*Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)*
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

# FOURIER ANALYSIS OF PARALLEL BLOCK-JACOBI SPLITTING WITH TRANSPORT SYNTHETIC ACCELERATION IN TWO-DIMENSIONAL GEOMETRY

**Massimiliano Rosa**
Department of Mechanical & Nuclear Engineering
The Pennsylvania State University
138 Reber Building, University Park, PA 16802, USA
mzr127@psu.edu

**James S. Warsa and Jae H. Chang**
Los Alamos National Laboratory
P.O. Box 1663, MS D409, Los Alamos, NM 87545, USA
warsa@lanl.gov; jhchang@lanl.gov

## ABSTRACT

A Fourier analysis is conducted in two-dimensional (2D) Cartesian geometry for the discrete-ordinates ($S_N$) approximation of the neutron transport problem solved with Richardson iteration (Source Iteration) and Richardson iteration preconditioned with Transport Synthetic Acceleration (TSA), using the Parallel Block-Jacobi (PBJ) algorithm. The results for the un-accelerated algorithm show that convergence of PBJ can degrade, leading in particular to stagnation of GMRES(m) in problems containing optically thin sub-domains. The results for the accelerated algorithm indicate that TSA can be used to efficiently precondition an iterative method in the optically thin case when implemented in the "modified" version MTSA, in which only the scattering in the low order equations is reduced by some non-negative factor $\beta < 1$.

*Key Words*: neutral particle transport, iterative acceleration, Fourier analysis, Transport Synthetic Acceleration, Parallel Block-Jacobi

## 1. INTRODUCTION

Fourier analysis is traditionally used to study transport iteration schemes in a homogeneous infinite medium. In fact, it represents a valuable tool to understand the behavior of the iteration error modes of various acceleration techniques, either in their continuous or spatially discretized forms. A Fourier analysis has been recently performed in slab geometry [1] for the discrete-ordinates ($S_N$) approximation of the steady-state one-group transport problem solved with Richardson iteration and preconditioned Richardson iteration, using the Parallel Block-Jacobi (PBJ) algorithm. Two types of Transport Synthetic Acceleration (TSA) have been considered as a preconditioner, the traditional "Beta" TSA (TTSA) and a modified TSA (MTSA).

In this paper the Fourier analysis for PBJ and for PBJ with TTSA and MTSA is extended to 2D Cartesian geometry. The spatial discretization considered is a Bilinear Discontinuous Finite Element Method (BLDFEM) and the scattering is assumed to be isotropic. The analysis is verified with results from a 2D transport code.

## 2. FOURIER ANALYSIS OF PBJ IN 2D GEOMETRY

The two-cell approach [1] that has proven to be effective in capturing the peculiar features of the PBJ algorithm into the Fourier analysis in slab geometry is naturally extended to 2D Cartesian geometry by considering four computational cells, sharing the interfaces between four adjacent processors, as schematically represented in Fig. 1.

