P(t) = M - (R(t)Q - R'(t))R^{-1}(t).$$

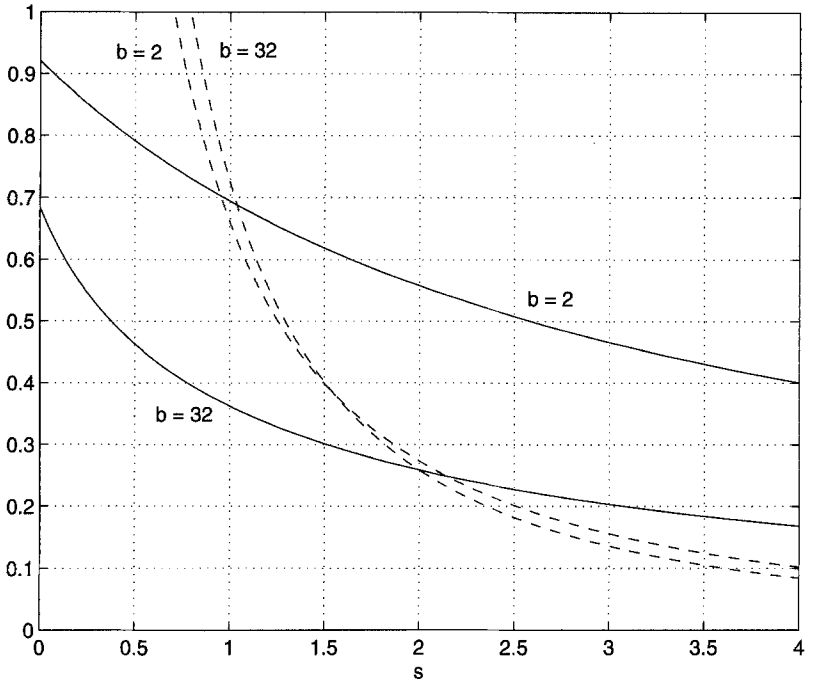

Figure 3.2: Spectral radii $\rho(K_N(s))$ and $\rho(K_P(s))$ for BJ scheme corresponding to two-dimensional heat equation.

Assume that

$$\begin{aligned} R(t) &= I + C_1 t + C_2 t^2 + \cdots, \\ P(t) &= \Delta_0 + \Delta_1 t + \Delta_2 t^2 + \cdots. \end{aligned}$$

Comparing the corresponding terms in the equation

$$P(t)R(t) = MR(t) - R(t)Q + R'(t)$$

we obtain the following relationship between C_i and Δ_i

$$C_{i+1} = \frac{1}{i+1}\left(C_i Q - MC_i + \sum_{j=0}^{i} \Delta_j C_{i-j}\right),$$

or

$$\Delta_i = (i+1)C_{i+1} + MC_i - C_i Q - \sum_{j=0}^{i-1} \Delta_j C_{i-j}.$$

Choosing $\Delta_0 = 0$, $C_1 = Q - M = D$ and $C_i = 0$ for $i \geq 2$ corresponds to approximating the exponential e^{Dt} by the polynomial $R(t) = I + Dt$ of the first degree which can be easily evaluated in parallel. In this case

$$\Delta_1 = MD - DQ,$$

and

$$\Delta_{i+1} = (-1)^i \Delta_1 D^i,$$

$i = 1, 2, \ldots$. Thus, in this case D should be chosen, if possible, so that $D^2 = 0$. Hence the error expansion in (3.6) will have only a contribution from the Δ_1 term. Similarly, it is easy to obtain relevant expressions when the function $R(t)$ represents rational preconditioning and has the form

$$R(t) = (I + D_1 t + D_2 t^2 + \ldots)^{-1}(I + C_1 t + C_2 t^2 + \ldots).$$

The hope here is that D_j and C_j can be chosen in such a way that $\Delta_1 = \Delta_2 = \ldots = \Delta_k = 0$ for some $k \geq 1$. In this case the leading term of $||\epsilon^{(\nu)}||_T$ is

$$\frac{A_{k+1}^{\nu}(T - t_0)^{\nu(k+2)}}{((k+2)!)^{\nu}\nu!}$$

and this will be a realistic bound on the error if $T - t_0$ is not too large.

