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Adjacent-Cell Preconditioners for Accelerating Multidimensional Neutron Transport Methods*

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ADJACENT-CELL PRECONDITIONERS FOR ACCELERATING MULTIDIMENSIONAL NEUTRON TRANSPORT METHODS

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ABSTRACT

The Adjacent-cell Preconditioner (AP) is derived for accelerating generic fixed-weight, Weighted Diamond Difference (WDD) neutron transport methods in multidimensional Cartesian geometry. The AP is determined by requiring: (a) the eigenvalue of the combined mesh sweep-AP iterations to vanish in the vicinity of the origin in Fourier space; and (b) the diagonal and off-diagonal elements of the preconditioner to satisfy a diffusion-like condition. The spectra of the resulting iterations for a wide range of problem parameters exhibit a spectral radius smaller than .25, that vanishes implying immediate convergence for very large computational cells. More importantly, unlike other unconditionally stable acceleration schemes, the AP is cell-centered and its spectral radius remains small when the cell aspect ratio approaches 0 or ∞. Testing of the AP and comparison of its rate of convergence to the standard Source Iterations (SI) for Burre's Suite of Test Problems (BSTeP) demonstrates its high efficiency in reducing the number of iterations required to achieve convergence, especially for optically thick cells where acceleration is most needed.

I. INTRODUCTION

Based on the results of the one-dimensional investigation of the Adjacent-cell Preconditioning (AP) acceleration method published in Ref. 1 we proceed to derive, analyze, implement, and test the AP for multidimensional problems.

The starting point for the derivation of the AP method in multidimensional Cartesian geometry is the steady-state, isotropic scattering, one-group, discrete-ordinates approximation of the transport equation, written in the fixed-weight, Weighted Diamond Difference (WDD) form. This comprises a J-dimensional neutron balance equation,

$$\sum_{j=1}^{J} \frac{\varepsilon_{m,j}}{2} \left[\psi_{m,j}^{o,l} - \psi_{m,j}^{i,l} \right] + \psi_m^l = c\ \phi^l, \tag{1}$$

and J weighted difference relations between the cell-averaged m^{th} angular flux, ψ_m^l, and the m^{th} angular flux evaluated on the incoming and outgoing j-edges of the cell, $\psi_{m,j}^{i,l}$ and $\psi_{m,j}^{o,l}$, respectively,

$$\alpha_{m,j}\ \psi_m^l = \left[\frac{\alpha_{m,j}+1}{2} \right] \psi_{m,j}^{o,l} + \left[\frac{\alpha_{m,j}-1}{2} \right] \psi_{m,j}^{i,l}. \tag{2}$$

In Eqs. (1) and (2) we use c to denote the scattering ratio, ϕ^l to denote the previous iterate of the

scalar flux, thus $\tilde{l}$ denotes the mesh sweep stage of the computation, and the dimensionality, J=1,2, or 3, for one-, two-, or three-dimensional, problems. Also we have defined the reciprocal of the cell optical half-thickness in the j-dimension, and k^{th} angular direction by,

$$\varepsilon_{m,j} \equiv 2|\mu_{m,j}|/\sigma\, a_j, \tag{3}$$

where a_j is the size of the cell in the j-dimension, σ is the macroscopic total cross section, and $\mu_{m,j}$ is the direction cosine of the m^{th} discrete ordinate with respect to the j-axis.

Several standard methods follow from the specific choice of the spatial weights, $\alpha_{m,j}$, in Eq. (2), e.g. Diamond Difference (DD) corresponds to $\alpha_{m,j}^{-1} = 0$, and the Step method corresponds to $\alpha_{m,j} = 1$. The 0-order Nodal Integral Method (0NIM) spatial weight approaches the DD (Step) method in the limit of optically thin (thick) cells, respectively.

The spectrum of the unaccelerated Source Iterations (SI) scheme, ν_{SI}, has been calculated previously[2] in terms of method and problem parameters as well as the Fourier variables r_j. It is well known [see for example Ref. 2] that for highly scattering media, $c \to 1$, the "flat" mode ($r_j \to 0$) eigenvalue approaches unity, thereby implying deterioration in the convergence rate of the SI algorithm. Of course, in a problem of finite size the continuum of eigenvalues resulting from the Fourier analysis is replaced with a discrete spectrum. In this case the thicker the computational cells, $a_j \to \infty$, and the larger the problem size, in other words the more the medium conserves neutrons, the closer the largest eigenvalue to unity, implying stability, but at a very slow rate of convergence. Hence reducing the magnitude of the eigenvalue near the origin in Fourier space, without adversely affecting the spectrum elsewhere, is the prime objective of acceleration methods.

