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An Acceleration of the Characteristics by a Space-Angle Two-level Method using Surface Discontinuity Factors

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Abstract

We present a non-linear space-angle two-level acceleration scheme for the method of the characteristics (MOC). To the fine level on which the MOC transport calculation is performed, we associate a more coarsely discretised phase space in which a low-order problem is solved as an acceleration step. Cross sections on the coarse level are obtained by a flux-volume homogenisation technique, which entails the non-linearity of the acceleration. Discontinuity factors per surface are introduced as additional degrees of freedom on the coarse level in order to ensure the equivalence of the heterogeneous and the homogenised problem. After each fine transport iteration, a low-order transport problem is iteratively solved on the homogenised grid. The solution of this problem is then used to correct the angular moments of the flux resulting from the previous free transport sweep. Numerical tests for a given benchmark have been performed. Results are discussed.

KEYWORDS: MOC, Non-linear Acceleration, Discontinuity Factors

1. Introduction

In recent years, the Method of Characteristics (MOC) has been widely used to model neutron transport problems in complicated geometries for modern heterogeneous reactor analysis. In the MOC approach [1], the phase space is discretised as follows: the geometrical domain $\mathcal{D}$ is decomposed into a set of homogeneous regions $\{D_i\}$ on which a flat-source approximation is done; a set of discrete angular directions and associated weights $\{\mathbf{\Omega}_n, \omega_n\}_{n=1,N}$ is chosen. For each direction a set of parallel trajectories is tracked. Although this method has proven to be very suitable to modern assembly-level transport problems, its efficient acceleration remains an open question. In previous works [2, 3], we have introduced a non-linear space-angle multigrid method to speed up the convergence rate of the inner iterations for the TDT solver in the APOLLO2 code [4]. This acceleration scheme presented two levels: a fine level on which the MOC transport calculation was performed and a more coarsely discretised phase space in which a low-order problem was solved as an acceleration step. Furthermore, it employed, on each homogenised mesh belonging to the so-called coarse level, two discontinuity factors

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(DFs) which were respectively applied to the outgoing and the incoming current. This ensured the equivalence between the heterogeneous and the homogenised problem [5–7].

Here, we propose a modification of the method in [3], the novelty being that surface discontinuity factors (SDFs) are employed on each coarse-mesh. This is expected to give better results for problems with strong heterogeneities. The two-level general framework is the same. The first step is to define a more coarsely discretised phase space. Coarsening affects both spatial and angular variable. For spatial discretisation, each coarse mesh $\mathcal{D}_I$ is obtained by fusing together fine meshes. We have:

$$\mathcal{D}_I = \underset{i\in I}{\cup}\mathcal{D}_i \quad \Rightarrow \quad V_I = \sum_{i\in I} V_i \; . \tag{1}$$

Flux-volume homogenised cross sections are used on the coarse level, which entails the non-linearity of the scheme. Further, a low-order angular quadrature formula is employed on the coarse level:

$$\{\mathbf{\Omega}_m, \omega_m\}_{m=1,M} \text{ with } M < N. \tag{2}$$

The acceleration step consists in solving, on the so-obtained more coarsely discretised phase space, a modified transport problem yielding a scalar flux $\{\phi_I^h\}$ while keeping the MOC-formalism. This flux is then used to reconstruct and accelerate the flux moments resulting from the previous free iteration $(n+1)$ as follows:

$$\left(\phi_i^{kl}\right)_{acc}^{(n+1)} = \left(\gamma_i^{kl}\right)^{(n+1)} \phi_I^h, \quad \forall \;\; i \in I \; . \tag{3}$$

To do this, we employ shape factors $\{\gamma_i^{kl}\}$ computed after each transport sweep. They are defined as:

$$\gamma_i^{kl} = \frac{\phi_i^{kl}}{\bar{\phi}_I}, \tag{4}$$

where $\bar{\phi}_I$ is the volume-averaged scalar flux:

$$\bar{\phi}_I = \frac{1}{V_I} \sum_{i\in I} \phi_i V_i \; . \tag{5}$$

This prolongation procedure [8, 9] requires that, once the convergence has been achieved, the following condition must be fulfilled:

$$\bar{\phi}_I = \phi_I^h \; . \tag{6}$$

This is achieved by introducing additional degrees of freedom such as discontinuity factors. In this work, the SDFs are employed in order to reconstruct, in the low-order balance equation, the partial currents of particles travelling from a coarse region I to its adjacent K through their common surface. In fact, because of homogenisation and source projection, partial currents computed by the low-order transport operator are a priori not consistent with the ones resulting from the high-order calculation. In particular, in a reference situation where the converged fine flux is available, the leakage term is not preserved on the two levels. On the coarse level isotropic sources are used. The projected inscatter or external sources, respectively $\bar{q}_I$ and $\bar{S}_I$, are obtained from the high-order ones by a space-angle restriction procedure which reads:

$$\bar{S}_I = \frac{1}{4\pi} \sum_n \omega_n \sum_{i\in I} V_i S_i \left(\mathbf{\Omega}_n\right) \; . \tag{7}$$

This kind of projection permits to avoid building a table of correspondence between the two angular representations.

