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Application of the DSA Preconditioned GMRES formalism to the Method of Characteristics - First Results

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The method of characteristics is well known for its slow convergence; consequently, as it is often done for S_N methods, the Generalized Minimal RESidual approach (GMRES) has been investigated for its practical implementation and its high reliability. GMRES is one of the most effective Krylov iterative methods to solve large linear systems. Moreover, the system has been "left preconditioned" with the Algebraic Collapsing Acceleration (ACA) a variant of the Diffusion Synthetic Acceleration (DSA) based on I. Suslov's former works.

This paper presents the first numerical results of these methods in 2D geometries with material discontinuities. Indeed, previous investigations have shown a degraded effectiveness of Diffusion Synthetic Accelerations with this kind of geometries. Results are presented for 9×9 Cartesian assemblies in terms of the speed of convergence of the inner iterations (fixed source) of the method of characteristics. It shows a significant improvement on the convergence rate.

KEYWORDS: Method of Characteristics, Krylov Subspace, GMRES, Diffusion Synthetic Acceleration

1. Projection on a Krylov Subspace

First, we establish the compatibility between the method of characteristics presented in Ref. 1 and the GMRES formalism as presented in Refs. 2–4.

The domain is first divided into N homogeneous regions with M boundary regions for which isotropic reflection is assumed. It is well known that the method of characteristics is totally equivalent to the collision probabilities method (one can find a proof in Ref. 12). Consequently, with linear algebra formalism, inner loop at fixed external sources (fission and scattering from other groups) $(F_i)_{1 \leq i \leq N}$ for a specific energy group can be written as

$$\mathbb{H}\vec{\Phi} = \mathbb{L}\vec{F} \tag{1}$$

where

$\vec{\Phi} = [\Phi \; J]^{\mathrm{T}}$: $(N+M)$ vector containing zonal scalar fluxes and outgoing currents

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$\vec{F} = [F]^{\mathrm{T}}$: N vector containing zonal sources

$\mathbb{H}$ and $\mathbb{L}$: $(N+M) \times (N+M)$ matrix and $(N+M) \times N$ matrix.

If we introduce an iteration index, (n), we can consider standard iterations

$$\begin{aligned} \vec{\Phi}^{(1)} &= \mathbb{P}\mathbb{L}\vec{F} \\ \vec{\Phi}^{(n+1)} &= \vec{\Phi}^{(1)} + (\mathbb{I} - \mathbb{P}\mathbb{H})\vec{\Phi}^{(n)} \end{aligned} \tag{2}$$

where $\mathbb{I}$ is the $(N+M) \times (N+M)$ identity matrix and $\mathbb{P}$ is a $(N+M) \times (N+M)$ left preconditionning matrix approaching $\mathbb{H}^{-1}$. This iteration will converge if one can find a norm definition such that $\|\mathbb{I} - \mathbb{P}\mathbb{H}\| < 1$.

We can express these iterations in a practical way in terms of the residual at the n^{th} iteration as

$$\mathbb{P}(\mathbb{L}\vec{F} - \mathbb{H}\vec{\Phi}^{(n)}) = \vec{\Phi}^{(n+1)} - \vec{\Phi}^{(n)} \tag{3}$$

This algorithm takes F and $\vec{\Phi}^{(n)}$ as inputs and delivers $\vec{\Phi}^{(n+1)}$ in output.

We implemented the method of characteristics in such a way that enables us to apply the Generalized Minimal RESidual formalism. The `GMRES` approach consists in a projection method on the Krylov subspace $K_m(r_{(o)}, \mathbb{P}\mathbb{H})$, where $r_{(o)}$ is the initial residual, with an orthogonalization of the final residual $r_{(m)}$ with respect to the subspace $\mathbb{P}\mathbb{H}K_m(r_{(o)}, \mathbb{P}\mathbb{H})$. In order to limit memory use, we have opted for the restarted version `GMRES`(m), which restarts the process every m iterations. A summary description of this method is given in Table 1.