The rest of this paper is organized as follows. In Sec. II we derive expressions for the AP elements, and explore its spectral properties via a Fourier mode analysis. In Sec. III we briefly discuss the implementation of AP in a test code, AHOT, and describe numerical experiments performed to verify the spectral analysis presented in Sec. II. Section IV includes a comparison between the speed of convergence of AP and SI for Burre's Suite of Test Problems (BSTeP) which covers a wide range in parameter space. We close with our conclusions in Sec. V.

II. CONSTRUCTION OF THE ADJACENT-CELL PRECONDITIONER

Following the same ideas used in the one-dimensional case,[1] we introduce a preconditioning stage at the conclusion of the mesh sweep, the result of which modifies the SI updating formula to effect rapid convergence. Denoting the preconditioner with the operator D the AP stage is formally represented by,[1]

$$\phi^{l+1} = \phi^{\tilde{l}} + D^{-1}\,(\phi^{\tilde{l}} - \phi^{l}). \tag{4}$$

[Thick-cell AP (KAP) which was shown[1] to be extremely successful in accelerating problems with optically thick cells in slab geometry is abandoned here due to its complexity and not-so-exceptional performance in multidimensions]. Considering AP operators that relate the scalar flux centered in each computational cell, e.g. ϕ^l, to the $2J$ adjacent cells in all J dimensions, e.g. $\phi^l(+a_j)$ and $\phi^l(-a_j)$ for the cells in the positive and negative j-direction, respectively, and applying Fourier mode decomposition to the resulting equation yields the AP spectrum,

$$\nu_{AP} = \frac{\Phi^{l+1}}{\Phi^{l}} = \nu_{SI} + \frac{\nu_{SI} - 1}{D_d + 2\sum_{j=1}^{J} D_{o,j}\cos(2r_j)}\,. \tag{5}$$

In Eq. (5) we use D_d to denote the diagonal element of the preconditioner matrix, and $D_{o,j}$ to denote its off-diagonal elements relating a computational cell to its adjacent neighbors in the j-dimension.

We note that the diagonal and off-diagonal elements of the preconditioner matrix in both cases must satisfy a "diffusion-like" condition to guarantee stability of the flat mode. In particular, as $r_j \rightarrow 0$, $\nu_{SI} \rightarrow c$, so that the last term in Eq. (5) vanishes as $c \rightarrow 1$, thereby implying slow convergence, unless the denominator of this term also vanishes in the same limit. Hence, for $c < 1$, we require that ν_{AP}, as given by Eq. (5,) vanishes in this limit, leading to,

$$D_d = \frac{1}{c} - 1 - 2 \sum_{j=1}^{J} D_{o,j}. \tag{6}$$

When $c=1$ the last term in Eq. (5) becomes indeterminate; however, in the vicinity of the origin the ratio is finite and determined by the $O(r_j^2)$ terms of the numerator and denominator. The AP operator when applied to the vector of cell-centered fluxes, under the stability condition, Eq. (6), produces a $(2J + 1)$-point expression that bears striking resemblance to a J-dimensional cell-centered diffusion relation. However, unlike traditional DSA formalisms, here this form is derived rather than presumed.

Another condition, in addition to Eq. (6), is necessary to fully determine the preconditioner matrix elements; thus we require the spectrum of the preconditioned iterations to approach zero as $r_j \rightarrow 0$. Asymptotic analysis of Eq. (5), after substituting the full expression of ν_{SI} and Eq. (6), results in,

$$D_{o,j} = \sum_{m=1}^{N} \omega_m \, \varepsilon_{m,j} \, (\frac{1}{\alpha_{m,j}} + \varepsilon_{m,j}) \, . \tag{7}$$

This guarantees vanishing of the $O(r_j^0)$ terms in the eigenvalue of the AP accelerated iterations as $r_j \rightarrow 0$. The diagonal elements of the preconditioner are obtained by substituting Eq. (7) into the stability condition, Eq. (6).

