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AN ALGEBRAIC MULTIGRID RESOLUTION STRATEGY FOR THE DP_N SYNTHETIC ACCELERATION OPERATOR

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In some recent papers[1,2,5], the DP_N operator has been introduced as a mean to accelerate free iterations for TDT code that is based on the Method of Characteristics (MOC). The quite complicated structure of this sparse matrix operator asks for an adapted numerical treatment. In the past many improvements of classical numerical algorithms, i.e. Krylov subspaces methods, have been proposed: these improvements consist basically in an adaptation of the standard algorithms to the specific form of DP_N operator. In this paper we conclude this task by presenting the impact of a newly implemented technique of Algebraic Multi-Grid (AMG). We present here an AMG method tailored for our specific application. We show that, by means of a preliminary elimination phase, we can obtain a reduced dimension operator, with exactly the same form of the full dimension one. The solution is then obtained by solving this reduced problem with the same techniques that have been previously developed.

KEYWORDS: .Characteristics method, synthetic acceleration, algebraic multigrid method.

1. Introduction

The DP_N equations are used to accelerate characteristics transport iterations and are derived in a consistent manner with respect to transport. I don't insist here on the similarities between the two operators [3], but I will detail only the DP_N geometrical form that is involved into the multigrid resolution strategy. For each region, the boundary is decomposed into surfaces, a surface α being typically the common interface with a neighboring region, and using a surface-wise constant approximation one writes:

$$\psi_{\pm}(r_s,\Omega) \sim \vec{A}_S(\Omega)\vec{\psi}_{\pm,\alpha}\ , r_s \in S_\alpha, \qquad (1)$$

where S_α stand for a generic surface in geometry. The quantities ψ_α will be called in the following "currents" or "partial currents", and this even if they are mostly related to fluxes rather than currents. The lower index S in $\vec{A}_S(\Omega)$ is used to indicate that the spherical harmonics vector for surfaces fluxes is not necessarily of the same order as that for volume sources. Indeed the order for surface fluxes is greater or equal to the index for volume fluxes, the reason for this will be apparent from the following equation (5). Development (1) is then used to express the following "projected currents":

$$J^{\rho}_{\pm,\alpha} = \int_{S_\alpha} dS \int_{(2\pi^{\pm})} d\Omega \left|\Omega \bullet n\right| A^{\rho}(\Omega)\psi_{\pm}(r_s,\Omega) = \sum_{\upsilon} A^{\rho\upsilon}_{\alpha,\pm}\psi^{\upsilon}_{\pm,\alpha}. \quad (2)$$

The projected currents are the physical quantities conserved in the DP_N synthetic method. I note that for the lowest moment this quantity is exactly the neutron current. The index "*N*" indicates that a "P_N" spherical harmonics development has been done in (1). Being strictly related to the MOC, the DP_N method uses the same set of tracking trajectories computed for this last. Boundary fluxes in (2) are expressed thank to the angular integral equation:

$$\psi_{+}(R,\Omega) = \psi_{-}(0,\Omega)e^{-\Sigma R} + \int_0^R dx\, e^{-\Sigma(R-x)} q\left(x,\Omega\right) \quad (3)$$

across the cell and along each trajectory, to derive a transmission equation for the exiting fluxes. In the last equation *R* is the trajectory chord length and the lower indexes + and – denote, respectively, the angular fluxes exiting and entering the cell along trajectory *t*, and *q* is the emission source. The integration of equation (3) is done in the framework of the characteristic method as is detailed in [2]. The substitution of (3) into (2) gives:

$$\sum_{\upsilon} A^{\rho\upsilon}_{\alpha,+}\psi^{\upsilon}_{+,\alpha} = \sum_{\beta,\upsilon} T^{\rho\upsilon}_{\alpha\beta}\psi^{\upsilon}_{-,\beta} + \sum_{\upsilon} E^{\rho\upsilon}_{\alpha i} V_i q^{\upsilon}_i, \quad (4)$$