For example, in the case of polynomial preconditioning, by choosing

$$C_1 = Q - M, \quad C_2 = \frac{1}{2}(C_1 Q - M C_1) = \frac{1}{2}(Q^2 - 2MQ + M^2), \quad C_i = 0, \qquad i \geq 3,$$

it follows that $\Delta_0 = \Delta_1 = 0$ and

$$\Delta_2 = MC_2 - C_2 Q, \qquad \Delta_n = (-1)^n \Delta_2 R_n, \qquad n > 2,$$

where

$$R_n - R_{n-1} C_1 + R_{n-2} C_2 = 0, \qquad R_1 = 0, \qquad R_2 = I.$$

3.4 Operator splitting.

The preconditioning approaches described in Section 2 bear some relationship to the concept of operator splitting. This approach consists of splitting a general problem

(3.9) $$y'(t) = F(y(t)),$$

into two equations

(3.10) $$\begin{cases} y'(t) = f(y(t)), \\ y'(t) = h(y(t)), \end{cases}$$

through the decomposition

$$F(y) = f(y) + h(y).$$

The hope here is that the equations given by (3.10) will be individually easier to integrate than the original equation (3.9) and can better reflect the structure of the underlying geometry (see Crouch and Grossman [5], for example). This approach can of course be generalized to spatially dependent splittings of the form

$$y' = F(y) = \sum_{j=0}^{k} f_j(y) h_j(y).$$

In the case of linear problem (1.1) (with $g(t) \equiv 0$), a natural splitting for Qy is

$$f(y) = Cy, \qquad h(y) = Dy$$

with $Q = C + D$. Hence, the solutions to the individual problems $y' = Cy$ and $y' = Dy$ corresponding to (3.10) are

$$e^{(t-t_0)C}y_1 \quad \text{and} \quad e^{(t-t_0)D}y_2$$

where y_1 and y_2 are appropriate initial conditions. The matrices C and D do not, in general, commute and we can show that

$$(3.11)\quad e^{(t-t_0)C}e^{(t-t_0)D} = e^{(t-t_0)Q+\frac{(t-t_0)^2}{2}[C,D]+\frac{(t-t_0)^3}{12}([C,[C,D]]+[D,[D,C]])+\cdots}$$

where $[C, D]$ is the commutator $CD - DC$. Thus, for example,

$$e^{\frac{t-t_0}{2}C}e^{(t-t_0)D}e^{\frac{t-t_0}{2}C} = e^{(t-t_0)Q+O((t-t_0)^3)},$$

and it follows that

$$(3.12)\qquad e^{\frac{t-t_0}{2}C}e^{(t-t_0)D}e^{\frac{t-t_0}{2}C}y_0 = e^{(t-t_0)Q}y_0 + O((t-t_0)^3).$$

The computation of the left hand side of (3.12) represents the solution of three different systems of equations and can be done, for example, by waveform relaxation methods. By using a pipelining approach with three processors, convergence will take place more rapidly than that for the original problem. The relation (3.11) is similar to the expression (3.3). Observe that the left hand side of (3.12) approximates $e^{(t-t_0)Q}$ if the size of the window of integration is not too large (compare also comments after the proof of Theorem 3). Note that more accurate approximations than that given by (3.12) can be obtained by increasing the number of splittings and hence the number of subproblems. The combination of operator splitting, preconditioning and waveform relaxation will be studied in a subsequent paper.

4 Overlapping the components of the system.

Waveform relaxation algorithms for ordinary differential equations, which allow the overlapping of components between different subsystems were proposed by Pohl [24] and further studied by Jeltsch and Pohl [9] and Frommer and Pohl [6] for linear differential systems. We illustrate this idea on the system of dimension 3

$$(4.1)\qquad y'(t) + Qy(t) = g(t), \quad t \in [t_0, T],$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}, \quad Q = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}, \quad g = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \end{bmatrix}.$$

Splitting (4.1) into two blocks consisting of the first two and the last two components, we obtain

$$\begin{bmatrix} y_1' \\ y_{2,1}' \end{bmatrix} + \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_{2,1} \\ y_2 \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \end{bmatrix},$$

and

$$\begin{bmatrix} y_{2,2}' \\ y_3' \end{bmatrix} + \begin{bmatrix} -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_{2,2} \\ y_3 \end{bmatrix} = \begin{bmatrix} g_2 \\ g_3 \end{bmatrix}.$$

These equations can be reformulated as the system of dimension 4 of the form

$$\tilde{y}'(t) + \widetilde{Q}\tilde{y}(t) = \tilde{g}(t), \quad t \in [t_0, T], \tag{4.2}$$

with

$$\tilde{y} = \begin{bmatrix} y_1 \\ y_{2,1} \\ y_{2,2} \\ y_3 \end{bmatrix}, \quad \widetilde{Q} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}, \quad \tilde{g} = \begin{bmatrix} g_1 \\ g_2 \\ g_2 \\ g_3 \end{bmatrix}.$$

After solving (4.2) the solution to (4.1) can be found from

$$y = \begin{bmatrix} y_1 \\ \alpha y_{2,1} + (1-\alpha) y_{2,2} \\ y_3 \end{bmatrix},$$

where α is any real number.