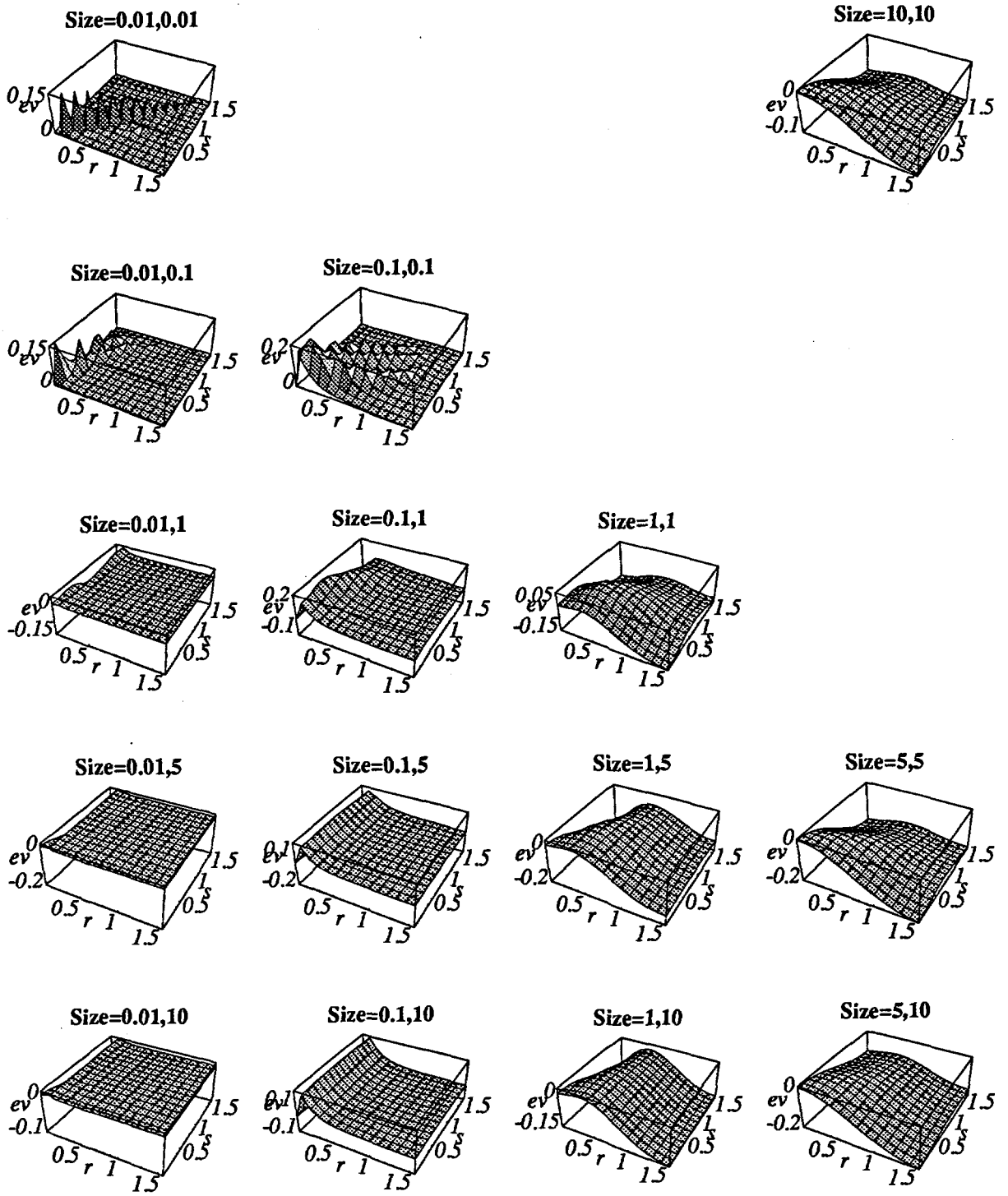
Spectra of the AP for the two-dimensional ONIM, with S_4 angular quadrature, $c = 1$, and various aspect ratios obtained by varying the x- and y-size of the computational cells, independently, between .01 and 10 *mfp* are shown in Fig. 1.

The behavior of the AP spectral radius for three-dimensional cells is similar to the two-dimensional case, shown in Fig. 1. Essentially the spectral radius increases as cell thickness increases from .01, then starts decreasing again beyond cell thickness 1, as previously observed in one-dimensional geometry.[1] The unique features of the AP spectrum that are not exhibited by many other acceleration methods in the literature are its cell-centered nature, and its small spectral radius for cells with very small or very large aspect ratios.

