



On the solution of systems of linear equations associated to the ADO method in particle transport problems

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Abstract

In this work, a study is carried out on the solution of large linear systems of algebraic equations relevant to establish a general solution, based on a spectral formulation, to the discrete ordinates approximation of the two-dimensional particle transport equation in Cartesian geometry. The number of discrete ordinates (discrete directions of the particles) is determined by the order of the quadrature scheme on the unity sphere used to approximate the integral term of the linear Boltzmann equation (also called the transport equation). A nodal technique is applied to the discrete ordinates approximation of this equation, yielding to a system of first order ordinary differential equations for average unknowns along the directions x and y . The developed formulation is explicit for the spatial variables. The order of the linear system is defined by the number of discrete directions as well as the number of the spatial nodes. High-quality solutions are expected as both, the number of discrete directions and the refinement of the spatial mesh, increase. Here, the performance of direct and iterative methods, for the solution of the linear systems, are discussed, along with domain decomposition techniques and parallel implementation. Alternative arrangements in the configuration of the equations allowed solutions to higher order systems. A dependence on the type of the quadrature scheme as well as the class of problems to be solved (neutron or radiation problems, for instance) directly affect the final choice of the numerical algorithm.

Keywords Boltzmann equation · Particle transport · Linear systems · Iterative methods · Domain decomposition

Mathematics Subject Classification 65F05 · 65F10 · 65M70 · 82D75 · 82A25

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1 Introduction

The Boltzmann equation (Cercignani 1988) is a fundamental mathematical model in the study and simulation of phenomena involving the transport of neutral particles, as is the case in optical tomography modeling, dose planning in radiotherapy, estimation of radiation sources, nuclear reactors shielding, and others. The complexity of its integrodifferential form reinforces the development of deterministic methods that can provide high-quality weak form solutions. In this context, the discretization of the spatial and angular variables of the equation is present in purely numerical or even analytical solution techniques.

The discrete ordinates method is well known and used in established codes (Lewis and Miller 1984) to treat angular variables. In the case of problems in two-dimensional Cartesian geometry, the object of this work, the discrete ordinates method reduces the integrodifferential equation to a system of first-order partial differential equations. The discrete directions are chosen according to a quadrature scheme that approximates the integral term of the equation. In the case of spatial variables, the so-called nodal methods (Badruzaman 1985) reduce the complexity of the model, following the idea of finite volume schemes, and are known to have better performance in coarser meshes. The connection between spatial and angular grids is usually made in the literature through sweep schemes (Lewis and Miller 1984) that demand high computational time.

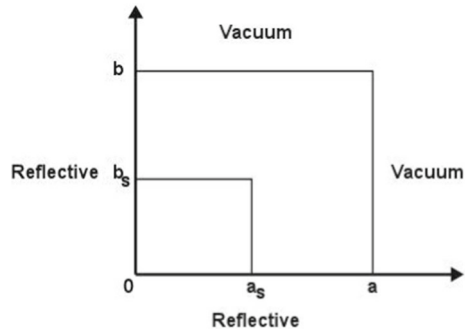
Recently, in this framework, the Analytical Discrete Ordinates-Nodal (ADO-Nodal) method was proposed for solving the discrete ordinates approximation of the two-dimensional linear Boltzmann (transport) equation (Barichello et al. 2011, 2017). The discrete ordinates equations are transversally integrated over a region (node) of the domain, yielding one-dimensional equations for average angular fluxes or intensities, in x and y -directions. The ADO method (Barichello and Siewert 1999) is then applied to the one-dimensional equations, with approximations for the unknowns (transverse leakage terms) on the contours of the regions, to derive explicit solutions for the spatial variables.

Due to the analytical characteristic of the ADO-Nodal method, as first proposed (Barichello et al. 2011), the integration procedure to generate the nodal equations was defined for the whole interval of the x and y variables definition, respectively. No division of the domain into nodes was carried out. More recently, the idea of local solutions was considered for the treatment of heterogeneous media problems (Barichello et al. 2017) where the physical domain is constituted by different materials.

