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# OPTIMAL $\rho$ PARAMETER FOR THE ADI ITERATION FOR THE SEPARABLE DIFFUSION EQUATION IN THREE DIMENSIONS

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## 1. Introduction

The ADI method was introduced by Peaceman and Rachford [6] in 1955, to solve the discretized boundary value problems for elliptic and parabolic PDEs. The finite difference discretization of the model elliptic problem

$$\begin{aligned} -\Delta u &= f, \qquad \Omega = [0,1] \times [0,1] \\ u &= 0 \qquad \text{on } \delta\Omega \end{aligned} \tag{1}$$

with 5-point centered finite difference discretization, with $n+2$ mesh-points in the $x$ - direction and $m+2$ points in the $y$ direction, leads to the solution of a linear system of equations of the form

$$Au = b \tag{2}$$

where $A$ is a matrix of dimension $N = n \times m$. Without loss of generality and for the sake of simplicity, we will assume for the remainder of this paper that $m = n$, so that $N = n^2$.

Writing the discretization in $x$ and $y$ direction into matrices $H$ and $V$ respectively, leads to a linear system of equations

$$(H+V)u = b \tag{3}$$

where both $H$ and $V$ are sparse and possess a special structure. In particular, with suitable reordering, $H$ and $V$ are *tridiagonal.*

Starting with some initial guess $u_0$, the Alternative Direction Implicit procedure for solving (3) generates a sequence of approximations $u_i, i = 1, 2, \ldots$ given by the following algorithm

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### 1.1. Peaceman-Rachford ADI(PR2-ADI)

1. Choose $u_0$
2. For $i = 1, \dots$ , Until Convergence Do

$$(H + \rho_i I)u_{i+1/2} = -(V - \rho_i I)u_i + b \tag{4}$$

$$(V + \rho_i I)u_{i+1} = -(H - \rho_i I)u_{i+1/2} + b, \qquad i \geq 0, \tag{5}$$

where $u_0$ is an arbitrary initial vector and $\{\rho_i,\ i \geq 0\}$ are positive constants called *acceleration parameters*, which are chosen to speedup the convergence of this process. Each of Eq. (4) and (5) forms $n$ sets of linear system of order $n$ where the $n$ linear systems are completely *decoupled.* Furthermore, the matrices $H$ and $V$ could be made *tridiagonal* with proper reordering. For example, under natural ordering in $x$ direction $H$ is tridiagonal, and with natural ordering in $y$ direction $V$ could be made tridiagonal. This ensures a minimum degree of parallelism of $n$, which makes PR2-ADI attractive in parallel computations. Also we note that Gaussian elimination method for the tridiagonal linear systems is very effective in terms of costs.

## 2. Convergence

We combine Eq. (4) and Eq. (5) into the form

$$u_{i+1} = T_\rho u_i + v \qquad i \geq 0, \tag{6}$$

where

$$T_\rho \equiv (V + \rho I)^{-1}(\rho I - H)(H + \rho I)^{-1}(\rho I - V), \tag{7}$$

and

$$v = (V + \rho I)^{-1}\{(\rho I - H)(H + \rho I)^{-1} + I\}b \tag{8}$$

We call $T_\rho$ the *Peaceman-Rachford matrix.* If $\varepsilon_i = u_i - u$ is the error at the $i$-th iteration, then $\varepsilon_{i+1} = T_\rho \varepsilon_i$, and in general

$$\varepsilon_l = \left( \prod_{j=1}^{l} T_{\rho_j} \right) \varepsilon_0, \quad l \geq 1, \tag{9}$$

where

$$\prod_{j=1}^{l} T_{\rho_j} \equiv T_{\rho_1} T_{\rho_2} \dots T_{\rho_l} \tag{10}$$

As for the convergence of Peaceman-Rachford iteration, we first consider the ***stationary*** case, where all the constants $\rho_i$ are equal. Then we have the following theorem[Va62]:

THEOREM 2.1. *Let $H$ and $V$ be $N \times N$ Hermitian nonnegative-definite matrices, where at least one of the matrices $H$ and $V$ is positive-definite. Then, for any $\rho > 0$, the stationary PR2-ADI iteration is convergent.*

Note that the above result still holds true without the assumption that $H$ and $V$ commute, i.e, $HV = VH$.