III. IMPLEMENTATION AND VERIFICATION OF THE SPECTRAL ANALYSIS

For non-model settings, i.e. finite media and heterogeneous material composition, we provide boundary conditions based on Larsen's prescription,[3] and the reciprocal averaging formula across material or mesh discontinuity. The resulting AP method is encoded in the AHOT code[4], restricted to ONIM, and implemented in 8 bit arithmetic on a Sun Sparc1+ workstation. For verification of the spectral analysis we employ a homogeneous region with $\sigma = 1$ and $c = 1$, vacuum boundary conditions on all external edges, and a uniform unit volumetric source in the lower left quadrant of the region. Three meshes are used in this test, 4×4, 8×8, and 16×16, where the cells are characterized

Fig. 1. Spectra of the AP for Two-dimensional 0NIM, with S_4, and c=1, and Various Cell Sizes Over the $(r,s) \equiv (r_1, r_2)$ Plane.



by three choices of the aspect ratio, $\rho \equiv a_2/a_1 = 1, .1$, and .01. The cell size in the x-direction, a_1, takes on one of six values, .01, .1, .5, 1, 5, and 10. The order and type of the angular quadrature were found to have no significant impact on the performance; in these numerical experiments we employ an S_4 quadrature. Table 1 presents the number of iterations required to achieve a pointwise relative convergence criterion of 10^{-4}.

Table 1. Number of Iterations Required to Achieve Convergence for the Verification Test Problem Using the AP Iterations in the AHOT Code.

ρ	Mesh	a_1					
		.01	.1	.5	1	5	10
1	4	4	5	6	5	6	5
	8	4	6	6	5	5	4
	16	5	7	5	5	5	4
.1	4	4	5	5	6	6	5
	8	5	6	7	8	6	5
	16	5	8	10	12	5	5
.01	4	3	4	4	4	5	6
	8	3	4	4	4	6	8
	16	4	4	5	7	9	12

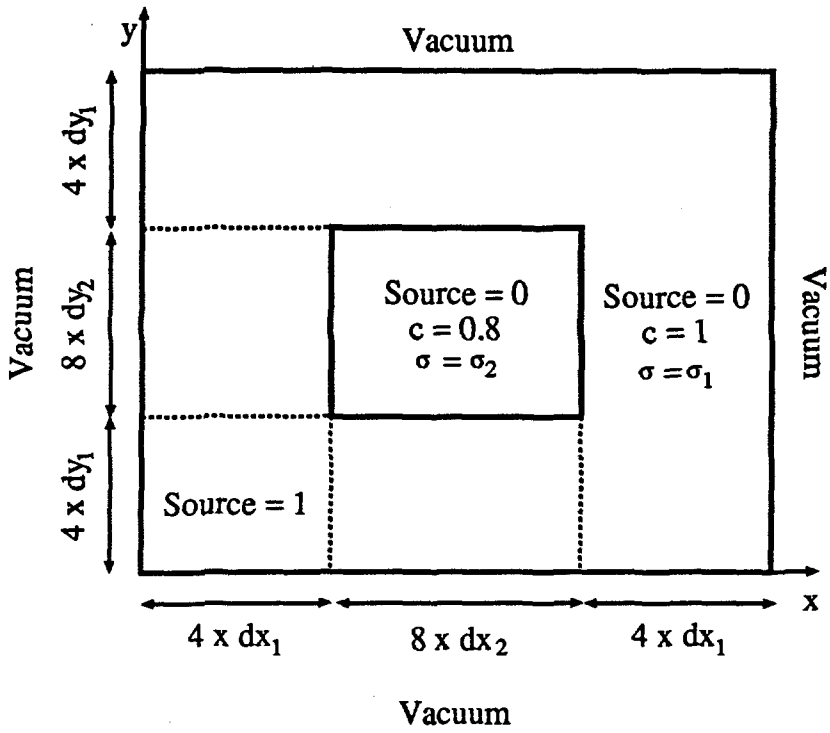
These results demonstrate the very good agreement between the spectral analysis and the observed convergence, i.e. the number of iterations for a given case in Table 1 $\sim -4/\log_{10}\rho_{AP}$, where $\rho_{AP} \equiv \max_{r_j} |\nu_{AP}|$ is the spectral radius for that case from Fig. 1. In particular the number of iterations initially increases with cell size, then starts decreasing again for large cells. This is true also for the $\rho = .01$ case even though this is not indicated by the results shown in Table 1.

IV. NUMERICAL TESTS EMPLOYING BSTeP

In order to evaluate the performance of the AP method in more realistic applications type settings we consider problems with mesh and material discontinuities. A suite of test problems, the Burre's Suite of Test Problem (BSTeP), covers a wide range in parameter space that includes sharp discontinuities and thus serves as a comprehensive test for AP. The geometric configuration of BSTeP is depicted in Fig. 2. Here we observed the number of SI and AP iterations required to achieve 10^{-4} relative pointwise convergence criterion as shown in Table 2.