Among the good features of this methodology, which is a spectral technique, one may cite: the solution of the transverse integrated one-dimensional equations, either in x and y -directions are explicitly written in terms of the spatial variables along with the fact that the associated eigenvalue problem is of reduced order, to only half of the number of discrete directions. With these features, the methodology applied to a wide class of neutron and radiation transport problems has advantages in providing fast and accurate solutions. In these problems, enhanced performance has been noted in coarser meshes compared with analogous methodologies.

The scheme does not use sweeping. Linear systems have to be solved to fully establish the general solutions. Considering a significant number of discrete directions in the simulations is theoretically recognized as an error control requirement between the discrete ordinate solution and the exact solution (Madsen 1971). Furthermore, from a physical perspective, problems in highly anisotropic scattering media (Barichello et al. 2022), for example, also impose such condition which means a choice of high-order quadrature schemes to approximate the integral term of the equation. This is a main factor that directly impacts the linear systems order.

Fig. 1 Typical configuration of a rectangular domain D for the benchmark problem



In this work, we present and discuss different approaches to solving the linear system associated with the ADO-Nodal formulation. We analyze the performance of the schemes applied to problems in different areas of particle transport, such as neutrons and radiation, as well as the influence of using different schemes for representing discrete ordinates.

The paper is organized as follows. In Sect. 2, we describe an earlier study for a neutron transport problem on a single domain (without domain decomposition), where the linear system that arises from the ADO formulation was solved using iterative methods. Section 3 describes a more recent study where a radiative heat transfer problem with high anisotropy degree was solved using the ADO method with domain decomposition, and the difficulties that arose while solving the linear system. We conclude in Sect. 4 with some remarks on our experiences and how we intend to address the difficulties so far encountered.

2 First large systems of linear equations: iterative solution

In da Cunha et al. (2015), we presented how the system of linear equations that arise in the ADO-Nodal method could be solved efficiently using iterative methods. There, the ADO method was applied to the solution of the time-independent neutron transport equation (1), which considers the distribution of the particles in a non-multiplicative homogeneous media on a rectangular domain D , defined by $[0, a] \times [0, b]$, with one group of energy and isotropic scattering. A typical configuration studied is a fixed-source problem (see Fig. 1) used as a benchmark in nuclear reactors shielding, where the source Q is defined in a smaller rectangle, defined by $[0, a_s] \times [0, b_s]$, embedded in D .

Following (Lewis and Miller 1984), the angular flux of neutrons $\Psi(x, y, \Omega_m)$ satisfies:

$$\begin{aligned} &\mu_m \frac{\partial}{\partial x} \Psi(x, y, \Omega_m) + \eta_m \frac{\partial}{\partial y} \Psi(x, y, \Omega_m) + \sigma_t \Psi(x, y, \Omega_m) \\ &= Q(x, y) + \sigma_s \sum_{k=1}^M w_k \Psi(x, y, \Omega_k), \quad m = 1, \dots, M \end{aligned} \tag{1}$$

where w_m are the weights associated to the $\Omega_m = (\mu_m, \eta_m)$ directions of the particles, σ_t and σ_s are, respectively, the total and scattering macroscopic cross-sections (parameters that indicate probabilities of absorption and scattering in the particle collision events) and $Q(x, y)$ is the isotropic neutron source term. The number of discrete ordinates directions M depends on the choice of the quadrature scheme. In that work, we considered the product quadrature proposed by Longoni and Haghghat (see Longoni and Haghghat 2001), whose technique