where q^{υ}_i is the moment υ of the source in region i, and all escape and transmission coefficients, *E* and *T*, obey many symmetry and anti-symmetry relations. [3] Since the source *q* contains flux moments, supplementary equations are needed to close the problem, such as the following balance relation:

$$\sum_{\alpha,\upsilon} A^{\rho\upsilon}_{\alpha,+}\left(\psi^{\upsilon}_{+,\alpha} - s^{\rho}s^{\upsilon}\psi^{\upsilon}_{-,\alpha}\right) + \Sigma_i V_i \phi^{\rho}_i = V_i \sum_{\upsilon} B^{\rho\upsilon} q^{\upsilon}_i, \quad (5)$$

where "*s*" stands for harmonic parity and *B* is an operator that takes into account the lack of numerical ortogonality for the spherical harmonics functions, and that would be the identity for exact integration. The number of currents is less or equal to the number of flux moments in (5), so that the anisotropy order for currents is always greater than for collision source. Equation (5) can be very ill conditioned when one deals with almost-vacuum situations or with a weak absorption. To enforce the numerical stability in a similar way as in [3], I write (5) as:

$$\sum_{\upsilon} M^{\rho\upsilon}_i \phi^{\upsilon}_i = 4\sum_{\beta\upsilon} E^{\rho\upsilon}_{\beta i} s^{\rho}s^{\upsilon}\psi^{\upsilon}_{-,\alpha} + \sum_{\upsilon} \frac{B^{\rho\upsilon}_i - E^{\rho\upsilon}_i}{\Sigma_i} S^{\upsilon}_i, \quad (6)$$

where $c^{\upsilon}_{s,i} = \dfrac{\Sigma^{\upsilon}_{s,i}}{\Sigma_i}$, $E^{\rho\upsilon}_i = \sum_{\alpha} E^{\rho\upsilon}_{\alpha i}$, *S* stands for the external source and

$M^{\rho\upsilon}_i = \delta_{\rho\upsilon} + \left(E^{\rho\upsilon}_i - B^{\rho\upsilon}\right)c^{\upsilon}_{s,i}$.

By replacing the flux moments from (6) in (4) and inverting matrix *A*, the final form of the problem is:

$$\psi_{+,\alpha}^{\rho} = \sum_{\beta \in i,\upsilon} \hat{T}_{\alpha,\beta}^{\rho\upsilon} \psi_{-,\beta}^{\upsilon} + \sum_{\upsilon} \hat{E}_{\alpha,i}^{\rho\upsilon} V_i S_i^{\upsilon} , \tag{7}$$

where the sum over β is done over all boundary surfaces of region *i*, and the sum over υ over all angular modes. In (7) all coupling coefficients *T* and *E* are no more physically established quantities but purely algebraic ones, so that no symmetry or reciprocity is valid for them. Equation (7) applies to each interface flux mode exiting the side of each region. A continuity condition is imposed between neighboring regions so that outgoing modes always equal entering ones in neighboring regions. General boundary conditions are treatable with specific equations.[4] In paper [5] there have been detailed some important improvements of standard Krylov subspace techniques applied to the problem (7). These improvements are strictly related to the specific geometrical form of (7). One of the major objectives of this paper is to show that the multigrid technique introduced here allows the adoption of the same strategies.

Once interface fluxes have been computed from (7), the average flux moments are computed by a re-arranged form of (6) which is written as:

$$\phi_i^{\rho} = \sum_{\beta \in i,\upsilon} H_{\beta,i}^{\rho\upsilon} \psi_{-,\beta}^{\upsilon} + \sum_{\upsilon} G_i^{\rho\upsilon} S_i^{\upsilon} , \tag{8}$$

where the following notation has been used :

$$H_{\beta}^{\rho\upsilon} = 4 \sum_{\upsilon'} M_{\rho\upsilon'}^{-1} E_{\beta i}^{\upsilon'\upsilon} s^{\upsilon'} s^{\upsilon}, \; G_i^{\rho\upsilon} = \sum_{\upsilon'} M_{\rho\upsilon'}^{-1} \frac{B_i^{\upsilon'\upsilon} - E_i^{\upsilon'\upsilon}}{\Sigma_i} ..$$