## 3. Optimal parameters for two dimensions

Assume that $HV = VH$ and further that $H$ and $V$ are diagonalizable, so that $H$ and $V$ have real eigenvalues. Then there exists a set of $n$ linearly independent vectors, $\{v_1, v_2, \dots, v_n\}$, which are common eigenvectors for $H$ and $V$. Let $v$ be any such vector, so that

$$Hv = \mu v \ , \quad Vv = \nu v$$

Then, we have

$$T_\rho v = (V + \rho I)^{-1} (\rho I - H)(H + \rho I)^{-1} (\rho I - V) v, \tag{11}$$

$$= \frac{(\mu - \rho)(\nu - \rho)}{(\mu + \rho)(\nu + \rho)} v \ . \tag{12}$$

Therefore, in general all the eigenvalues of the operator in (10) are given by

$$\prod_{i=1}^{l} \frac{(\mu - \rho_i)(\nu - \rho_i)}{(\mu + \rho_i)(\nu + \rho_i)} \tag{13}$$

where $\mu$ and $\nu$ belong to the set of eigenvalues of $H$ and $V$ with a common eigenvector. Let $T_l$ denote the operator in (10), and let $a \leq \mu, \nu \leq b$. Also let $S_p(A)$ denote the spectral radius of the matrix $A$. Then, we have

$$S_p(T_l) = \max_{a \leq \mu,\ \nu \leq b} \prod_{i=1}^{l} \left| \frac{(\mu - \rho_i)(\nu - \rho_i)}{(\mu + \rho_i)(\nu + \rho_i)} \right| \tag{14}$$

Hence minimizing the spectral radius of $T_\rho$ is a *minimax* problem of finding $\{\rho_1, \dots, \rho_l\}$ such that (14) is minimized.

For $l = 1$ we have

THEOREM 3.1. *Spectral radius of $T_1$ is minimized when $\rho = \sqrt{ab}$, with the corresponding $S_p(T_1) = (\frac{\sqrt{ab}-a}{\sqrt{ab}+a})^2$.*

For the model problem

$$a = 4\sin^2\left(\frac{\pi}{2(n+1)}\right),\ b = 4\sin^2\left(\frac{n\pi}{2(n+1)}\right) \tag{15}$$

so that $S_p(T_1) = (\frac{1-\tan(\pi/2(n+1))}{1+\tan(\pi/2(n+1))})^2$, which turns out to be that of SOR with optimal $\omega = \frac{2}{1+\sin(\pi/(n+1))}$.

For $l > 1$ the exact solutions are given in terms of elliptic functions[Wa66,To67].

THEOREM 3.2. *The sequence of optimal $\rho$ parameters is given by*

$$\rho_i{}^* = b\ dn\left(\frac{2(l-i)+1}{2l}K,\ k\right), \qquad i = 1, \dots, l, \tag{16}$$

*where $dn(u,k)$ is an elliptic function defined by*

$$\begin{aligned} dn(u,k) &== \sqrt{1 - k^2x^2} \\ x &== \sin\phi\ . \end{aligned} \tag{17}$$

*Here, $\phi$ is implicitly defined by*

$$\int_0^\phi (1 - k^2\sin^2\theta)^{-1/2} d\theta = u$$

$$k = \sqrt{1-c^2},\ \ c = a/b$$

$$K = \int_0^{\pi/2} (1 - k^2\sin^2\theta)^{-1/2} d\theta\ .$$

## 4. Three dimensional extension

PR2-ADI iteration in two dimensions depends on the fact that $A$ can be written as $A = H + V$, where $H$ and $V$ can be made into tridiagonal matrix by a suitable permutation. In three dimensions with the 7-point Laplacian for the second order derivatives $A$ can be written as $A = H + V + W$, where $H, V$ , and $W$ contain the $x$-, $y$-, $z$-, directional derivatives, respectively. As in two dimensions the matrices $H$, $V$, and $W$ can be made tridiagonal by suitable permutations. So writing

$$\begin{aligned} A =&(H + \rho_i I) + (A - H - \rho_i I) = (V + \rho_i I) + (A - V - \rho_i I) \\ =&(W + \rho_i I) + (A - W - \rho_i I), \end{aligned}$$

we can get the following analogue of Peaceman-Rachford ADI in three dimensions.