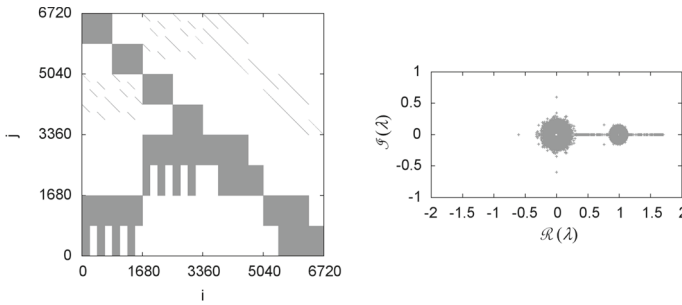


Fig. 2 Structure of a matrix of order $n = 6720$ and its eigenvalue distribution when solving the benchmark problem ($\sigma_t = 1, \sigma_s = 0.5$)

is developed using the same arrangement of directions as the classical Level symmetric quadrature (Lewis and Miller 1984) but allowing higher orders. This scheme is defined as the product of one-dimensional Legendre and Chebyshev quadratures with orders $N1$ and $N2$, respectively; here $M = N1(N2 + 2)/2$ with $N1 = N2$.

Following the transverse integrations in the x and y variables, we arrived at two systems of one-dimensional equations, depending on x and on y , respectively. The general (homogeneous plus particular) solution of the problem, is written in terms of eigenvalues and elementary solutions. To fully describe this solution, in da Cunha et al. (2015), a total of $8M$ coefficients have to be determined; these are obtained by solving a system of n linear equations $\mathbf{Ax} = \mathbf{b}$. These equations are written down according to the equations for the general solution, boundary conditions, interface conditions and unknown angular fluxes on the contours; these fluxes were approximated by constants. For details on the general derivation of the ADO formulation for two-dimensional neutron transport problems, see Barichello et al. (2017).

The largest system studied in da Cunha et al. (2015) has $n = 6720$ equations. It is sparse and nonsymmetric. Solving it by traditional, direct methods like a LU factorization, may become unfeasible depending on the available computation resources, due to the amount of memory required to hold the factors caused by excessive fill-in. The coefficient matrix of the system for $n = 6720$ and $\sigma_t = 1, \sigma_s = 0.5$ has the structure and eigenvalues λ as shown in Fig. 2 (other tests were made with $\sigma_t = 1$ and different values of σ_s and are reported in da Cunha et al. 2015). It is readily noticeable that the eigenvalues are distributed in the complex plane in two main clusters, with some outlying eigenvalues (both real and complex). Krylov subspace methods like GMRES and other iterative methods are known to diverge in this case (see (Saad 2003, p. 339)).

The approach we used to solve the system resorted to using the normal equations, $\mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b}$, and then computing a simple, fast Jacobi preconditioner \mathbf{J} ,

$$\mathbf{J} = \text{diag}(\mathbf{A}^T \mathbf{A})^{-1} \tag{2}$$

$$\mathbf{J}_{i,i} = ((\mathbf{A}_i)^T \mathbf{A}_i)^{-1}, \quad 1 \leq i \leq n, \tag{3}$$

where \mathbf{A}_i indicates the i th column of \mathbf{A} . Applying the preconditioner to the left of both sides of the normal equations, we write

$$\mathbf{JA}^T \mathbf{Ax} = \mathbf{JA}^T \mathbf{b} \tag{4}$$

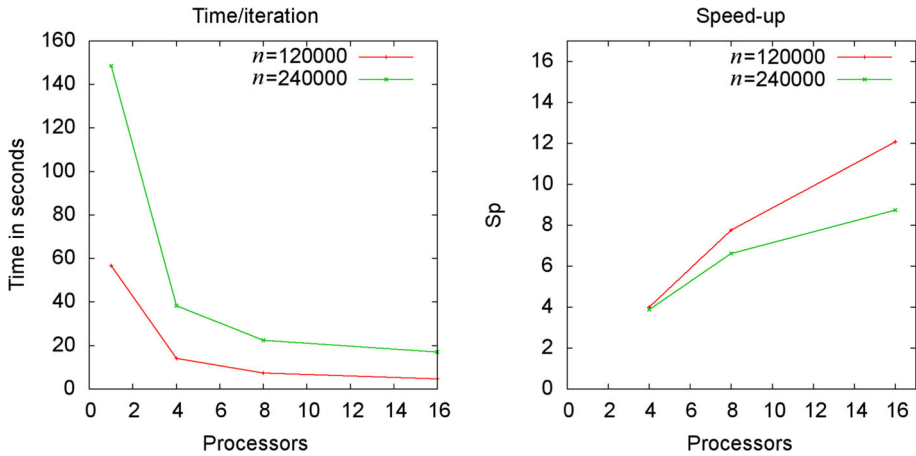


Fig. 3 Performance of the iterative solution of two systems of linear equations using the LGMRES method, one with $n = 120,000$ and the other with $n = 240,000$ equations