Assume that (4.1) and (4.2) are solved by block-Jacobi waveform relaxation methods corresponding to the splittings

$$Q = M - N, \qquad \widetilde{Q} = \widetilde{M} - \widetilde{N}$$

with

$$M = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \qquad N = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

and

$$\widetilde{M} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}, \qquad \widetilde{N} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

We have

$$\rho(\widetilde{M}^{-1}\widetilde{N}) = \frac{1}{3} < \frac{\sqrt{3}}{3} = \rho(M^{-1}N),$$

and we can expect that the block-Jacobi iterations on the overlapped system (4.2) will converge faster than the corresponding iterations on the original system (4.1).

This process can be generalized to any vector of block sizes

$$b = [b_1, b_2, \ldots, b_r]T,$$

and vector of overlaps

$$o = [o_1, o_2, \ldots, o_r]^T,$$

such that

$$\sum_{i=1}^{r} b_i - \sum_{i=1}^{r-1} o_i = n,$$

where n is the dimension of Q. The MATLAB program to compute the new matrix $\tilde{Q}$ of dimension $\sum_{i=1}^{r} b_i$ can be obtained from the second author at `jackiewi@math.la.asu.edu`.

Denote by $Q = M - N$ and $\widetilde{Q} = \widetilde{M} - \widetilde{N}$ the splittings of the matrices Q and $\widetilde{Q}$ corresponding to waveform relaxation block Jacobi methods. We have verified that for all but one test case considered in the next section

$$\rho(\widetilde{M}^{-1}\widetilde{N}) < \rho(M^{-1}N) < 1$$

which indicates that the convergence of the iterations corresponding to the overlapped system should be faster than the convergence of the iterations corresponding to the original system. This was indeed observed in our numerical experiments presented in the next section.

Comparison results for certain splittings of the matrix Q have been studied by Frommer and Pohl [6].

5 Numerical experiments.

5.1 Heat equation in one space variable.

Discretizing the heat equation in one space variable leads to the linear system of the form

$$\begin{cases} y'(t) + Qy(t) = 0, & t > 0, \\ y(0) = y_0, \end{cases} \tag{5.1}$$

where

$$y = [y_1, y_2, \ldots, y_N]^T,$$

$$Q = \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \ddots \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix} \in R^{N \times N}.$$

The system (5.1) also describes the interconnect resistor-capacitor (RC) line. Such systems have been examined by Leimkuhler [10] and Leimkuhler and Ruehli [11].

We have studied the behavior of the errors of waveform relaxation iterations resulting from applications to the system (5.1) of block Jacobi (BJ), preconditioned

block Jacobi (PBJ), block Jacobi with overlapping (BJO), and preconditioned block Jacobi with overlapping (PBJO). These modes are ideally suited for parallel implementation. We assumed that the starting iterations $y_i^{(0)}(t)$ were chosen in such a way that the initial errors $\epsilon_i^{(0)}(t) = y_i(t) - y_i^{(0)}(t)$ satisfy $\epsilon_i^{(0)}(t) = t$ for $i = 1, 2, \ldots, N$. The integrals in the resulting error equations were discretized by the composite trapezoidal rule with stepsize $\Delta t = 0.01$. The computation of the iterations corresponding to PBJ and PBJO modes involves the evaluation of the matrix exponentials e^{Dt_μ}, e^{-Dt_μ}, $e^{\widetilde{D}t_\mu}$ and $e^{-\widetilde{D}t_\mu}$ for the discrete set of points $t_0, t_1, \ldots$, where $D = Q - M$, $\widetilde{D} = \widetilde{Q} - \widetilde{M}$, and the matrices M and $\widetilde{M}$ are block-diagonal (compare with sections 2 and 4). It is easy to verify that the matrix D corresponding to the system (5.1) has the following block-diagonal structure