The BSTeP most difficult cases, as one can expect, occur when the material discontinuity, as represented by σ_1 and σ_2, is largest, i.e. the 10 and .01 cases. The results shown in Table 2, confirm this expectation especially that most acceleration methods experience similar difficulties in such cases. In particular, the upper right corner cases of Table 2, i.e. $\sigma_1 = 10$, $\sigma_2 = .01$, converge in far more AP iterations than can possibly be explained by the spectral analysis. In order to exclude arithmetic precision as the cause for this discrepancy we solved the BSTeP case which consumes the largest number of AP iterations, namely $\sigma_1 = 10$, $\sigma_2 = .01$, $dy_1 = .1$, and $dy_2 = .01$, using a single precision version of the AHOT code described above. The observed number of iterations

Fig. 2. Geometric Configuration of the Burre's Suite of Test Problems (BSTeP).



Mesh: 16 x 16 $dx_1 = 1 = dx_2$

σ_1, σ_2 : {.01,.1,1,10} dy_1, dy_2 : {.01,.1,1}

S_6 Angular Quadrature

did not show sensitivity to the arithmetic precision employed. The fact that the boundary conditions perform well in model problem configurations, and in most of the cases included in Table 2, especially where the material discontinuity is not too sharp, excludes them as the reason for the deterioration in the spectral properties. Spectral analysis of a problem configuration with a single periodic interface across which mesh and material discontinuities are permitted provides evidence that the diffusion-like coupling stencil imposed by AP is responsible for this poor behavior. This should not be too surprising because the diffusion approximation is known to be invalid near sharp material discontinuities. Alternative coupling schemes capable of faster convergence, and comparison of AP performance to that of other acceleration methods is under investigation.

V. CONCLUSION

We have derived the Adjacent-cell Preconditioner for the general Weighted Diamond Difference discretization of the neutron transport equation in multidimensional Cartesian geometry. We performed a spectral analysis of the AP iterations in model problem settings and demonstrated its small spectral radius for a wide range of nuclear properties and cell aspect ratios. The AP opera-

Table 2. Number of Iterations Required to Achieve Convergence for Burre's Suite of Test Problems Using AP (top) and SI (bottom) Algorithms in AHOT with 0NIM.

			σ_1											
			.01			.1			1			10		
		dy_1	.01	.1	1	.01	.1	1	.01	.1	1	.01	.1	1
σ_2		dy_2	4	5	5	4	8	7	7	14	10	15	37	13
		.01	3	5	6	4	8	15	8	26	158	57	317	1515
			5	5	5	7	9	8	11	21	15	18	36	22
	.01	.1	5	6	6	7	9	15	23	50	153	223	482	1465
			6	5	5	8	10	8	10	12	12	13	15	13
		1	7	7	7	13	18	15	79	76	149	633	813	1309
			4	5	5	5	7	7	7	11	6	13	18	6
		.01	4	5	6	5	9	15	8	29	158	59	354	1511
			7	7	6	6	8	7	10	12	8	15	18	10
	.1	.1	7	7	7	7	11	15	27	48	151	299	476	1436
			8	9	7	7	7	7	8	9	9	10	11	10
		1	15	15	11	15	15	17	70	77	136	635	763	1173
			6	7	6	6	8	7	6	12	5	11	10	5
		.01	6	7	7	7	10	15	8	38	156	46	385	1472
			11	13	10	9	11	9	10	11	5	11	7	6
	1	.1	17	16	13	17	19	19	29	52	141	253	464	1287
			10	11	11	8	8	9	6	6	5	6	6	5
		1	46	43	39	45	50	39	109	92	142	669	762	1242
			10	14	11	9	12	9	7	10	5	10	5	5
		.01	13	16	14	14	17	20	15	38	141	51	337	1280
			10	13	10	7	11	9	8	11	6	7	6	5
	10	.1	60	59	40	60	58	40	67	76	126	166	451	1234
			8	10	9	8	9	9	8	9	6	7	7	6
		1	73	75	63	73	74	63	99	112	140	587	801	1389

tor is cell-centered, a very important feature in multidimensional and high order implementation in production codes. We implemented our new method in a special version of the test code AHOT and successfully verified the spectral analysis using a simple configuration with homogeneous material composition and a uniform mesh. To fully test the method we applied it to Burre's Suite of Test Problems which covers a wide range in parameter space and found AP to be extremely efficient in reducing the number of iterations required to achieve convergence. However, some cases are too slow to converge in contradiction with the spectral analysis of the method. These cases are characterized with very sharp material and mesh discontinuities that are not taken into consideration in the spectral analysis. Other acceleration methods have been found to run into similar difficulties in such cases. The question now is: does there exist another sparse preconditioner that is unconditionally stable even in the presence of sharp discontinuities?

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