2. Left Preconditioning

We based our preconditioning on the Algebraic Collapsing Acceleration, developed by I. Sulsov[5,6] and based on H. Khalil's work described in Ref. 7. It performs a correction of the flux at the n^{th} iteration using

$$\begin{aligned} \vec{\Phi}^{(n+\frac{1}{2})} &= \mathbb{L}\vec{F} - \mathbb{H}\vec{\Phi}^{(n)} + \vec{\Phi}^{(n)} \\ \vec{\Phi}^{(n+1)} &= \vec{\Phi}^{(n+\frac{1}{2})} + \vec{\Psi}^{(n+1)} \end{aligned} \tag{4}$$

where $\vec{\Psi}^{(n+1)}$ is the correction term which satisfies

$$\mathbb{D}\vec{\Psi}^{(n+1)} = \mathbb{E}\left(\vec{\Phi}^{(n+\frac{1}{2})} - \vec{\Phi}^{(n)}\right) \tag{5}$$

where $\mathbb{D}$ and $\mathbb{E}$ are $(N+M) \times (N+M)$ matrices.

This approach will be practical only if system (5) is easy to solve and if matrices $\mathbb{D}$ and $\mathbb{E}$ are sparse. This is achieved by constructing this system on a low order approximation for the angular variable. We therefore assumed

$$\psi(\vec{r}, \hat{\Omega}) + \psi(\vec{r}, -\hat{\Omega}) = 2 \times \Psi(\vec{r}). \tag{6}$$

It is easy to verify that this acceleration stands for a left preconditioning of the original system (1) and that

$$\begin{aligned} \vec{\Phi}^{(n+1)} - \vec{\Phi}^{(n)} &= \vec{\Phi}^{(n+\frac{1}{2})} - \vec{\Phi}^{(n)} + \vec{\Psi}^{(n+1)} \\ \vec{\Phi}^{(n+1)} - \vec{\Phi}^{(n)} &= \mathbb{P}(\mathbb{L}\vec{F} - \mathbb{H}\vec{\Phi}^{(n)}) \end{aligned} \tag{7}$$

where $\mathbb{P} = \mathbb{I} + \mathbb{D}^{-1}\mathbb{E}$.

Consequently, the association of this method with `GMRES` is possible and represents a preconditioned `GMRES` approach to solve the transport equation.

initialisation

choose initial guess $\vec{\Phi}^{(o)}$ and calculate the first vector of the othonormal basis of $K_m(r_{(o)}, \mathbb{PH})$ $v_1 = \dfrac{r_{(o)}}{\left\|r_{(o)}\right\|}$

iterations: for $j = 1, \ldots, m$ while $(r_{(j)} \leq \varepsilon \left\|\vec{\Phi}^{(j)}\right\|)$ do:

Calculation of $\mathbb{PH}v_j$ (i.e. a transport calculation with the method of characteristics)
Arnoldi process to update the orthonormal basis

$$\begin{aligned} h_{ij} &= \langle \mathbb{PH}v_j, v_i \rangle \text{ for } i \in [1, j] \text{ (scalar product)} \\ \hat{v}_{j+1} &= \mathbb{PH}v_j - \sum_{i=1}^{j} h_{ij} v_i \\ h_{j+1\,i} &= \|\hat{v}_{j+1}\| \\ v_{j+1} &= \frac{\hat{v}_{j+1}}{h_{j+1\,i}} \end{aligned}$$

Updating the QR decomposition of the upper Hessenberg matrix

$$\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1j} & \left\|r_{(o)}\right\| \\ h_{21} & h_{22} & \cdots & h_{2j} & 0 \\ & \ddots & \ddots & \vdots & \vdots \\ 0 & & h_{j\,j-1} & h_{j\,j} & \vdots \\ 0 & \cdots & \cdots & h_{j+1\,j} & 0 \end{bmatrix} = \mathbb{Q}_j \mathbb{R}_j$$

where $\mathbb{Q}_j$ is an orthonormal matrix and $\mathbb{R}_j$ is an upper triangular matrix of dimensions $((j+1) \times (j+1))$

Calculation of $r_{(j)}$ **and** $\vec{\Phi}^{(j)}$ based on the $\mathbb{R}_j$ calculation

convergence reached ?