### 4.1. Peaceman-Rachford ADI in three dimensions(PR3-ADI)

(18)
$$\begin{aligned} (H + \rho_i I)u_{i+1/3} &= -(V + W - \rho_i I)u_i + b \\ (V + \rho_i I)u_{i+2/3} &= -(H + W - \rho_i I)u_{i+1/3} + b \\ (W + \rho_i I)u_{i+1} &= -(H + V - \rho_i I)u_{i+2/3} + b \end{aligned}$$

The convergence behavior of this algorithm is quite different from that of PR2-ADI in two dimension. Assume that $H$, $V$, and $W$ are pairwise-commutative, and that

$$a \le S_p(H), S_p(V), S_p(W) \le b.$$

For example, with Poisson equation in three dimensions

$$a = 4\sin^2\left(\frac{\pi}{2(n+1)}\right), \quad b = 4\sin^2\left(\frac{n\pi}{2(n+1)}\right)$$

where $N = n^3$.

Let $T_\rho$ be the operator associated with PR3-ADI. Then,

$$T_\rho = (W+\rho I)^{-1}(H+V-\rho I)(V+\rho I)^{-1} (H+W-\rho I)(H+\rho I)^{-1}(V+W-\rho I). \tag{19}$$

Since the given equation is separable, $HV = VH$, $HW = WH$, and $VW = WV$ and H, V, and W share common set of eigenvectors. Let $v$ be any such vector, and

$$Hv = \mu v,\ Vv = \nu v, Wv = \omega v.$$

Then,

$$T_\rho v = \frac{(\mu+\nu-\rho)(\nu+\omega-\rho)(\mu+\omega-\rho)}{(\mu+\rho)(\nu+\rho)\ (\omega+\rho)} v\ . \tag{20}$$

Then, the spectral radius of $T_\rho$ is given by

$$S_p(T_\rho) = \max_{a\le\mu,\nu,\omega\le b} \left| \frac{(\mu+\nu-\rho)(\nu+\omega-\rho)(\mu+\omega-\rho)}{(\mu+\rho)(\nu+\rho)(\omega+\rho)} \right|\ . \tag{21}$$

This expression is quite different from that in two dimensions as in Eq. (14). While in two dimensions for any positive $\rho$ the spectral radius was smaller than 1, here this is not true.

Now, we are looking for $\rho$ such that (21) becomes smaller than 1. For the following discussion we will assume that $a < \rho < b$, and $a$ small enough so that $b/2 > 2a$. Now, we introduce several functions. Let

$$\phi_1(\rho) = \max_{a\le\mu,\nu,\omega\le b} \left| \frac{\nu+\omega-\rho}{\mu+\rho} \right|\ , \tag{22}$$

$$\phi_2(\rho) = \max_{a\le\mu,\nu,\omega\le b} \left| \frac{\mu+\omega-\rho}{\nu+\rho} \right|\ , \tag{23}$$

$$\phi_3(\rho) = \max_{a\le\mu,\nu,\omega\le b} \left| \frac{\mu+\nu-\rho}{\omega+\rho} \right|\ , \tag{24}$$

and

$$\psi_1(\rho) = \max_{a\leq\mu,\leq b}\left|\frac{2\mu-\rho}{\mu+\rho}\right| , \tag{25}$$

$$\psi_2(\rho) = \max_{a\leq\nu,\leq b}\left|\frac{2\nu-\rho}{\nu+\rho}\right| , \tag{26}$$

$$\psi_3(\rho) = \max_{a\leq\omega,\leq b}\left|\frac{2\omega-\rho}{\omega+\rho}\right| . \tag{27}$$

By symmetry, we see

$$\phi_1(\rho) = \phi_2(\rho) = \phi_3(\rho) ,$$

and

$$\psi_1(\rho) = \psi_2(\rho) = \psi_3(\rho).$$

Note that

$$S_p(T\rho) \leq \phi_1(\rho)^3 ,$$

and

$$\psi_1(\rho)^3 \leq S_p(T\rho),$$

since the latter is an expression for $S_p(T_\rho)$ over the subset $\{\mu = \nu = \omega\}$. For the ADI iteration to converge, $\psi_1(\rho)$ need to be smaller than 1. So we have $\frac{2b-\rho}{b+\rho} < 1$, which leads to $\rho > b/2$.