which can be recast as

$$(\mathbf{JA}^T) \mathbf{Ax} = (\mathbf{JA}^T) \mathbf{b} \tag{5}$$

where \mathbf{JA}^T is the preconditioner applied to $\mathbf{Ax} = \mathbf{b}$.

The system (5) was solved using the GMRES (Saad and Schultz 1986), LGMRES (Baker et al. 2003) and TFQMR (Freund and Szeto 1992) iterative methods implemented on NUMERICO (Cunha 2015). The package allows for the parallel solution of the system using MPI (MPI forum, 1993) seamlessly by the user, who does not have to write parallel-specific code; the user just specifies how the matrix is stored in memory and how it is to be partitioned across the processors.

The Eq. (1) was later applied to the solution of the same problem but using a nodal formulation, subdividing the domain into several regions, with the aim of improving the numerical quality of the solution using the ADO method (Barichello et al. 2017). Typical results are given in Fig. 3, where we show the execution times in seconds normalized per iteration, for systems of order $n = 120,000$ and $240,000$, and the speed-ups (S_p) achieved on an SGI Altix cluster at the National Supercomputing Centre/UFRGS, equipped with 64 blades each with two dodeca-core 2.3 GHz AMD Opteron processors and 64 GB RAM. The blades are interconnected by an InfiniBand 4 GB/s network. The program used double precision floating-point arithmetic and was compiled with optimization turned on using GNU Fortran v. 4.3.4 and linked with the SGI MPI v. 2.0 library. We used a maximum of 16 processors and achieved speed-ups of over 12 for LGMRES.

In a later, related work, Moura et al. (2018) investigated how the iterative solution of systems of linear equations derived from the same ADO-Nodal solution to a similar neutron transport problem was affected by using other quadrature schemes, namely the Quadrangular Legendre–Chebyshev (Longoni and Haghghat 2001) and the Quadruple Range (QR) quadrature schemes (Abu-Shumays 2001). The results given in Moura et al. (2018) show that the use of different quadrature schemes for the same problem does not affect adversely the iterative solution of the systems, though in some cases less iterations are required for convergence.

The ADO formulation applied in Barichello et al. (2017) uses domain subdivision, dividing the region in meshes. The order of the system of linear equations was much higher (the largest solved consisting of $n = 259,200$ equations for a 30×30 mesh) and therefore the structure and eigenvalues of the coefficient matrix changed considerably from that on da Cunha et al. (2015). However, the same normal equations-Jacobi preconditioner was used and the results in terms of the number of iterations required for convergence very much similar to those reported on da Cunha et al. (2015), with LGMRES(30,5) solving the largest system in just 19 iterations.

3 Systems derived from the application of the ADO method to a radiative transfer problem

In another application of the ADO method, which was extended to high degree of anisotropy scattering media, this time to solve a radiative heat transfer problem (see Barichello et al. 2022), the previous approach failed to provide an appropriate solution, and different approaches were taken to obtain the solution of the system of linear equations that arise in the method.