2 Two-level algebraic multigrid method

The two-level algebraic method reduces the computational effort needed to solve the synthetic problem by reducing the number of unknowns involved in the iteration procedure. It is important to note that the method introduced here is purely algebraic, in the sense that no approximation is made in the resolution strategy adopted. Actually, I will build a second-level operator that gives an exact solution to the problem, but on a reduced number of unknowns. This reduced operator will have the same response-matrix form and will be amenable to undergo the same numerical treatment as that for the fine mesh operator.

The algebraic reduction of unknowns is similar to the one done in exact domain decompositions using Schur' complements. [6]

The first step is to choose a partition of the unknowns in different subsets. Every subset is so subdivided into two different parts of unknowns. The first part contains all the unknowns that are coupled only with other unknowns of the subset. All the unknowns that have external couplings constitute the second part. In order to formalize this procedure we can work with regions.

Let denote with *D* the set of regions that constitute this geometry, that is to say $D = \{i, i \in [1, N_r]\}$, where N_r is the number of regions in the geometry. A « macro region » « *I* » is defined as a subset of connected regions of *D*.

In the following I will use upper case letters for macro regions and lower case letters for simple regions. For $i \in I$ the partial fluxes exiting this region will be denoted in three

different manners :

$$\psi_{+,\alpha}^{in,in}, \psi_{+,\alpha}^{ex,in}, \psi_{+,\alpha}^{in,ex}, \tag{9}$$

according to whether the current goes from an internal region to another, from an external region to an internal one, from an internal region to an external one. Note that the set of internal currents is transformed into itself by the operator *P* that reverses the direction of the currents, i.e. that changes outgoing into ingoing currents and vice versa. Equation (7) written for currents that are on the interfaces between two internal regions reads:

$$\vec{\psi}_{+}^{in,in} = \left(I - T_{i,i}P\right)^{-1}\left[T_{i,e}\vec{\psi}_{-,ex} + E^{in}\vec{V}\vec{S}\right], \tag{10}$$

where $T_{i,i}$ is the part of the transmission matrix that couples internal currents with internal currents, $T_{i,e}$ is that part which couples external currents with internal ones, E^{in} is the matrix which gives the escape of the collision source for all internal regions through internal faces, $\vec{S}$ is the vector of all internal sources and $\vec{V}$ is the diagonal operator multiplying source element times the region volume. I define:

$$\hat{T}_{i,e} = \left(I - T_{i,i}P\right)^{-1} T_{i,e}\ , \quad \hat{E}_{i,i} = \left(I - T_{i,i}P\right)^{-1} E_{\alpha i}^{in},$$

so that Eq. (10) can be written for a current on a surface dividing two macro regions, briefly denoted as a grid current « gr », as :

$$\vec{\psi}_{\alpha,gr}^{+} = \underbrace{\left[T_{e,e} + T_{i,e}\hat{T}_{i,e}\right]}_{\hat{T}_{e,e}}\vec{\psi}_{\alpha,gr}^{-} + \underbrace{\left[T_{e,i}\hat{E}_{i,i} + E_{e,i}^{\alpha}\right]}_{\hat{E}_{e,i}}\vec{V}\vec{S}\,, \tag{11}$$

where $T_{e,e}$ is the part of the transmission matrix which couples external to other external currents. Equation (11) is a reduced form of the transmission equation acting only on grid unknowns. This equation has the same response-matrix form of Eq. (7) written for the reference geometry. The only difference is the exclusive presence of currents connecting macro regions instead of standard currents. This permits the use not only of the same program routines but also of the same acceleration techniques already established for the basic equation (7). Once grid currents have been determined, by solving problem (11), all other currents, that couple only internal regions, are computed by (10), rewritten here as:

$$\vec{\psi}_{+,\alpha}^{in,in} = \sum_{\beta\in\partial I}\hat{T}_{i,e}^{\alpha\beta}\vec{\psi}_{-,\beta}^{ex} + \sum_{j\in I}\left(\hat{E}_{ii}\right)_{\alpha i}^{j} V_j S_j, \tag{12}$$

which is valid for all surfaces α internal to macro-region *I*. The only set of unknowns to be still computed is that of flux moments. Introducing the “macro regions” partition of unknowns into Eq. (8) one can write :

$$\phi_{i,\rho} = \sum_{(\beta,\rho)\in\partial i^{-}et(\beta,\rho)\in\partial I^{-}} H_{\beta}^{\rho\upsilon}\psi_{-,\beta}^{\upsilon} + \sum_{\substack{(\beta,\upsilon)\in\partial I^{-}\\(\beta',\upsilon')\notin\partial I^{-}}} H_{\beta'}^{\rho\upsilon'}\left(\hat{T}_{i,e}\right)_{\beta'\upsilon'}^{\beta\upsilon}\psi_{-,\beta}^{\upsilon} + \sum_{\substack{j\in I,\\(\beta,\upsilon')\in\partial i^{-},(\beta,\upsilon')\notin\partial I^{-}}}\left(H_{\beta}^{\rho\upsilon'}\left(\hat{E}_{i,e}\right)_{\beta,ij}^{\upsilon'\upsilon} + G_i^{\rho\upsilon}\delta_{ij}\right)V_j S_j^{\upsilon},$$

which results from the elimination of all currents relating internal regions. It is then possible to give the following definitions :

$$\hat{H}_{\beta}^{\rho\upsilon} = H_{\beta}^{\rho\upsilon} + \sum_{(\beta',\upsilon')\notin\partial I^{-}} H_{\beta'}^{\rho\upsilon'} \left(\hat{T}_{i,e}\right)_{\beta'\upsilon'}^{\beta\upsilon}, \hat{G}_{ij}^{\rho\upsilon} = \sum_{\substack{(\beta,\upsilon')\in\partial i^{-} \\ (\beta,\upsilon')\notin\partial I^{-}}} \left(H_{\beta}^{\rho\upsilon'} \left(\hat{E}_{i,e}\right)_{\beta,ij}^{\upsilon'\upsilon} + G_{i}^{\rho\upsilon}\delta_{ij} \right),$$

and the equation for the flux will be more simply written as :

$$\phi_{i,\rho} = \sum_{(\beta,\rho)\in\partial I^{-}} \hat{H}_{\beta}^{\rho\upsilon} J_{-,\beta}^{\upsilon} + \sum_{\upsilon,j\in I} \hat{G}_{ij}^{\rho\upsilon} V_j Q_j^{\upsilon}, \tag{13}$$

which has the same form as Eq. (8). Once again no particular specialization is needed at this level to implement the multigrid method in the standard program.

It is important to note that the critical point for this algebraic multigrid method to work is that the multiple inversion procedure involved with the computation of matrixes $\left(I - T_{i,i}P\right)^{-1}$ present in Eq. (10) must be a very fast one. This operation is done once for all in a preparatory initial phase, and it is then exploited in multigroup iterations.

In order to achieve a higher efficiency I adopt, inside each macro region, an ICM (Inverse Cuthill-McKee [6]) renumbering of the regions and I compute then, on the renumbered system, an LU factorization for $I\text{-}T_{i,i}P$ that preserves the front of the matrix. Each factorization is then stored with the standard CSR algorithm.[6] With this LU factorization the action of $\left(I - T_{i,i}P\right)^{-1}$ is obtained by inverting, over matrixes $T_{i,e}$ and $E_{\alpha i}^{in}$, the lower and upper part separately. Some tests have proven that this procedure is much more faster than a crude LU gaussian factorization done over the non-reordered local matrixes. The difference is already sensible for macro regions of more than 10 regions. As this number increases the time of gaussian factorization raises faster than linearly. On the contrary, after applying the ICM reordering, the sparse LU factorization time increases almost as a linear function of regions.