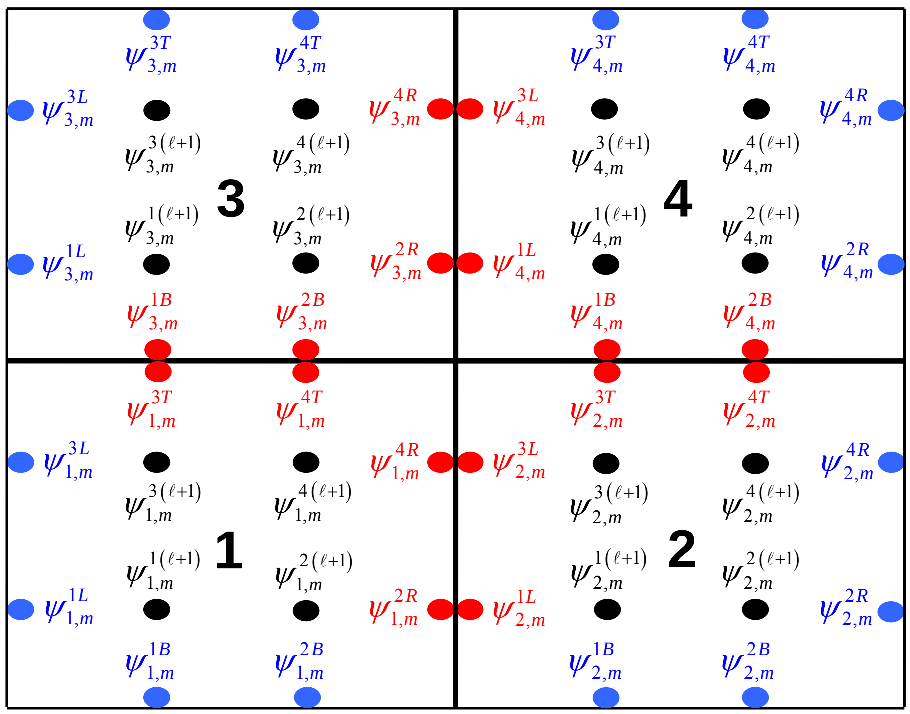


**Figure 1. Four-cell system for the Fourier analysis of PBJ.**

### 2.1. Fourier Analysis

The formulation of the problem in terms of angular fluxes only is initially convenient in order to devise a Fourier analysis for the PBJ algorithm. It is then possible to cast the Fourier analysis in terms of the variables actually utilized in the numerical implementation of PBJ in the 2D transport code, namely scalar fluxes and interface angular fluxes, introducing suitable projection operators that map the angular fluxes into the interface angular fluxes.

The equations representing the fixed-source-free BLDFEM [2] spatial discretization of the $S_N$ approximation to the 2D homogeneous transport problem are written for the four-cell system of Fig. 1. The relationships representing the extension to 2D geometry of the interface conditions and of the Fourier ansatz [1] are presented in Eqs. (1,2) and in Eqs. (3,4) respectively, for the discrete-ordinates with positive cosines $\mu_m$ and $\eta_m$. Analogous expressions are introduced for the discrete ordinates in the remaining three quadrants.

Interface Conditions $\left(\mu_m > 0, \eta_m > 0\right)$

$$\psi_{i,m}^{1,3L} = \psi_{(i-1),m}^{2,4(\ell)},\ i = 2,4 \tag{1}$$

$$\psi_{i,m}^{1,2B} = \psi_{(i-2),m}^{3,4(\ell)},\ i = 3,4 \tag{2}$$

Fourier Ansatz $\left(\mu_m > 0, \eta_m > 0\right)$

$$\psi_{(i-1),m}^{1,3L} = \psi_{i,m}^{2,4(\ell+1)} \exp\left(-j\lambda_x \sigma 2\mathrm{dx}\right),\ i = 2,4 \tag{3}$$

$$\psi_{(i-2),m}^{1,2B} = \psi_{i,m}^{3,4(\ell+1)} \exp\left(-j\lambda_y \sigma 2\mathrm{dy}\right),\ i = 3,4 \tag{4}$$

In the previous equations, $j = \sqrt{-1}$ represents the imaginary unit, $\sigma$ is the macroscopic total cross section, while $\mathrm{dx}$ ($\mathrm{dy}$) is the width of a cell in the *x* (*y*) direction. Finally, $\lambda_x$ ($\lambda_y$) is the wave-number of the Fourier modes in the *x* (*y*) direction.