The paper is structured as follows: in section 2 we give the basic equations of the MOC; in section 3 we introduce the low-order problem and the MOC-like formalism which is used to iteratively solve it; in section 4 some numerical results are presented and discussed; closing conclusions are given in section 5.

2. The Characteristics

We give here the basic equations of the method of the characteristics. More details can be found in [1, 10]. The method is based upon two main equations: a balance equation for the angular flux on each region i, and a propagation equation giving the angular flux leaving the region i in terms of the incoming angular flux and the internal source. The propagation equation along a trajectory t parallel to the discrete direction $\mathbf{\Omega}_n$ crossing a region i is:

$$\psi_{+,i}\left(t,\mathbf{\Omega}_n\right)=\psi_{-,i}\left(t,\mathbf{\Omega}_n\right)+\beta_i\left(t,\mathbf{\Omega}_n\right)\left[q_i\left(\mathbf{\Omega}_n\right)-\sigma_i\psi_{-,i}\left(t,\mathbf{\Omega}_n\right)\right]\ , \tag{8}$$

where the escape coefficient is:

$$\beta_i\left(t,\mathbf{\Omega}_n\right)=\frac{1-e^{-\sigma_i R_i\left(t,\mathbf{\Omega}_n\right)}}{\sigma_i}\ , \tag{9}$$

and $R_i\left(t,\mathbf{\Omega}_n\right)$ is the length of the trajectory within the region. The average emission density $q_i\left(\mathbf{\Omega}_n\right)$ is written as:

$$q_i\left(\mathbf{\Omega}_n\right)=C_i\left(\mathbf{\Omega}_n\right)+S_i\left(\mathbf{\Omega}_n\right)\ , \tag{10}$$

where $S_i\left(\mathbf{\Omega}_n\right)$ is the average external source and $C_i\left(\mathbf{\Omega}_n\right)$ is the within-group transfer. The latter is given by:

$$C_i\left(\mathbf{\Omega}_n\right)=\sum_{k=0}^{K_i}\sigma_{s_{k,i}}\sum_{l\leq|k|}A^{kl}\left(\mathbf{\Omega}_n\right)\phi_i^{kl}\ , \tag{11}$$

where K_i is the degree of anisotropy in region i. The moments ϕ_i^{kl} of the angular flux are obtained as follows:

$$\phi_i^{kl}=\sum_n w_n A^{kl}\left(\mathbf{\Omega}_n\right)\psi_i\left(\mathbf{\Omega}_n\right)\ . \tag{12}$$

The balance equation is obtained by integration of the integral-differential form of the transport equation over the volume of a region i:

$$\sum_{t\shortparallel\mathbf{\Omega}_n,t\cap i}w_\perp\left(t,\mathbf{\Omega}_n\right)\left[\psi_{+,i}\left(t,\mathbf{\Omega}_n\right)-\psi_{-,i}\left(t,\mathbf{\Omega}_n\right)\right]+\sigma_i\psi_i\left(\mathbf{\Omega}_n\right)V_i=q_i\left(\mathbf{\Omega}_n\right)V_i\ , \tag{13}$$

the sum in t being done for all trajectories with direction $\mathbf{\Omega}_n$ that intersect region i,

3. Low-order problem

After a transport sweep which can be summarised as follows:

$$q_i^{(n)}\left(\mathbf{\Omega}_n\right)\rightarrow\psi_i^{(n+1)}\left(\mathbf{\Omega}_n\right)\rightarrow\phi_i^{(n+1)}\ , \tag{14}$$

a low-order problem is iteratively solved as an acceleration step. Let be p the iteration index, we have the following steps:

1. The source term is updated as follows:

$$q_I^{h,(p)} = \frac{1}{4\pi}\sigma_{s_I}^h \phi_I^{h,(p)} + \bar{S}_I \ , \tag{15}$$

where the coarse-level scattering cross section is given by a flux-volume homogenisation procedure:

$$\sigma_{s_I}^h = \frac{1}{\bar{\phi}_I V_I} \sum_{i \in I} \sigma_{s_i}^0 \phi_i V_i \ . \tag{16}$$

