Two Conjectures on the Crisis of Cell-Centered Diffusive Operators for the Iterative Acceleration of Neutron Transport Methods in the PHI Configuration

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A recent study examined the asymptotic behavior of the elements of the integral transport matrix **B** in the thick-cell limit for homogeneous configurations in 2D [1]. It was shown that **B** acquires a sparse structure, implying a strong local coupling of a cell-averaged scalar flux with only its nearest Cartesian neighbors. Here we extend this work to the Periodic Horizontal Interface (PHI) configuration, where layers of two different materials are stacked in the y direction in an alternating fashion. The asymptotic properties of **B** lead to the formulation of two conjectures on the structural deficiency of the Adjacent-cell Preconditioner (AP) [2,3], and potentially of other diffusive operators, notably Diffusion Synthetic Acceleration (DSA) [4,5], in PHI. The two conjectures are verified by devising two novel acceleration schemes, named APB and OAP. A loss of unconditional robustness has been observed, both for AP and DSA, in strongly heterogeneous multidimensional configurations. In this respect, the verification of the above conjectures represents a first step in understanding and possibly resolving the crisis of diffusive operators in such configurations.

Integral Transport Matrix in PHI. For PHI we seek estimates for the strength of coupling of a cell-averaged scalar flux for a cell in the thick (K) or thin (N) layer with the fluxes in its neighbors. We consider an even number of layers, J, comprising I computational cells along the x-axis. The cells' properties are:

$$\text{K cell}, j \text{ even}: \ \delta_x, \delta_y, \Sigma_K = \sigma_K \Delta, c_K$$

$$\text{N cell}, j \text{ odd}: \ \delta_x, \delta_y, \Sigma_N = \sigma_N / \Delta, c_N$$

The scattering ratios c_l, with $l = \text{N, K}$, are fixed parameters, and a uniform mesh with fixed cell size δ_x, δ_y is assumed. The total cross sections Σ_l are scaled according to the dimensionless parameter Δ, vanishing like Δ^{-1} in the N layer and diverging like Δ in the K layer as $\Delta \to \infty$. The results pertaining to an N cell are of particular relevance. Hence, the results summarized in Fig. 1 refer to cell (1,1) in an N layer. Denoting the cell aspect ratio $R \equiv \delta_x / \delta_y$ the behavior of the **B** elements for square cells, $R = 1$, is distinct from their behavior for rectangular cells, $R \neq 1$. The results in Fig. 1 indicate that the coupling of an N cell's scalar flux with

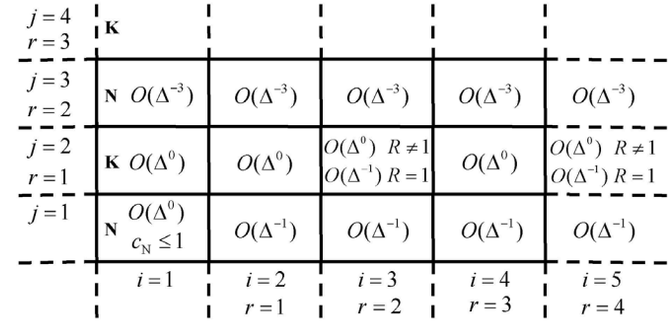

Fig. 1. Strength of coupling of N cell's flux with its neighbors for PHI.

the fluxes in the next K layer (interlayer coupling) can be of the same order as self-coupling and coupling with the first Cartesian neighbors. Also, the coupling of an N cell's scalar flux with the fluxes in the same N layer (intralayer coupling) is of the same order, independent of the distance between the cells in the layer. The long-range nature of the latter coupling plays an important role in the loss of robustness of AP.

APB. The AP ignores the strong cross-derivative coupling between a cell and its diagonal neighbors, displayed by the full **B**. Therefore, we conjecture, and establish via numerical experiments, that extended low-order operators that account

for cross-derivative coupling can recover acceleration robustness in PHI. Specifically, the APB extends AP by including cross-derivative coupling in a nine-point stencil operator that was implemented in the AP2 code [2]. The L_2 estimates of the spectral radius ρ obtained from the code with increasing mesh size for vacuum boundary conditions are contrasted with the values predicted from the Fourier analysis for a model PHI in Table 1. In the model $c_{K,N} = 1 - 10^{-8}$, $\delta_{x,y} = \sigma_{K,N} = 1$, and S_6 level symmetric angular quadrature are used. The number of iterations consumed to achieve 10^{-5} convergence of the scalar fluxes for the same problem driven by a uniform unit fixed source is also reported in Table 1. The APB's spectral radius is bounded below 0.55 for all Δ, whereas AP's approaches 1 as $\Delta \rightarrow \infty$. Indeed, in contrast to APB, which converges for all values of Δ, AP did not converge in 50 iterations for $\Delta > 10^2$. Results of further testing beyond the model problem indicate that robustness of APB decreases with increasing R, with ρ exceeding 0.8 for R larger than 4:1. This behavior appears consistent with the dependence on R of the asymptotic results in Fig. 1.

Table 1. Spectral radius and APB iterations in PHI.

	Δ					
$I \times J$	10^0	10^1	10^2	10^3	10^4	10^5
10 × 10	0.103 5	0.392 12	0.460 13	0.468 14	0.468 14	0.468 14
20 × 20	0.117 5	0.444 12	0.515 14	0.523 15	0.524 15	0.523 14
40 × 40	0.123 5	0.463 13	0.534 15	0.542 15	0.543 15	0.542 15
80 × 80	0.124 5	0.468 13	0.539 15	0.547 15	0.548 15	0.547 15
160 × 160	0.124 5	0.470 13	0.540 15	0.548 15	0.549 15	0.548 15
Fourier	**0.125**	**0.471**	**0.541**	**0.549**	**0.550**	**0.549**

OAP. A second conjecture we propose attributes the crisis of AP to its overestimating the strength of intralayer coupling in an N layer. The OAP maintains the five-point stencil of AP while optimizing the value of the elements exerting intralayer coupling in the N and K layers. The optimization procedure is time consuming and was performed only for Δ equal to 10^4 and 10^5, to test the validity of the conjecture in the asymptotic regime. The L_2 estimates of ρ and the iterations consumed to achieve 10^{-5} convergence of the scalar fluxes are contrasted with the values predicted from Fourier analysis for the model problem in Table 2. The OAP is more resilient to adverse effects of material discontinuities than APB. Though numerical results beyond the model problem show that its robustness is also conditional with respect to R—namely, it is guaranteed that ρ does not exceed 0.8 up to an aspect ratio of 5:1. Further research is envisioned for a nine-point OAP that holds promise to improve the spectral properties of OAP by incorporating cross-derivative coupling. We also wish to find a prescription for computing the optimization coefficients from the geometric and material properties of the transport problem.

Table 2. Spectral radius and OAP iterations in PHI.

	Δ			
	10^4		10^5	
$I \times J$	ρ	*It*	ρ	*It*
10 × 10	0.282	9	0.281	9
20 × 20	0.341	9	0.340	9
40 × 40	0.369	10	0.363	10
80 × 80	0.378	10	0.381	10
160 × 160	0.388	10	0.388	10
Fourier	**0.390**		**0.390**	

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Funding Acknowledgments
LANL Directed Research and Development Program