Substitution of the interface conditions and of the Fourier ansatz into the original BLDFEM equations and the use of suitable projection operators produce, after considerable algebra, the iteration matrix $\mathbf{T}_{PBJ}$ for the PBJ algorithm in the scalar and interface angular flux formulation. Given a certain quadrature order, and values for $\sigma$ and the scattering ratio *c*, the spectral radius $\rho$ of $\mathbf{T}_{PBJ}$ and the minimum eigenvalue $\Lambda$ of the symmetric part of $\left(\mathbf{I} - \mathbf{T}_{PBJ}\right)$ are finally obtained as a function of $\mathrm{dx}$ and $\mathrm{dy}$:

$$\rho\left(\mathrm{dx},\mathrm{dy}\right) = \max_{\lambda_x,\lambda_y}\left(abs\left(Eig\left(\mathbf{T}_{PBJ}\left(\mathrm{dx},\mathrm{dy},\lambda_x,\lambda_y\right)\right)\right)\right) \tag{5}$$

$$\Lambda\left(\mathrm{dx},\mathrm{dy}\right) = \min_{\lambda_x,\lambda_y}\left(Eig\left(\frac{1}{2}\left[\left(\mathbf{I} - \mathbf{T}_{PBJ}\right) + \left(\mathbf{I} - \mathbf{T}_{PBJ}\right)^*\right]\right)\right) \tag{6}$$

If $\Lambda$ is positive, matrix $\left(\mathbf{I} - \mathbf{T}_{PBJ}\right)$ is positive definite and a Krylov method like GMRES is guaranteed to converge. However, if $\Lambda$ is negative, GMRES is not guaranteed to converge.

In Fig. 2, we plot the spectral radius as a function of cell widths obtained for a level-symmetric $S_4$ quadrature with equal weights, assuming $\sigma = 1$ and $c = 0.5$. The plot for $\Lambda$ is presented in Fig. 3. The results in Fig. 2 point to the fact that convergence of the PBJ algorithm can degrade for problems containing optically thin sub-domains, even for values of the scattering ratio *c* less than unity. In fact the spectral radius, as the cell widths are decreased, is independent from the value of *c*. The results in Fig. 3 indicate that restarted GMRES, GMRES(m), may stagnate for optically thin problems because $\Lambda$ becomes negative.