$\dfrac{r_{(j)}}{\left\|\vec{\Phi}^{(j)}\right\|}$ less than convergence criterion ?

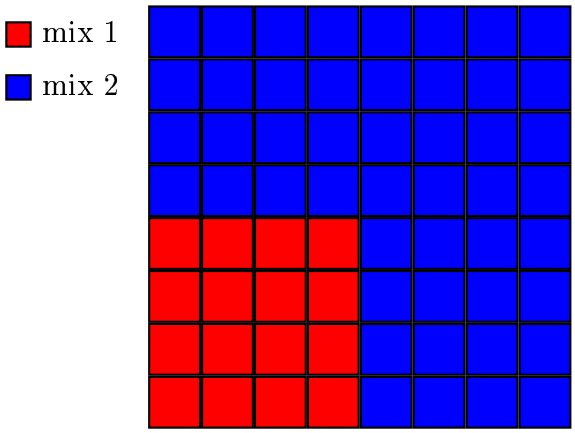
if it isn't reached, go back to "initialisation step" with $r_{(o)} \longleftarrow r_{(j)}$ to compute v_1

Table 1: the `GMRES` method

3. Convergence Behaviour

The implementation of these techniques has been made in a development version of the DRAGON lattice code.[8] The tracks are computed with the standard EXCELL module[9] and the fluxes are integrated using a modified implementation of MCCG. First, we have looked at the convergence behaviour of our code with respect to the tracking refinement and have compared it to the behaviour of the normalized collision probabilities method of DRAGON in terms of the k_{eff}. We present it for a simple 2D Cartesian geometry with reflective boundary conditions in a first test and void boundary conditions in a second one. This geometry is presented in Figure 1.

On one hand, we have kept the track density constant equal to 20 cm^{-1} and have made the number of tracking angles vary from 4 to 40 and on the other hand, we have kept the number of tracking angles constant equal to 20 and have made the track density vary from 10 cm^{-1} to 50 cm^{-1}. The results of these simulations are presented in Table 2. One can see that the expected convergence is reached and moreover, the standard deviation of these calculations is less for the method of characteristics than for the collision probabilities method which is encouraging.



	mix 1	mix 2
Σ_t (cm^{-1})	0.75	0.75
Σ_s (cm^{-1})	0.5	0.5
$\nu\Sigma_f$ (cm^{-1})	1.0	0.0

Figure 1: Cross sections and geometry of the the simple 2D assembly

		reflective boundary conditions		void boundary conditions	
		P_{ij}[‡]	MOC	P_{ij}	MOC
20 tracks/cm	4 angles	1.705191	1.695116	0.690604	0.673160
	8 angles	1.692570	1.695428	0.673710	0.676904
	12 angles	1.694056	1.693313	0.680735	0.677918
	16 angles	1.691667	1.690712	0.683299	0.678508
	20 angles	1.686074	1.687489	0.679424	0.677984
	24 angles	1.685090	1.688032	0.674056	0.678276
	28 angles	1.686792	1.687350	0.678723	0.678561
	32 angles	1.687022	1.688383	0.679727	0.679114
	36 angles	1.691646	1.691634	0.680721	0.679057
	40 angles	1.686726	1.689284	0.677024	0.678884
20 angles	10 tracks/cm	1.696328	1.694205	0.685364	0.680670
	15 tracks/cm	1.691408	1.694158	0.672897	0.678527
	20 tracks/cm	1.686074	1.687489	0.679424	0.677984
	25 tracks/cm	1.684106	1.685853	0.677120	0.678392
	30 tracks/cm	1.689995	1.690512	0.678447	0.677992
	35 tracks/cm	1.687363	1.688290	0.678278	0.678068
	40 tracks/cm	1.686387	1.687996	0.677405	0.678071
	45 tracks/cm	1.685779	1.686615	0.678526	0.677895
	50 tracks/cm	1.687346	1.687868	0.679013	0.677946
average value		**1.689559**	**1.689986**	**0.679184**	**0.678101**
standard deviation ($\times 10^3$)		**5.1**	**4.1**	**4.1**	**1.4**