Thermal synthetic acceleration

The speed up permitted by the algebraic multilevel method allows a further application of the DP_N method. Indeed to apply it to the thermal problem. I recall here the form of this problem and show that synthetic acceleration is applicable to it quite naturally.

The classic Gauss-Seidel iteration strategy for thermal iterations can be written as:

$$L_g \phi_g^{(l+1)} = H_{g\leftarrow g}\phi_g^{(l+1)} + \sum_{g'<g} H_{g\leftarrow g'}\phi_{g'}^{(l+1)} + \sum_{g'>g} H_{g\leftarrow g'}\phi_{g'}^{(l)} + F_g \,. \tag{14}$$

Operator *L* stands for the one-group transport operator, while operators "*H*" are the slowing down operators acting on the direction indicated by the arrows. Finally *F* is the fission source for group g. The index "l" refers to the iteration process. The up-scattering contribution, inside Eq. (14), is computed by fluxes coming from the preceding iteration. One can apply the synthetic acceleration recipe to (14), so that making the difference between (14) and a converged solution one can obtain for the correction the following equation:

$$L_g \delta\phi_g = H_{g\leftarrow g}\delta\phi_g + \sum_{g'<g} H_{g\leftarrow g'}\delta\phi_{g'} + \sum_{g'>g} H_{g\leftarrow g'}\delta\phi_{g'} + \sum_{g'>g} H_{g\leftarrow g'}\Delta\phi_{g'}. \tag{15}$$

One readily recognizes the standard synthetic problem. In the multigroup thermal iterations one can compute the source once the difference between two transport iterations is available.

After that problem (15) is solved with the synthetic operator, the estimated correction is inserted in the multigroup flux for the next transport sweep.

3 Numerical results

To show the effectiveness of our approach we report calculation times for the C5G7 benchmark calculation [7], done with TDT (~20000 regions). All computing parameters for the MOC calculation as well as comparaisons of results with a reference Monte Carlo result are provided in [8]. The synthetic acceleration operator adopted in these calculations is the DP_1 one. In every case the synthetic problem is solved with a ILU0 preconditioning and with all renumbering strategies illustrated in [5]. Table 1 shows calculation times for three different phases, that is the phase of acceleration matrix (and other transport auxiliaries) building, the phase of a full multigroup initialization done with the synthetic operator and finally the phase of the accelerated transport calculation. All computing times are expressed in seconds and calculations have been done on a Pentium 4 2.1 Ghz machine.

The new AMG method is very efficient in the two last phases but implies a great overhead for matrix building. Nevertheless the adoption of the AMG method greatly improves the total computing time since it permits (in the case without synthetic thermal acceleration) to reduce it from ~1800 seconds to ~1100 seconds. As for thermal synthetic synthetic acceleration its results are shown in the fourth row of table 1. This strategy permits a great diminution of the number of internal iteration (reduced from 752 to 448). Anyway, for this benchmark, the total time gain is only of ~100 seconds, so that even if this method is better performing the advantage is not too great.

Table 1 Results for the C5G7 benchmark. All computing times are expressed in seconds. The figures are to be interpreted as follows: “a” is the number of external iterations, “b” is the total number of internal iterations, “c” is the computing time needed for transport calculation (building and initializing phases excluded), “d” , between parenthesis, is the time needed for initialization.

Keff=1.18641	AMG	No AMG
Building Phase	237	136
No Thermal Synthetic	16[a] 752[b] 813[c] (85[d])	15 726 1293 (339)
Thermal Synthetic	15 448 776 (81.9)	

4. Conclusion

In this paper a new method is introduced to improve the solution of the DP_N synthetic acceleration problem. This method is based on the well known idea of multilevel partition of unknowns. Thank to this partition an algebraic elimination of the unknowns is done that permit to obtain a lower dimension operator that has the same form as the original one. This

feature allows one to adopt the same resolution techniques used for the standard operator but on a reduced system. Results on C5G7 benchmark show the efficiency of the technique.

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