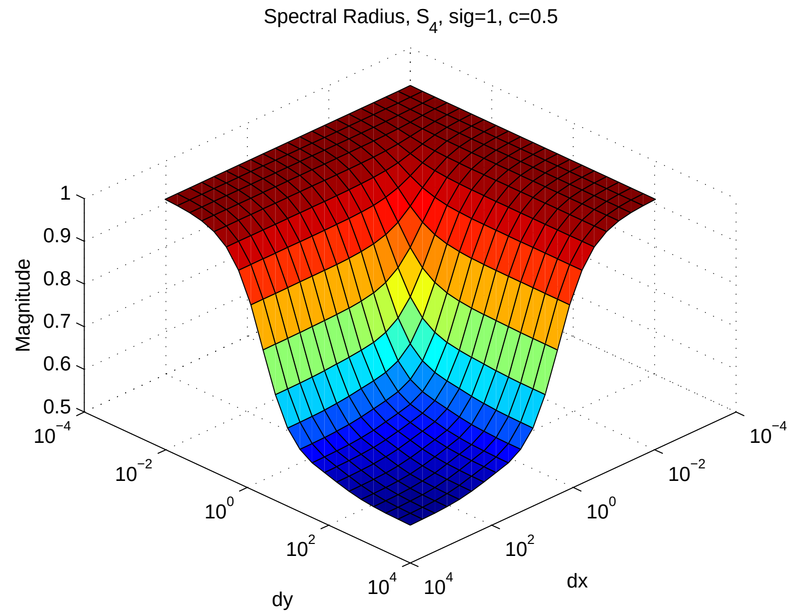


**Figure 2. Fourier analysis for PBJ: ρ.**

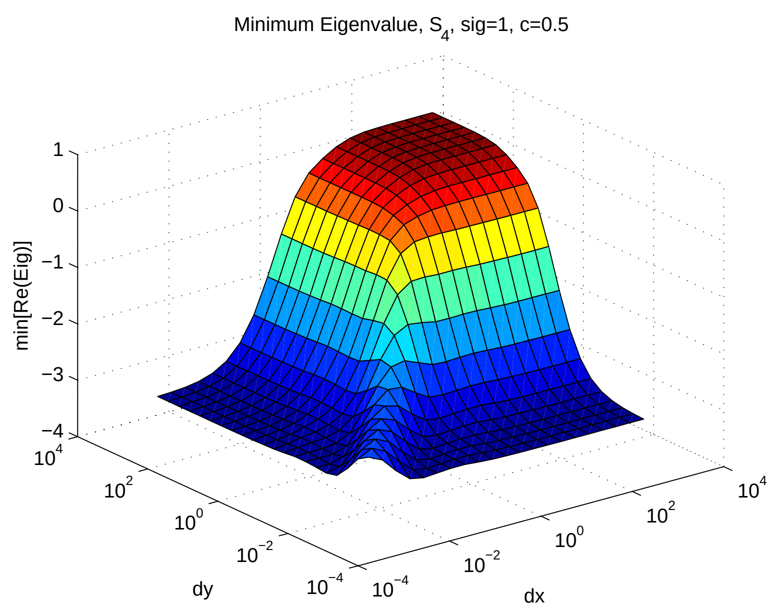


**Figure 3. Fourier analysis for PBJ: Λ.**

The predictions from the Fourier analysis for PBJ have been compared with the numerical results obtained from the 2D transport code. For the purpose of this comparison, the code has the capability of building the $(\mathbf{I}-\mathbf{T})$ matrix for the 2D problem treated. The spectral radius and the minimum eigenvalue can then be determined and compared with the results of the Fourier analysis. Notice that the Fourier analysis refers to the case of an infinite medium treated by an infinite number of processors. To reproduce the conditions of the Fourier analysis, the 2D transport code ran on four processors with four computational cells per processor (Nx = Ny = 2) and with reflective boundary conditions on all four boundaries, in order to eliminate the effect of leakage. The results for ρ and Λ obtained for a level-symmetric $S_4$ quadrature with equal weights, a unitary total macroscopic cross-section and a scattering ratio of 0.5 are compared with the Fourier analysis in Table I and in Table II, respectively. In both cases it may be noticed that the numerical results are very close to the predicted theoretical values.

**Table I: Theoretical and computed ρ for a problem with reflective boundaries (Nx=Ny=2)**

| dx = dy | $10^{-3}$ | $10^{-2}$ | $10^{-1}$ | $10^{0}$ | $10^{+1}$ | $10^{+2}$ | $10^{+3}$ |
|---|---|---|---|---|---|---|---|
| **Fourier** | 0.9991 | 0.9910 | 0.9195 | 0.6600 | 0.5509 | 0.5097 | 0.5010 |
| **Code** | 0.9991 | 0.9910 | 0.9196 | 0.6622 | 0.5376 | 0.5050 | 0.5005 |

**Table II: Theoretical and computed Λ for a problem with reflective boundaries (Nx=Ny=2)**

| dx = dy | $10^{-3}$ | $10^{-2}$ | $10^{-1}$ | $10^{0}$ | $10^{+1}$ | $10^{+2}$ | $10^{+3}$ |
|---|---|---|---|---|---|---|---|
| **Fourier** | -2.5745 | -2.5305 | -2.1376 | -0.4881 | 0.3136 | 0.4874 | 0.4906 |
| **Code** | -2.4958 | -2.4520 | -2.0642 | -0.4471 | 0.4340 | 0.4900 | 0.4907 |

The number of iterations and the residual are reported in Table III for different values of the restart parameter. A maximum number of 1000 iterations and a tolerance of $10^{-5}$ have been pre-set in the calculations. The results show that GMRES(m) may stagnate for a value of the restart parameter equal to the square root of the number of processors, which is number of steps needed to propagate the information across the full problem domain.