Table 2: convergence behaviour with respect to tracking refinement

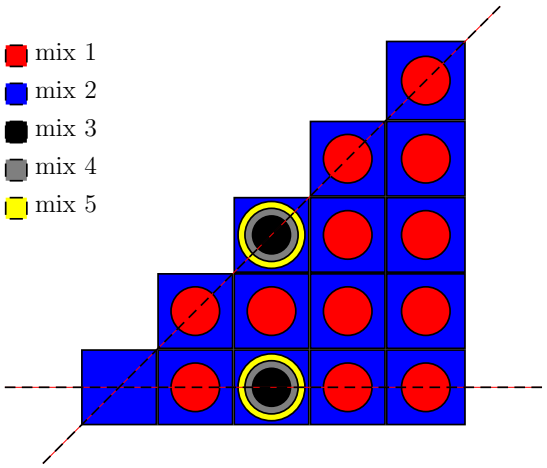
4. Acceleration of the Convergence

To evaluate the performance of these techniques, numerical tests based on 9×9 assemblies in 2D with three types of cells, using mono-energetic cross sections and isotropic sources were performed. Huge discontinuities between mixes and scattering ratio ($c = \Sigma_s/\Sigma_t$) close to 1 have been chosen to reproduce the difficulties highlighted in previous works with diffusion synthetic accelerations.[10,11] Figure 2 details these configurations. We have performed fixed source calculations with isotropic reflection at the boundaries. The following stopping criterion is used

$$\frac{\left\| \vec{\Phi}^{(n+1)} - \vec{\Phi}^{(n)} \right\|_2}{\left\| \vec{\Phi}^{(n)} \right\|_2} \leq \epsilon$$

where ϵ is set to 10^{-5}.

[‡] P_{ij} stands for the collision probabilities method and MOC stands for the method of characteristics.



	case 1 ($c = 0.999$)	case 2 ($c = 0.999$)	case 3 ($c = 0.9999$)
Σ_{t1} (cm^{-1})	1000.0	1.0	1.0
Σ_{t2} (cm^{-1})	0.1	0.01	0.01
Σ_{t3} (cm^{-1})	1000.0	1000.0	1000.0
Σ_{t4} (cm^{-1})	0.1	1000.0	1000.0
Σ_{t5} (cm^{-1})	1000.0	1000.0	1000.0