THEOREM 4.1. *Assume that $H$, $V$, and $W$ are pairwise-commutative, and that $\rho > b/2$, and $b/2 > 2a$. Then,*

$$\phi_1(\rho) \equiv \psi_1(\rho)$$

*Proof.* Note that if a real valued function is monotonically increasing or decreasing, the absolute value of that function on a closed interval takes its maximum at one of the endpoints of that interval. For a given $\rho$ the function $\frac{2\mu-\rho}{\mu+\rho}$ is a monotonically increasing function of $\mu$, so the absolute value of that function takes its maximum at $\mu = a$ or $b$. So

$$\psi_1(\rho) = \max\left\{\frac{\rho-2a}{a+\rho}, \frac{2b-\rho}{b+\rho}\right\} = \begin{cases} \frac{2b-\rho}{b+\rho}, & \text{if } \rho < \rho^* \\ \frac{\rho-2a}{a+\rho}, & \text{if } \rho > \rho^* \end{cases} \tag{28}$$

where

$$\rho^* = \frac{a + b + \sqrt{(a+b)^2 + 32ab}}{4}.$$

For $\phi_1$ the function $\frac{\mu+\nu-\rho}{\mu+\rho}$ is monotonically decreasing in $\mu$ and monotonically increasing in $\nu$, so the maximum happens at the boundary $\mu = a$ or $b$ and $\nu = a$ or $b$. Also note that for $\rho > b/2$, $\frac{2b-\rho}{b+\rho} > \frac{a+b-\rho}{a+\rho}$. Then,

(29)

$$\begin{aligned}
\phi_1(\rho) &= \max\left\{\frac{\rho - 2a}{a+\rho}, \frac{a+b-\rho}{a+\rho}, \frac{a+b-\rho}{b+\rho}, \frac{a+b-\rho}{b+\rho}, \frac{2b-\rho}{b+\rho}\right\} \\
&= \max\left\{\frac{\rho - 2a}{a+\rho}, \frac{a+b-\rho}{a+\rho}, \frac{2b-\rho}{b+\rho}\right\} \\
&= \max\left\{\frac{\rho - 2a}{a+\rho}, \frac{2b-\rho}{b+\rho}\right\} \quad \text{since} \quad \rho > b/2 \\
&= \begin{cases} \frac{2b-\rho}{b+\rho}, & \text{if } \rho < \rho^* \\ \frac{\rho-2a}{a+\rho}, & \text{if } \rho > \rho^* \end{cases}
\end{aligned}$$

By comparing above equations (28) and (29) we complete the proof.

COROLLARY 4.1. *With the same hypotheses as in theorem 4.1 the necessary and sufficient condition that the PR3-ADI iteration is convergent is that* $\rho > b/2$.

*Proof.* $S_p(T_\rho) = \phi_1(\rho)^3$, hence if $\rho > b/2$ then $S_p(T_\rho) < 1$.

COROLLARY 4.2. $\rho$ *minimizing* $S_p(T_\rho)$ *is given by* $\rho = \rho^*$.

*Proof.*

$$\frac{\partial \phi_1}{\partial \rho} = -\frac{a+b}{(a+\rho)^2} < 0, \quad \rho < \rho^*$$

and

$$\frac{\partial \phi_1}{\partial \rho} = \frac{3a}{(a+\rho)^2} > 0, \quad \rho > \rho^*.$$

So, the minimum is obtained when $\rho = \rho^*$.

If $N$ is large enough then accordingly $a$ will be small so the condition that $b/2 > 2a$ is not unpractical. And the optimum value, $\rho^*$ is not linearly proportional to $h$, the meshsize, as in two dimensions, but rather **constant** throughout various meshsizes.

The above optimum $\rho$ is actually quite close to $b/2$, the lower bound for convergence.

## 5. Conclusion

In three dimensions for the separable diffusion equation the optimal $\rho$ parameter for the stationary case was determined. It turns out to be very close to $b/2$, the lower bound for the convergence. This might have been one of the important reasons why the ADI has not been so popular in three dimensions. However, as a preconditioner to a Krylov subspace method our result might turn out to be useful, for example, when used with the heuristic in [5].

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