**Table III: Number of iterations and residual for GMRES(m)**

| dx = dy | $10^{-3}$ | $10^{-2}$ | $10^{-1}$ | $10^{0}$ | $10^{+1}$ | $10^{+2}$ | $10^{+3}$ |
|---|---|---|---|---|---|---|---|
| **m=40** | 10<br>4.272e-8 | 9<br>9.527e-6 | 9<br>7.105e-7 | 7<br>4.441e-7 | 5<br>9.818e-7 | 3<br>3.237e-6 | 2<br>2.067e-7 |
| **m=4** | >1000<br>1.065(†) | >1000<br>2.547e-3(†) | 39<br>7.825e-6 | 10<br>6.217e-6 | 6<br>2.484e-6 | 3<br>3.237e-6 | 2<br>2.067e-7 |
| **m=3** | >1000<br>1.080(†) | >1000<br>1.021(†) | >1000<br>4.167e-5(†) | 11<br>2.475e-6 | 5<br>4.857e-6 | 3<br>3.237e-6 | 2<br>2.067e-7 |
| **m=2** | >1000<br>1.083(†) | >1000<br>1.071(†) | >1000<br>1.607(†) | 13<br>3.247e-6 | 6<br>2.478e-6 | 3<br>3.268e-6 | 2<br>2.067e-7 |

(†) The residual stagnates.

## 3. FOURIER ANALYSIS OF PBJ WITH TSA IN 2D GEOMETRY

The results shown in the previous section indicate that preconditioning of the PBJ algorithm is needed to improve its spectral properties, especially for optically thin problems. In this section, we present preliminary results of Fourier analysis of PBJ accelerated using both traditional TSA (TTSA) and modified TSA (MTSA) as preconditioners in 2D Cartesian geometry. Since the effective scattering ratio $c'$ is a measure of the actual computational effort required by each acceleration method, the comparison of the two methods is again carried out for equal values of this parameter. In particular, the results presented in this section refer to the case $c'=0$ $(\beta=1)$ that gives an upper bound for the spectral radius.

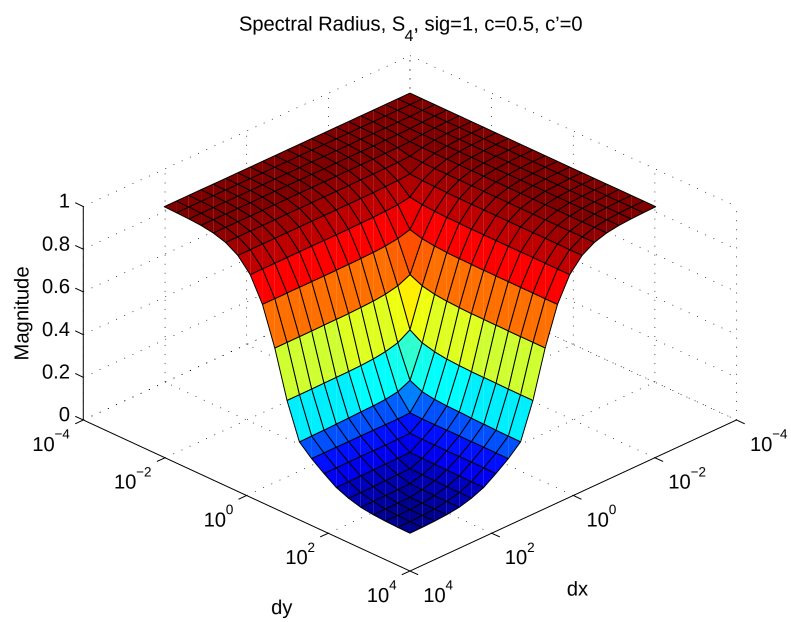


**Figure 4. Fourier analysis for PBJ with TTSA: ρ.**

The surfaces are obtained by plotting the spectral radius ρ from the Fourier analysis as a function of the cell widths, Fig. 4 for TTSA and Fig. 5 for MTSA, respectively. TTSA appears extremely effective for thick problems, for which the spectral radius tends to zero. However, the spectral properties degrade for thin problems. Also, for values of the scattering ratio *c* greater than 0.5, the spectral radius may become greater than one leading to instability, unless the $\beta$ parameter is properly selected. MTSA is slightly less effective than TTSA for thick problems, where the spectral radius tends to a small value greater than zero. The spectral properties are better for thin problems. As a matter of fact, the spectral radius is always bounded from above by the value of the scattering ratio *c*, for $\beta=1$. MTSA is therefore unconditionally stable.