2. A MOC propagation equation is employed:

$$\hat{\psi}_{+,I}^{(p+1)}\left(t, \mathbf{\Omega}_m\right) = \hat{\psi}_{-,I}^{(p+1)}\left(t, \mathbf{\Omega}_m\right) + \beta_I^h\left(t, \mathbf{\Omega}_m\right)\left[q_I^{(p)} - \sigma_I^h \hat{\psi}_{-,I}^{(p+1)}\left(t, \mathbf{\Omega}_m\right)\right] \ , \tag{17}$$

the escape coefficient $\beta_I^h\left(t, \mathbf{\Omega}_m\right)$ being defined in an analogous way to the fine case:

$$\beta_I^h\left(t, \mathbf{\Omega}_m\right) = \frac{1 - e^{-\sigma_I^h R_I(t, \mathbf{\Omega}_m)}}{\sigma_I^h} \ , \tag{18}$$

where σ_I^h is the homogenised total cross section defined as:

$$\sigma_I^h = \frac{1}{\bar{\phi}_I V_I} \sum_{i \in I} \sigma_i \phi_i V_i \ , \tag{19}$$

and $R_I\left(t, \mathbf{\Omega}_m\right)$ is the length of the chord intersected in the macro-region I by the trajectory t.

3. The partial current from a region I to its neighbour K is built up as follows:

$$\hat{J}_{I \to K} = \sum_{m=1}^{M/2} \omega_m \sum_{\substack{t \| \mathbf{\Omega}_m \\ t \cap \partial\mathcal{D}_{IK}}} \omega_\perp\left(t\right) \hat{\psi}_{+,I}\left(t, \mathbf{\Omega}_m\right) \ , \tag{20}$$

where $\partial\mathcal{D}_{IK} = \partial\mathcal{D}_I \cap \partial\mathcal{D}_K$.

4. The coarse scalar flux is obtained from the following modified balance equation using the SDFs:

$$\sum_{K \in \mathcal{N}(I)} \left[f_{K \to I} \cdot \hat{J}_{K \to I}^{(p+1)} - f_{I \to K} \cdot \hat{J}_{I \to K}^{(p+1)}\right] + \sigma_I^h \phi_I^{h,(p+1)} V_I = Q_I^{h,(p)} V_I \ , \tag{21}$$

where the sum is done over all the neighbours of I, the weight $w_\perp(t)$ represents the orthogonal area associated with the trajectory, and $Q_I^h = \sum_m \omega_m q_I^h$. The so-obtained coarse scalar flux is the used to update the coarse source.

The SDFs are dynamically computed: their evaluation is done after performing a transport iteration and before solving the associated low-order problem. For each surface, they are computed as a ratio between the heterogeneous current $J_{I \to K}$ depending on angular flux in (14) and the current $\hat{J}_{I \to K}$ produced by the low-order operator in a reference situation. We have:

$$f_{I \to K} = \left.\frac{J_{I \to K}}{\hat{J}_{I \to K}}\right|_{ref} \ . \tag{22}$$

We note that the evaluation of the currents $\{\hat{J}_{I\to K}\}$ consists in solving a fixed-source transport problem on the coarse level with:

$$q_I^h = \bar{q}_I^{(n)} \ . \tag{23}$$

This requires to perform one transport sweep.

4. Results

Tests have been performed in order to test the effectiveness of our method. We present here the case of a BWR assembly benchmark using a 6 group P1 cross sections library [11].