$$D = \operatorname{diag}(D_1, D_2, \ldots, D_q),$$

for block sizes equal to 2, 4, 8, 16 and 32, where each block D_i is a 1×1 or 2×2 zero matrix or the matrix of the form

$$\Gamma = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

Since

$$e^{\Gamma t} = I \cosh t - \Gamma \sinh t,$$

where I is the 2×2 identity matrix, the computation of e^{Dt} or e^{-Dt} is trivial. (For block size equal to one the PBJ scheme converges in one iteration, but in this case the computation of e^{Dt} and e^{-Dt} is more costly.) The situation is even simpler in the PBJO mode. In this case $\widetilde{D}^k = 0$ for some integer $k > 1$ and $e^{\widetilde{D}t}$ is equal to the polynomial

$$e^{\widetilde{D}t} = I + \widetilde{D}t + \frac{\widetilde{D}^2 t^2}{2!} + \cdots + \frac{\widetilde{D}^{k-1} t^{k-1}}{(k-1)!}$$

which can be evaluated efficiently in parallel.

We have monitored the speed of convergence for BJ, PBJ, BJO and PBJO iterations for $N = 64$ and for many block sizes and various overlap patterns. We present in Table 5.1 the results for block size $s = 4$ and block pattern corresponding to the vectors of block sizes b and overlaps o given by

$$b = [5, 6, \ldots, 6, 5] \in R^{16}, \qquad o = [2, 2, \ldots, 2] \in R^{31}.$$

The entries in this table represent the ratios r_3 and r_6 at $t = 0.25$, 0.5, 1 and 2, where r_i defined by

$$r_i = \sqrt[i]{\frac{\epsilon_i - \epsilon_0}{\epsilon_1 - \epsilon_0}}, \tag{5.2}$$

is the rate of convergence observed over the first i sweeps (compare [10]).

Table 5.1: Convergence ratios, one dimensional case

mode	$t = 0.25$		$t = 0.5$		$t = 1$		$t = 2$	
	r_3	r_6	r_3	r_6	r_3	r_6	r_3	r_6
BJ	0.179	0.094	0.265	0.159	0.374	0.258	0.501	0.391
PBJ	0.060	0.021	0.147	0.064	0.350	0.203	0.612	0.680
BJO	0.021	0.001	0.049	0.003	0.109	0.010	0.220	0.038
PBJO	0.041	0.001	0.097	0.004	0.218	0.016	0.473	0.065

Table 5.2: Number of iterations, one dimensional case

mode	$t = 0.25$		$t = 0.5$		$t = 1$		$t = 2$	
	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}
BJ	4	7	5	9	7	11	9	14
PBJ	3	5	4	6	6	9	12	16
BJO	2	3	3	4	3	5	4	6
PBJO	3	4	3	4	4	5	5	6

To get further insight into convergence properties of various modes of block Jacobi iterations we present in Table 5.2 the number of iterations needed to reduce the errors on the time intervals $[0, 0.25]$, $[0, 0.5]$, $[0, 1]$, and $[0, 2]$ below the required tolerances, TOL $= 10^{-4}$ and 10^{-8}. We have also plotted in Figure 5.1 the errors of the first six iterations for all considered waveform relaxation modes. Analyzing the results in these tables and the corresponding plots in Figure 5.1 we observe that the preconditioning technique described in Section 2 improves the speed of convergence of the resulting PBJ iterations on the time interval $[0, 1]$. This is consistent with our theoretical results presented in Section 3. We were surprised, however, by the fast convergence of block Jacobi iterations with overlapping. The convergence was so fast that, in most cases, further application of preconditioning did not result in further acceleration of convergence. On the contrary, the convergence of PBJO iterations was somewhat slower than that of BJO iterations. However, this did not affect too much the number of iterations needed to reduce the error below the prescribed tolerance.

In an attempt to understand the fast convergence of BJO iterations as compared with BJ mode we computed the spectral radii of the matrices $M^{-1}N$ and $\widetilde{M}^{-1}\widetilde{N}$, where $Q = M - N$ and $\widetilde{Q} = \widetilde{M} - \widetilde{N}$ are the corresponding splittings of the matrices Q and $\widetilde{Q}$ (see Section 4). Those radii, which represent rates of convergence of the corresponding iterations at infinity (compare [16]), are $\rho(M^{-1}N) = 0.9953$ and $\rho(\widetilde{M}^{-1}\widetilde{N}) = 0.9861$.