The radiation intensity $I(x, y, \Omega_i)$ is given by the discrete ordinates approximation to the two-dimensional radiative transfer equation in a rectangular domain $(x, y) \in [0, a] \times [0, b]$, for M discrete directions (Barichello et al. 2022):

$$\begin{aligned} \mu_i \frac{\partial}{\partial x} I(x, y, \Omega_i) + \eta_i \frac{\partial}{\partial y} I(x, y, \Omega_i) + \beta I(x, y, \Omega_i) &= \kappa I_b(x, y) \\ + \frac{\sigma_s}{4\pi} \sum_{l=0}^L \sum_{\substack{p=0 \\ (l+p \\ \text{even})}}^l (2 - \delta_{0,p}) C_l^p P_l^p(\xi_i) \sum_{k=1}^M w_k P_l^p(\xi_k) \cos[p(\varphi_k - \varphi_i)] &I(x, y, \Omega_k), \end{aligned} \quad (6)$$

where $1 \leq i \leq M$ and w_k are the weights (normalized to 4π) associated to the angular directions $\Omega_i = (\mu_i, \eta_i, \xi_i)$, defined in accordance with a numerical quadrature scheme. The coefficients κ and σ_s are the absorption and scattering coefficients of the medium and $\beta = \kappa + \sigma_s$ is the extinction coefficient; $I_b(x, y)$ is the intensity of radiation from a blackbody; $\delta_{0,p}$ is the Kronecker delta and the P_l^p 's are the associated Legendre polynomials of order l and $C_l^p = C_l(l-p)!/(l+p)!$.

The boundary conditions imposed are

$$I(x, y, \Omega_i) = \epsilon_w I_{bw}(x, y) + \frac{\rho}{\pi} \sum_{\mathbf{n} \cdot \Omega_j > 0} w_j I(x, y, \Omega_j) | \mathbf{n} \cdot \Omega_j |, \quad (7)$$

for (x, y) in the contour, where ϵ_w is the surface emissivity; ρ is the surface reflectivity; Ω_i (with $\mathbf{n} \cdot \Omega_i < 0$, \mathbf{n} being the unit outer normal vector at the boundary) denote the incoming flux directions and Ω_j are the outgoing flux directions ($\mathbf{n} \cdot \Omega_j > 0$).

The equations for the nodal scheme were written down according to a subdivision of the domain $(x, y) \in [0, a] \times [0, b]$ into a mesh of $H \times K$ rectangular regions (nodes) along the x and y axes, respectively, such that each region $r = 1, \dots, R$ is defined by $x \in [a_{h-1}^r, a_h^r]$ and $y \in [b_{k-1}^r, b_k^r]$ with $0 \leq a_{h-1}^r < a_h^r \leq a$ and $0 \leq b_{k-1}^r < b_k^r \leq b$, where $h = 1, \dots, H$ and $k = 1, \dots, K$ are the subdivisions in the x and y axes, respectively, as seen in Fig. 4. The domain regions are listed from left to right and from bottom to top.

Fig. 4 Domain subdivided into a mesh of $H \times K$ rectangular regions

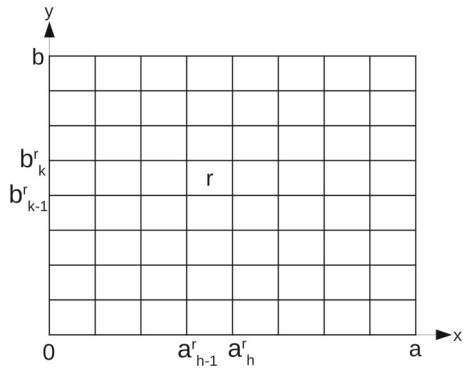
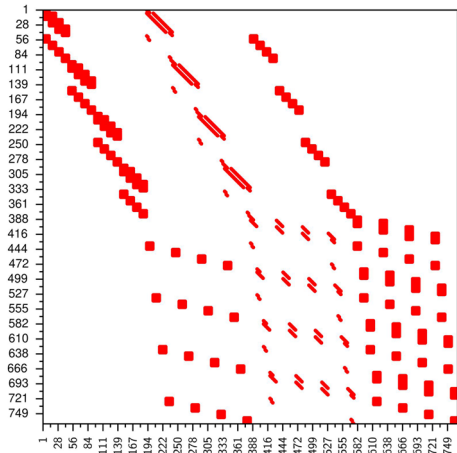


Fig. 5 Typical matrix structure of the system of linear equations, with the earlier ordering used