Figure 2: Cross sections and geometry of the 9×9 heterogeneous assemblies

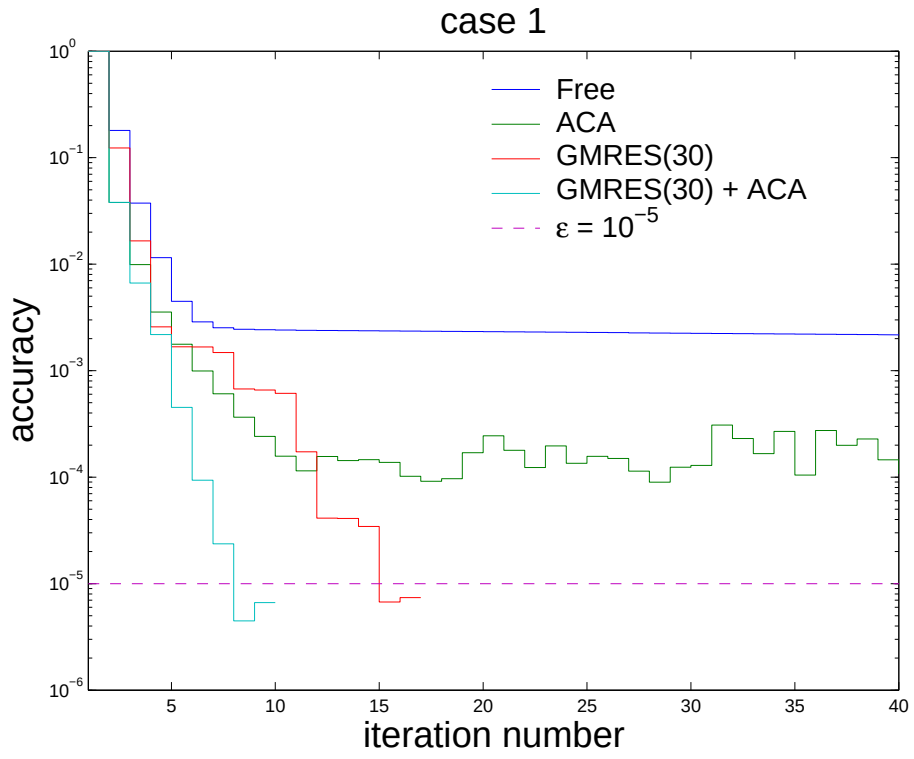


Figure 3: Convergence histogram for case 1

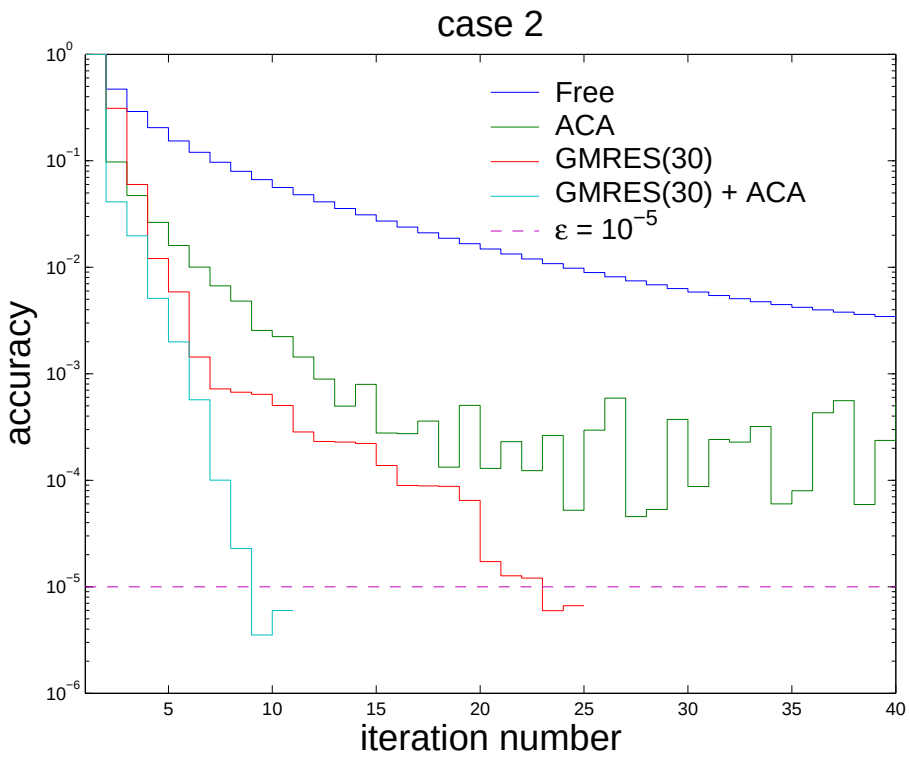


Figure 4: Convergence histogram for case 2

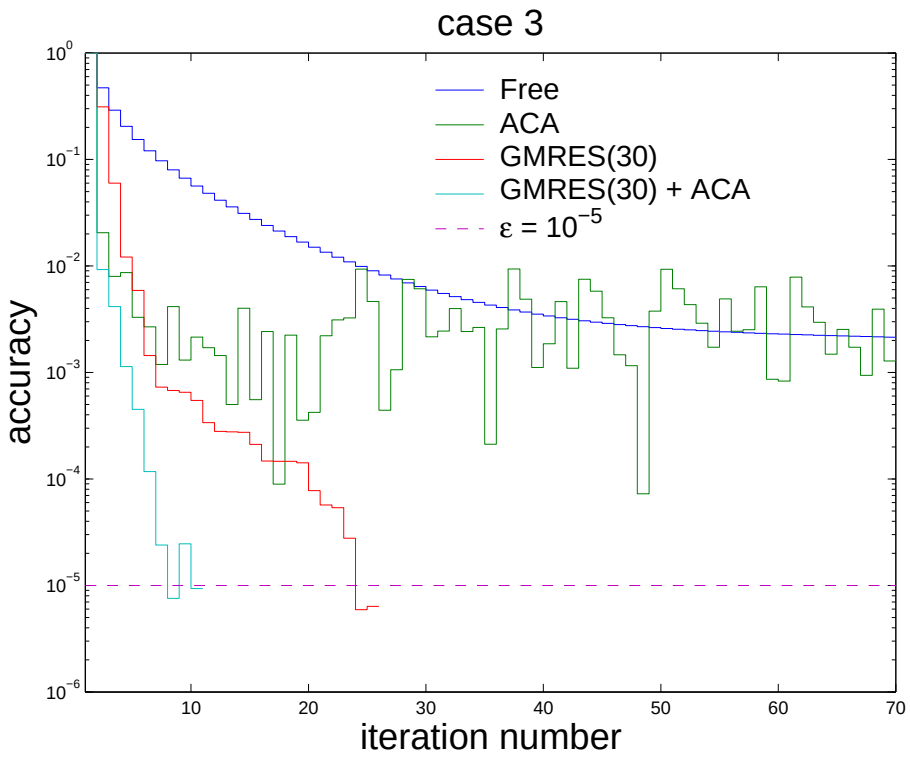


Figure 5: Convergence histogram for case 3

Figures 3, 4, 5 show the convergence speed of the different methods in these three cases. When GMRES is used, the calculation stops when the accuracy predicted by GMRES is less than ϵ but because of numerical round-offs, this value may differ from the real accuracy so, to insure the convergence, when GMRES stops, a calculation of the real error is performed and is included in figures. In the two first examples, this difference is about 2×10^{-6} and don't compromise the convergence but in the third case, the real accuracy is more than ϵ and an additional free iteration is recquired to reach the convergence. This phenomenon explains the last three values of the accuracy in Figure 5.

The degraded effectiveness of the ACA technique is well shown in these examples: oscillations appear which generally don't enable accuracy to reach the target value.

Although the ACA technique present some problems of numerical stability, it remains a good preconditioner: expressing explicitly the matrices of these three configurations enables us to calculate the 2-norm condition numbers of these systems

	case 1	case 2	case 3
ACA not used	2249.5	3683.2	35094
ACA used	3.96	9.59	9.83

and shows that ACA performs well in reducing the condition numbers of hugely ill-preconditioned problems.

Concerning GMRES the results are convincing: this technique significantly accelerates the convergence and overcomes the difficulties that ACA encounters. While a hundred free iterations only reach an accuracy of 1.9×10^{-3} in the third case, GMRES formalism ensures convergence in 25 iterations.

Moreover, preconditioning GMRES with ACA succeeds in improving the convergence rate: the number of iterations to reach the target accuracy is divided by more than 2 in the third test compared to GMRES alone although an additional free iteration is recquired. The ACA preconditioned GMRES approach avoids oscillations that encounters ACA alone and effectively reduces the condition number.

5. Conclusions and Future Works

As the examples presented show, our first attempt at using the ACA preconditioned GMRES formalism with the method of characteristics is successful and promising. Problems encountered by diffusion synthetic accelerations aren't reproduced with GMRES approach and the combination of these techniques hugely accelerate the convergence.

Obviously, these results have to be confirmed with other configurations and multigroups calculations to evaluate concretely the improvement in terms of CPU time. Moreover, we want to investigate other preconditioning techniques such as the self-collision rebalancing technique developed by G. J. Wu and R. Roy[12] in order to evaluate and compare different types of algorithms.

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