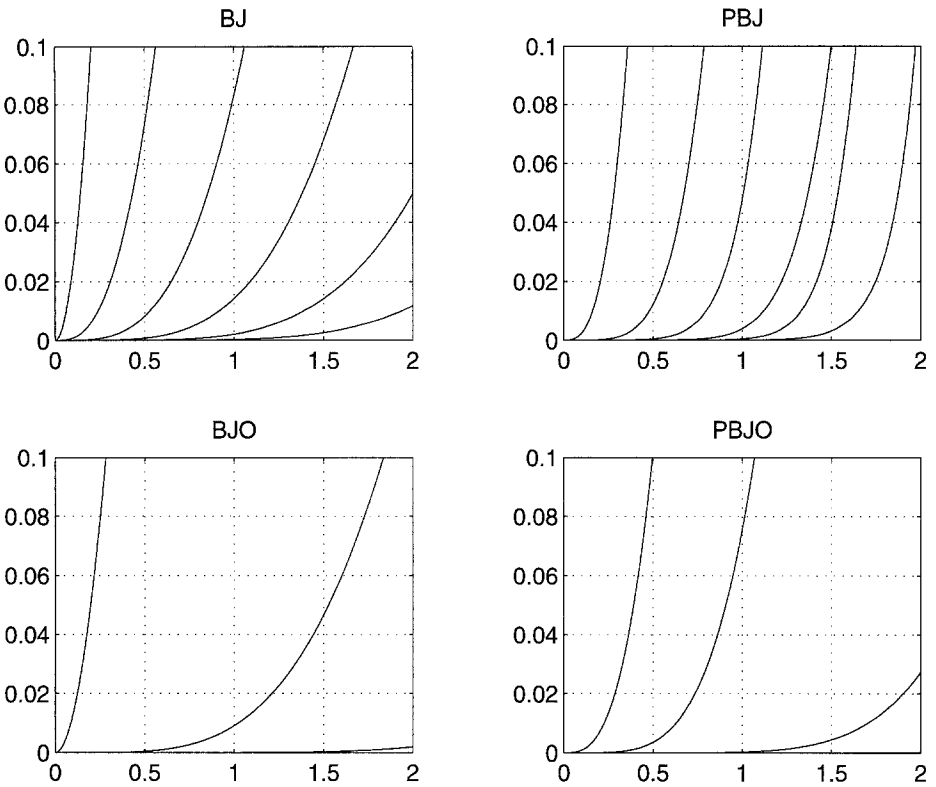

Figure 5.1: Errors of waveform relaxation block Jacobi iterations for one-dimensional heat equation.

We have also tested the convergence of waveform relaxation block Gauss-Seidel (BS) and preconditioned block Gauss-Seidel (PBS) iterations. As expected, the BS iterations converge faster than the corresponding BJ iterations and this is reflected in the smaller value of the spectral radius $\rho(M^{-1}N) = 0.9907$ for the BS mode than for the BJ mode. We have also observed that, with the exception of block size 1, the preconditioning does not improve the speed of convergence of PBS iterations and even decelerates it a little. This can be partially explained by the fact that the norm of the matrix Δ_1 given by (3.4), which corresponds to the dominant term in the error equation (3.5), is $||\Delta_1||_\infty = 1$ for block size 1 and $||\Delta_1||_\infty = 2$ for all other block sizes used in our numerical experiments (2, 4, 8, 16 and 32). On the other hand, for the BS mode we have $||N||_\infty = 1$ for all block sizes where the matrix N corresponds to the splitting $Q = M - N$.

5.2 Heat equation in two space variables.

Discretizing the heat equation in two space variables leads to a linear system of the form (5.1), where I is the identity matrix of dimension N, and

$$Q = \begin{bmatrix} T & -I & & & \\ -I & T & -I & & \\ & \ddots & \ddots & \ddots & \\ & -I & T & -I & \\ & & -I & T & \end{bmatrix} \in R^{N^2 \times N^2},$$

$$T = \begin{bmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{bmatrix} \in R^{N \times N}.$$