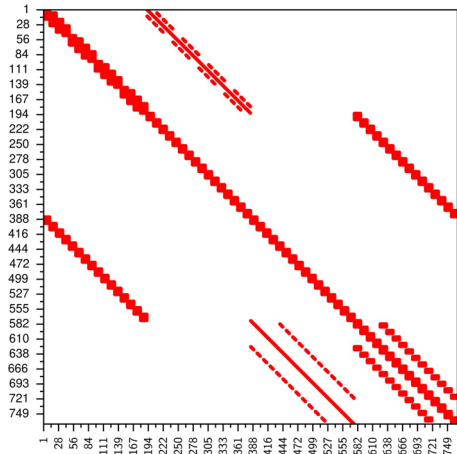


After writing the one-dimensional transverse-integrated equations in the x and y directions for each region r and using constant functions to properly express the radiation intensities in the contours of a node, we solve two eigenvalue problems to obtain separation constants to describe the homogeneous solutions and finally obtain the equations describing the general solutions for the average intensity along the x and y directions in each node. For details on this derivation, see Barichello et al. (2022).

To compute these average intensities, a system of linear equations needs to be solved to provide $4M$ arbitrary coefficients (half coming from the homogeneous solutions and half from the particular solutions) in each node and, therefore, a system of order $n = 4M(HK)$ needs to be solved. This system has its equations derived from auxiliary equations that approximate unknown intensities in the contours; equations for defining the particular solution (since the source is unknown as it depends on the intensities in the contours); the boundary conditions; and the continuity conditions at the interfaces of the regions.

However, there are different ways to write down the equations of the linear system, according to not only how each auxiliary and particular equations and boundary and continuity equations are considered in each region and along which direction. In previous work (Rui et al. (2020)), the ordering used led to a system of linear equations that had the structure as shown in Fig. 5. Being sparse, an iterative solution was attempted, as it had been proved very efficient. However, possibly due to the nature of the test problem where a pure scattering

Fig. 6 Typical matrix structure of the system of linear equations with the reordering of the equations



medium is assumed, the iterative methods used before failed to achieve convergence to the necessary tolerance (a residual less than 10^{-12}).

We, therefore, had to seek an alternative method to solve the system. At first, we used the DGESVX subroutine from LAPACK (Anderson et al. 1999), but the memory requirements to hold the factors from the LU factorization precluded us from using combinations of number of directions M and mesh sizes $H \times K$ that lead to systems of large order n . This was due to the structure exhibited by the coefficient matrix, which caused an excessive amount of fill-in on the LU factors.

It is known that matrices that exhibit a diagonal or banded structure (with a bandwidth that is less than n) will have less fill-in than an equivalent matrix with a different structure. There are some implementations of LU factorization tailored to diagonal or banded matrices, one such being the HSL_MA48 subroutine from the HSL Mathematical Software Library (HSL 2013).

To use this subroutine, we had to rearrange the equations and their coefficients (Rui et al. 2021). We swept the mesh along its lines and then its columns, writing the equations for the left and right contours of each region (boundary or continuity equations); the set of linear equations of the particular solution in the x direction; the set of linear equations of the particular solution in the y direction; and the equations for the bottom and top contours of each region (boundary or continuity equations). With this reordering, we obtained an equivalent system of linear equivalents that exhibited the structure shown in Fig. 6.

The structure and sparsity exhibited by the reordered coefficient matrix allowed us to solve problems on mesh sizes with $H = K = 60$ and $M = 128$ number of directions, which lead to a system of linear equations of order $n = 1,843,200$ on a computer with an Intel Core i7 processor at 2.8 GHz and with 16 GB of RAM. Typical CPU times to obtain the solution using $L = 8$ and the LQN quadrature, for $N = 8$ are as follows: 18.59 s for the 10×10 mesh, and 1943.74 s for the 40×40 mesh. Although we have experimented with solving the reordered system using ScaLAPACK (Blackford et al. 1997) on a distributed, shared-memory parallel computer, the results were not ideal, since there is not a specific routine in that package to deal with a coefficient matrix with the structure of the reordered system. Thus, we experienced similar limitations as when using LAPACK.