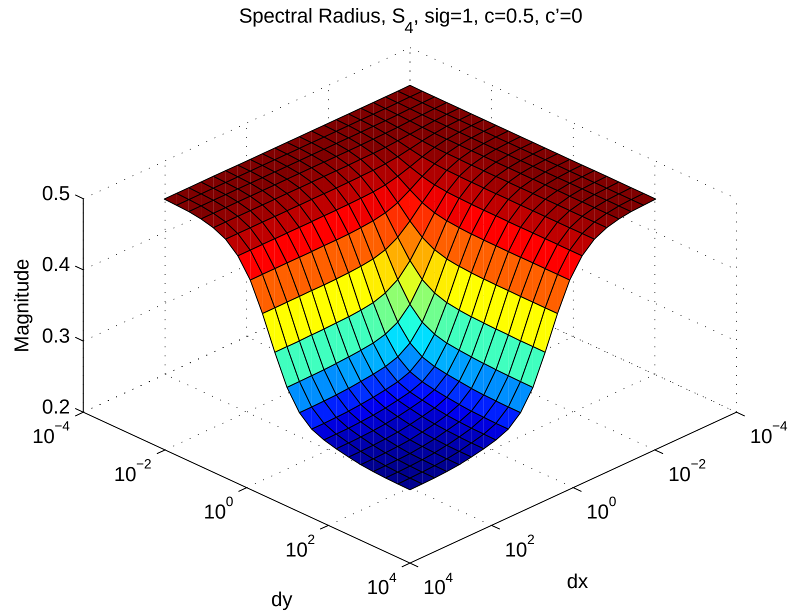


**Figure 5. Fourier analysis for PBJ with MTSA: ρ.**

## 4. CONCLUSIONS

A Fourier analysis has been implemented for the Parallel Block-Jacobi (PBJ) algorithm and for PBJ with both traditional TSA (TTSA) and modified TSA (MTSA). The results for the un-accelerated algorithm show that convergence of PBJ can degrade and lead to stagnation of GMRES(m) in problems with optically thin sub-domains. These predictions have in turn been successfully verified against the 2D transport code.

Preliminary results of the Fourier analysis for the accelerated PBJ algorithm indicate that PBJ with TTSA can be effective provided the β parameter is properly tuned for a given scattering ratio *c*, but is potentially unstable. Compared to TTSA, MTSA is less sensitive to the choice of β, more effective for the same computational effort ($c'$), and it is unconditionally stable. In the future these predictions will be verified with the numerical 2D transport code.

## ACKNOWLEDGMENTS

This information has been authored by employees of the Los Alamos National Security, LLC (LANS) operator of Los Alamos National Laboratory under contract No DE-AC52-06NA25396 with the U.S. Department of Energy.

## REFERENCES

1. M. Rosa, J. S. Warsa, J. H. Chang, "Fourier Analysis of Parallel Inexact Block-Jacobi Splitting with Transport Synthetic Acceleration in Slab Geometry," *Proc. Int. Topical Mtg. PHYSOR-2006*, Vancouver, BC, Canada, Sep. 10-14, 2006, on CD-ROM, ANS, LaGrange Park, IL (2006).

2. M. L. Adams, "Discontinuous Finite Element Transport Solutions in Thick Diffusive Problems," *Nucl. Sci. Eng.*, **137**, pp.298-333 (2001).