In Tables 5.3 and 5.4 we present for the two-dimensional case, $N^2 = 64$, equivalent results to Tables 5.1 and 5.2 for the one-dimensional case. The same block size and block pattern as in the one-dimensional case are used. We have also plotted in Figure 5.2 the errors of the first six iterations. Analyzing the results in these tables and additional data not presented here we observe that PBJ mode is much more efficient than BJ mode on the window approximately equal to $[0, 1.2]$. We further note that the overlapping of the components does not have such a dramatic effect as in the one-dimensional case and leads only to the modest improvement of the rate of convergence of the resulting BJO iterations as compared with BJ mode. Additional insight into this is provided by spectral radii of $M^{-1}N$ and $\widetilde{M}^{-1}\widetilde{N}$, where $Q = M - N$ and $\widetilde{Q} = \widetilde{M} - \widetilde{N}$ are the splittings of the matrices Q and $\widetilde{Q}$ corresponding to BJ and BJO modes, respectively. These radii are $\rho(M^{-1}N) = 0.9062$ and $\rho(\widetilde{M}^{-1}\widetilde{N}) = 0.8951$.

Observe that the spectral radius $\rho(\widetilde{M}^{-1}\widetilde{N})$ is only marginally smaller than the corresponding radius $\rho(M^{-1}N)$.

As in the one-dimensional case the computations related to PBJ and PBJO schemes involve the evaluation of e^{Dt_μ}, e^{-Dt_μ}, $e^{\widetilde{D}t_\mu}$ and $e^{-\widetilde{D}t_\mu}$ for the discrete set of points t_μ, $\mu = 0, 1, \ldots$, where $D = Q - M$ and $\widetilde{D} = \widetilde{Q} - \widetilde{M}$. It turns out that the matrix D corresponding to the system (5.3) has, for block sizes 2, 4, 16, and 32, the following block diagonal structure

$$D = \operatorname{diag}(D_1, D_2, \ldots, D_q),$$

where each block D_i is an $N \times N$ or $2N \times 2N$ zero matrix or the matrix of the form

$$\Gamma = \begin{bmatrix} 0 & -I \\ -I & 0 \end{bmatrix}$$

and I is the identity matrix of dimension N. Therefore, e^{Dt_μ} and e^{-Dt_μ} can be efficiently computed by utilizing the identity

$$e^{\Gamma t} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \cosh t - \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \sinh t.$$

Table 5.3: Convergence ratios, two dimensional case

mode	$t = 0.25$		$t = 0.5$		$t = 1$		$t = 2$	
	r_3	r_6	r_3	r_6	r_3	r_6	r_3	r_6
BJ	0.340	0.209	0.496	0.344	0.668	0.528	0.780	0.714
PBJ	0.051	0.018	0.115	0.054	0.242	0.154	0.307	0.489
BJO	0.332	0.185	0.488	0.313	0.665	0.498	0.786	0.699
PBJO	0.081	0.029	0.185	0.088	0.419	0.282	0.848	0.672

Table 5.4: Number of iterations, two dimensional case

mode	$t = 0.25$		$t = 0.5$		$t = 1$		$t = 2$	
	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}
BJ	6	9	8	12	11	16	16	23
PBJ	3	5	4	6	5	9	10	14
BJO	5	9	7	11	10	15	14	20
PBJO	3	4	4	7	7	11	18	24

We can also see that the PBJO scheme is much more efficient than the BJO method although not as efficient as the PBJ mode.

The PBJ scheme converges in one iteration for block sizes equal to $s = 1$ and $s = 8$ (this follows from the fact that $M - e^{Dt}Me^{-Dt} \equiv 0$ for $s = 1$ and $s = 8$). However in these cases the matrix D does not have the structure described above and the computation of e^{Dt} and e^{-Dt} is more costly. This is also the case for the PBJO method. It can be verified that $\widetilde{D}^k \neq 0$ for any $k \geq 0$ and as a consequence the resulting error equation (3.5) possesses an infinite number of terms. This explains why the overlapping is not as effective as in the one-dimensional case.

We have also experimented with BS and PBS modes for which we observed that, contrary to the one-dimensional case, the preconditioning improves significantly the speed of convergence of the resulting PBS iterations as compared with BS iterations on the window approximately equal to $[0, 1.2]$ for block sizes 1, 2, 4, and 8 and the improvement is most dramatic for block size equal to one. The BS mode is more efficient than the BJ scheme and this is reflected in much smaller values of the spectral radius $\rho(M^{-1}N) = 0.8213$ (for block size $s = 4$) for the BS mode as compared with the BJ method.