These difficulties motivated the use of non-overlapping domain decomposition using Schur’s complement formulation (Smith et al. 1996). In general, a system of linear equations

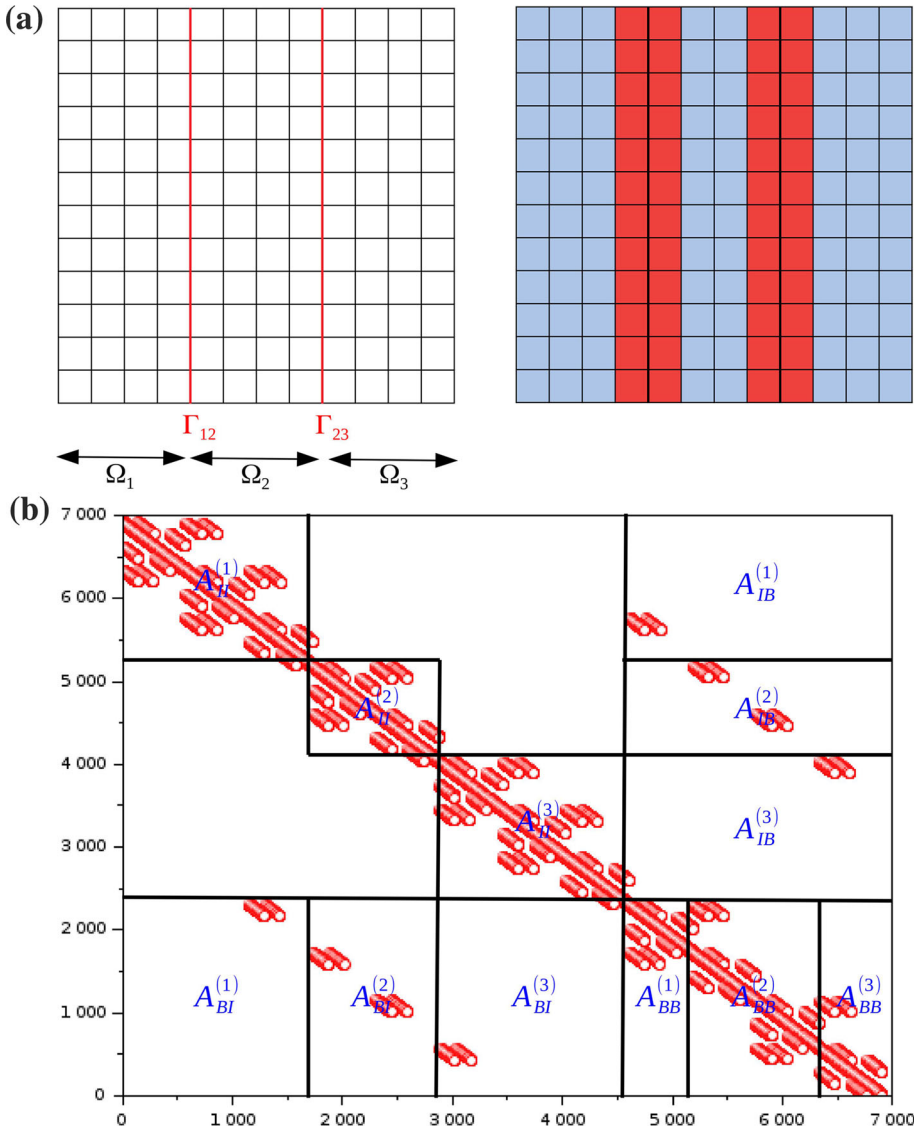


Fig. 7 **a** Non-overlapping domain decomposition of a 12×12 mesh with internal cells in gray and border cells in dark gray; **b** Corresponding block matrix Image presented in Rui (2021) (color figure online)

obtained following this decomposition and formulation may be expressed as

$$\begin{bmatrix} \mathbf{A}_{II} & \mathbf{A}_{IB} \\ \mathbf{A}_{BI} & \mathbf{A}_{BB} \end{bmatrix} \begin{bmatrix} \mathbf{x}_I \\ \mathbf{x}_B \end{bmatrix} = \begin{bmatrix} \mathbf{b}_I \\ \mathbf{b}_B \end{bmatrix} \tag{8}$$

where “I” and “B” indicate internal or border cells.