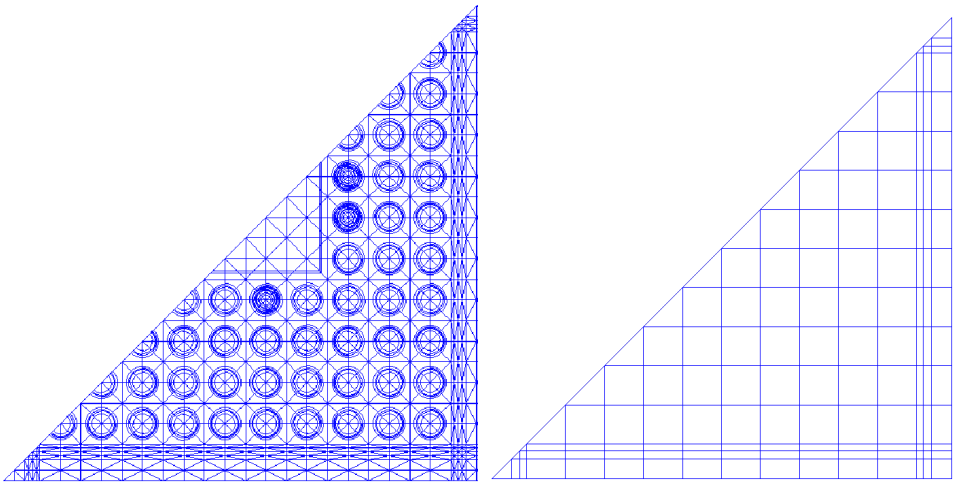

Figure 1: Fine and coarse spatial discretisation for Atrium benchmark

For our fine level MOC calculation, we use a 3052-region discretisation. Because of the enforced specular boundary conditions on all the three sides, a set of cyclic trajectories [10] has been used. The trajectories have been tracked for all the directions in a product angular quadrature formula comprising 20 uniformly spaced azimuthal angles in $(0, \pi)$ and three polar angles derived from a Bickley-Naylor formula [12] in $(0, \pi/2)$. On the coarse level we have 136 meshes, with a ratio of fine to coarse meshes of ~ 22.4 (see Fig. 1). A poorer angular quadrature formula has been considered on this level. All the tracking parameters for the two levels can be found in Table 1.

Level	Regions	Azimutal angles	Polar angles	Spacing	Trajectories	Tracks
Fine	3052	20 (uniform)	3 (Bickley)	0.02	1084	954,466
Coarse	136	4 (uniform)	2 (Bickley)	0.06	113	11,301

Table 1: Tracking parameters for tracking on fine and coarse level. The number of tracks is the total number of intersections of trajectories with regions.

All the calculations have been converged to the same solution (eigenvalue $k_{eff} = 1.12854$) with a relative precision of 10^{-5} on inner iterations and eigenvalue, and a relative precision of 10^{-4} on thermal iterations and fission rates. For all the accelerated calculations, the following iterative strategy has been adopted: only one transport iteration per group is performed for

each outer iteration, and the maximum number of inner iterations for the low-order problem is a priori fixed to 15. Results are given in Table 2.

$k_{eff} = 1.12854$	Free	DFs	SDFs
building time	5.85	4.30	4.21
solving time	555.24	55.36	60.07
(fine+coarse+other)		(36.76+2.72+15.88)	(42.00+2.77+15.30)
total time	561.09	59.66	64.28
# transport sweeps	1403	88	88

Table 2: Atrium assembly benchmark. Results are given for the old version (DFs) and the new version (SFDs) of the presented two-level acceleration scheme. A reference to the unaccelerated case is also supplied. All times are expressed in seconds.

This table gives global computation parameters such as the total computing time and the total number of transport sweeps. Total calculation time is divided into the different phases of the calculation: building (which includes reading geometry, tracking, and computing MOC parameters), and the solution of the *k*-eigenvalue multi-group problem. For the latter, the contributions from fine-level and coarse-level calculation are given between parenthesis. We give results for the old version (using global incoming and outgoing DFs) and the new version (using SDFs) of our acceleration scheme. Furthermore, all the calculations are compared to the free-iteration results.

Both accelerations give the same total number of transport sweeps and total computing times are similar. In particular, the total computing time for the new version results to be slightly bigger. This is due to the fact that, in the new version, each transport iteration requires some more work than the old one to compute and store currents on each surface of the coarser discretisation. And, since the total number of transport iterations is not reduced, the overall cost becomes more expensive. For the Atrium benchmark, the extension of our method to SDFs seems not to bring any benefits.

5. Conclusions

In this work, we have presented an extension of a previous space-angle two-level acceleration for the MOC. This new implementation consists in using surface discontinuity factors (SDF) on the coarse level instead of global incoming and outgoing discontinuity factors (DFs). In both cases, those factors are employed to correct partial currents in the balance equation for the coarse homogenised scalar flux. The latter is then used to reconstruct the moments of the fine angular flux.

Intuitively, we would expected this extension to lead to an improvement of our acceleration scheme, especially for a class of problems with much strong heterogeneities. However, the tests that we have performed on the Atrium benchmark have not give the expected results so far. Work is in progress to better understand this behaviour. Cases with stronger heterogeneities should be taken into consideration.

Furthermore, as we already pointed out in [2,3], work is under way to extend this acceleration

technique to more levels for reactor-core-size transport problems. In this perspective, SDFs could play an important role to ease the implementation task.

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