6 Concluding remarks.

We have studied the effect of preconditioning on the rate of convergence of the waveform relaxation iterations resulting from application of various modes

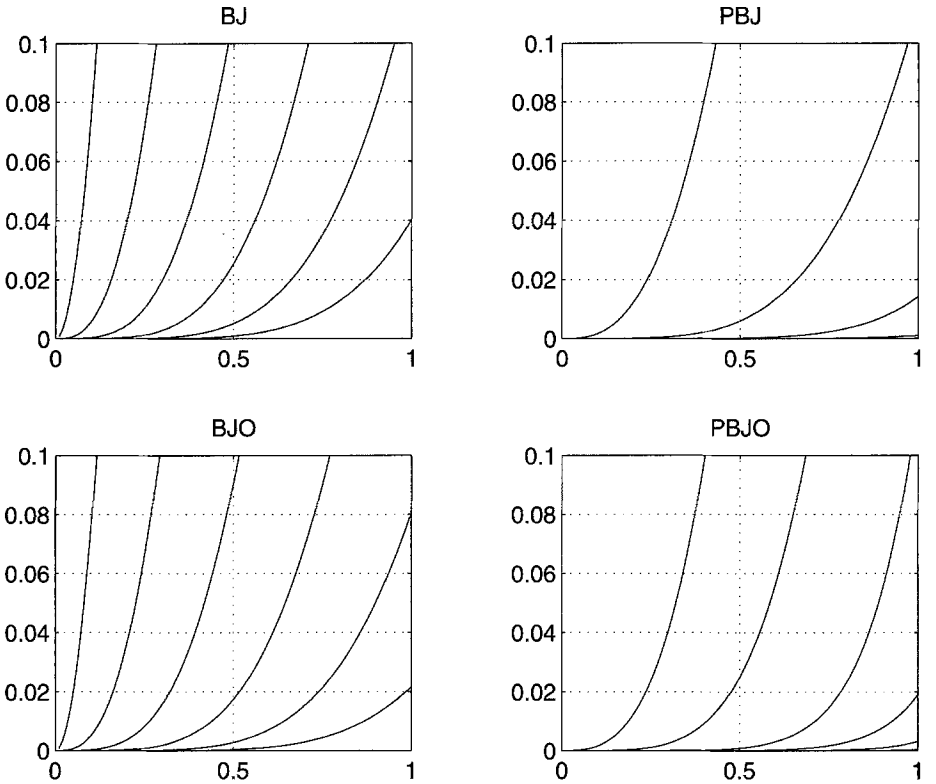

Figure 5.2: Errors of waveform relaxation block Jacobi iterations for two-dimensional heat equation.

of block Gauss-Jacobi and block Gauss-Seidel to linear differential systems of equations. The preconditioning technique is described in Section 2. The error bound is derived in Section 3.1 which suggests that preconditioning should generate faster schemes than the original one if the window of integration is not too large. This conclusion also follows from the Laplace transform error analysis presented in Section 3.2. The results of the extensive numerical experiments presented in Section 5 are in good agreement with the theoretical results derived in Sections 3.1 and 3.2. These experiments were carried out on sparse linear differential systems obtained from finite difference approximation to the heat conduction equation in one and two space variables. We examined waveform relaxation block Jacobi and block Seidel modes denoted by BJ, PBJ, BJO, PBJO, BS, and PBS, when P stands for preconditioning and O for overlapping. These modes are defined in Section 5 and the overlapping algorithm is described in Section 4. It turns out that overlapping of the block Jacobi scheme as described in Section 4 is very effective on differential systems approximating the one-dimensional heat equation and that in this case further application of preconditioning does not lead to further increase of the rate of convergence of

the resulting iterations. On the other hand, preconditioning is more effective on differential systems approximating the heat equation in two space variables, and overlapping in this case leads only to a modest gain in efficiency of the resulting schemes. We can conclude that preconditioning and overlapping are two powerful techniques of accelerating the convergence of the waveform relaxation processes but the right combination of them depends on the type of differential system under consideration.

We have also examined the effect of using more general preconditioners which are polynomial or rational approximations to the matrix exponential function. These preconditioners are ideally suited for parallel implementation. Our preliminary numerical results, which will be reported elsewhere, indicate that this approach seems to be well suited for dense differential systems resulting from application of pseudospectral methods to partial differential equations of hyperbolic type. Finally, we briefly describe in Section 3.4 the new approach to accelerating the convergence of the waveform relaxation method by the concept of operator splitting of the right hand side of the differential system. This approach and its combination with preconditioning and overlapping will be the subject of future work.

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