In Rui (2021), Rui divided the domain in vertical panels, as in Fig. 7a. Using the reordered equations and writing them down in terms of the cells belonging to each subdomain leads to a block matrix shown in Fig. 7b, where \mathbf{A}_{II}^i is a block matrix that refers to the internal

cells to subdomain i ; \mathbf{A}_{IB}^i and \mathbf{A}_{BI}^i are block matrices that refer to the interfaces between the internal and border cells of subdomain i ; and \mathbf{A}_{BB}^i is a block matrix that refers to the border cells of subdomain i .

The main reason for using this formulation is that it offers various sources of parallelization. Note that \mathbf{A}_{II} is a block diagonal matrix where each block is \mathbf{A}_{II}^i ; \mathbf{A}_{IB} and \mathbf{A}_{BI} are block column and block row matrices; and \mathbf{A}_{BB} is also a block row matrix, the blocks being related to each subdomain. To solve Eq. (8), one forms a system $\mathbf{S}\mathbf{x}_B = \mathbf{g}$ and solve for the variables on the border cells. The Schur complement matrix \mathbf{S} is obtained by computing expressions involving $(\mathbf{A}_{II}^i)^{-1}\mathbf{A}_{IB}^i$, solving i independent block systems. The system $\mathbf{S}\mathbf{x}_B = \mathbf{g}$ in itself is then solved for \mathbf{x}_B . Finally, with \mathbf{x}_B at hand, the variables \mathbf{x}_I^i are obtained by solving i independent block systems with \mathbf{A}_{II}^i as their coefficient matrices.

Note that there are two steps which require the solution of systems involving \mathbf{A}_{II}^i , one to form the Schur complement matrix \mathbf{S} and the other to solve for \mathbf{x}_I^i . Being not dependent on each other, these may be farmed out to individual processors, this being close to optimal parallelization. The solution of the system $\mathbf{S}\mathbf{x}_B = \mathbf{g}$ can be obtained either sequentially or in parallel, depending on how large is \mathbf{S} .

In her thesis, Rui provided results that show that by a suitable choice of the number of subdomains, the size of the largest system to be solved with this formulation— $\mathbf{S}\mathbf{x}_B = \mathbf{g}$ —is between 2.5 and 3 times smaller than the reordered system. This provides a gain by itself in that it will be solved faster (perhaps even more if using parallelism). However, we have yet to provide a parallel implementation to fully take advantage of this approach, and this is an ongoing work.

4 Concluding remarks

Solutions of large linear systems of algebraic equations were investigated via direct and iterative methods. The relevant systems arise when developing spectral solutions for two-dimensional particle transport problems in applications of neutron transport and radiation transfer problems. The order of the systems is related to the number of discrete ordinates associated to the angular discretization and the number of nodes in a domain subdivision.

Iterative methods such as GMRES, LOOSE GMRES and TFQMR were successful in neutron applications, for different choices of quadrature schemes. For the radiative transfer problem discussed here, those methods were unable to solve the linear system and the alternative was to try to obtain its solution via direct methods (LU factorization). Due to its high sparsity, which lead to unacceptable levels of fill-in the factorization, a reordering of the equations of the system was necessary to allow an application of a sparse block diagonal subroutine.

Ongoing research is focused on domain decomposition techniques to allow the solution of higher order systems due to the high execution times experienced using the latter approach. Such study seeks to enhance the chance of avoiding as much as possible the use of sweeping procedures to deal with angular and spatial discretization for these types of problems.

In grateful memory of Dr. Marco Antonio Raupp.

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Data availability No data to share at this time

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