A HIGHLY PARALLEL MULTILEVEL NEWTON-KRYLOV-SCHWARZ METHOD WITH SUBSPACE-BASED COARSENING AND PARTITION-BASED BALANCING FOR THE MULTIGROUP NEUTRON TRANSPORT EQUATIONS ON 3D UNSTRUCTURED MESHES

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Abstract. The multigroup neutron transport equations have been widely used to study the motion of neutrons and their interactions with the background materials. Numerical simulation of the multigroup neutron transport equations is computationally challenging because the equations is defined on a high dimensional phase space (1D in energy, 2D in angle, and 3D in spatial space), and furthermore, for realistic applications, the computational spatial domain is complex and the materials are heterogeneous. The multilevel domain decomposition methods is one of the most popular algorithms for solving the multigroup neutron transport equations, but the construction of coarse spaces is expensive and often not strongly scalable when the number of processor cores is large. A scalable algorithm has to be designed in such a way that the compute time is almost halved without any comprise on the solution accuracy when the number of processor cores is doubled. In this paper, we study a highly parallel multi-level Newton-Krylov-Schwarz method equipped with several novel components, such as subspace-based coarsening, partition-based balancing and hierarchical mesh partitioning, that enable the overall simulation strongly scalable in terms of the compute time. Compared with the traditional coarsening method, the subspace-based coarsening algorithm significantly reduces the cost of the preconditioner setup that is often unscalable. In addition, the partition-based balancing strategy enhances the parallel efficiency of the overall solver by assigning a nearly-equal amount of work to each processor core. The hierarchical mesh partitioning is able to generate a large number of subdomains and meanwhile minimizes the off-node communication. We numerically show that the proposed algorithm is scalable with more than 10,000 processor cores for a realistic application with a few billions unknowns on 3D unstructured meshes.

Key words. Neutron transport equations, Newton-Krylov-Schwarz, mesh partitioning, workload balancing, parallel computation, multilevel domain decomposition methods

AMS subject classifications. 65N55, 65Y05, 65N25, 65N30

1. Introduction. The multigroup neutron transport equations is employed to describe the motion of neutrons and their interactions with the background materials [21]. The fundamental quantity of interest is the statistically averaged neutron distribution, referred to as “flux”, in a high dimensional phase space (1D in energy, 2D in angle, 3D in space). We consider the time-independent version of the equations here so that the time dimension is not taken into account. The neutron flux is a scalar quantity physically representing the total length traveled by all free neutrons per unit time and volume. For solving the neutron transport equations, some fundamental nuclear data (referred to as “cross sections”) describing the likelihood per unit path length of neutrons interacting with the background materials is required. The cross sections depend on the energy and temperature of the background materials in a complicated manner [21]. The neutron transport equations can behavior as hyperbolic and elliptic forms under simple changes in cross sections (material properties) that may occur in realistic applications [10]. Because of the large dimensionality, the complicated solution behaviors, the complex computational domain and the heterogeneous materials, the neutron simulations are among the most memory and computation intensive in all of computational science. Therefore, a scalable parallel solution

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approach that takes advantages of modern supercomputers plays a critical role in the transport simulations. In this paper, we propose a scalable parallel nonoverlapping Newton-Krylov-Schwarz (NKS) method for the high-resolution simulation of the multigroup neutron transport equations. The performance of NKS is almost completely determined by the preconditioner. To achieve a high-performance neutron simulation, we develop a multilevel domain decomposition method with including a novel subspace-based coarsening scheme, a partition-based balancing strategy and a hierarchical mesh partitioning approach.

The development of efficient algorithms for the neutron simulations has been an active research topic for a couple of decades, and many solvers were studied. Multilevel domain decomposition and algebraic multigrid (AMG) methods are ones of the most popular algorithms for the numerical solution of the neutron transport equations. We briefly review the multilevel and AMG methods here, and for other popular methods such as the transport sweeps, interested readers are referred to [21, 35]. With the development of supercomputers, the domains decomposition methods become attractive because they are naturally suitable for parallel computations. In [31], the second-order even-parity form of the time-independent Boltzaman transport equations is solved with fGMRES preconditoned by an one-level overlapping domain decomposition method, where ILU together with CG is chosen as a local subdomain solver. The algorithm is numerically demonstrated to scale up to a few hundreds processor cores, but the scalability drops significantly when using 1,000 processor cores. In [8], a nonoverlapping domain decomposition with Robin interface conditions is studied for the simplified transport approximation, and the parallel efficiency is reported using up to 25 processors cores. In [10], the parallel computation is implemented using a space-angle-group decomposition method, where the “within-group” equation is solved using a Richardson iteration. A two-level overlapping Schwarz preconditioner is developed for the multigroup neutron diffusions equations in [19].

The algebraic multigrid (AMG) methods can be implemented in space, angle or energy. A spatial multigrid algorithm is presented for the isotropic neutron transport equations with a simple 2D geometry in [4], where the algorithm works well for homogeneous domains but the convergence need to be improved for heterogeneous domains. In [30], an angular multigrid method is used as a preconditioner for the GMRES method for the problems with highly forward-peaked scattering, and the method is numerically shown to be more efficient than an analogous DSA-preconditioned (diffusion synthetic acceleration [1]) Krylov subspace method. A multigrid-in-energy preconditioner (MGE) together with a Krylov subspace solver is proposed in [26]. The MGE preconditioner reduces the number of Krylov iterations in both the fixed source and eigenvalue problems.

The multilevel and AMG methods are used for a wide range of problems in the neutron transport, but the construction of coarse spaces is challenging and often unscalable when the number of processor cores becomes large. To have scalable simulations, we take an attempt to address these issues using the NKS method equipped with two important ingredients, subspace-based coarsening and partitioned-based balancing. In this paper, the multigroup transport equations is discretized in space using the first order continuous finite element method and in angle using the discrete ordinates approach. The resulting algebraic system of equations is solved with Jacobian-free Newton-Krylov (PJFNK) [11], where the preconditioning matrix is formed with the streaming and collision operator. During each Newton iteration, the Jacobian system is calculated by a Krylov subspace method such as GMRES precondi-
tioned by a multilevel nonoverlapping Schwarz. The coarse spaces can be constructed either geometrically or algebraically. In our previous works [13, 14, 15], some boundary preserving coarse spaces are constructed geometrically, and they are shown to work well for elasticity problems and fluid-structure interaction problems. Unfortunately, the geometric coarsening method is unavailable for the targeting application since the computational domain, shown in Fig. 1, used in this work includes many different regions that are meshed using different element types. Instead, an algebraic coarsening algorithm is employed to construct coarse spaces for the multilevel Schwarz method. However, if the traditional coarsening method is employed, the overall algorithm performance will be deteriorated and the strong scalability can not be maintained. To overcome the difficulty, we introduce a novel subspace-based coarsening algorithm that reduces the preconditioner setup time significantly compared with the traditional coarsening method, which makes the overall algorithm scalable with more than 10,000 processor cores. In addition, a partition-based balancing scheme is included to enhance the parallel efficiency, and a hierarchical mesh partitioning approach is studied to generate a large number of subdomains.

The rest of this paper is organized as follows. In Section 2, the multigroup neutron transport equations and its spatial and angular discretizations are described in detail. And a highly parallel Newton-Krylov-Schwarz framework is presented in Section 3. A novel subspace-based coarsening algorithm is introduced, in Section 4, to construct coarse spaces for building an efficient Schwarz preconditioner. In Section 5, some numerical tests are carefully studied to demonstrate the performance of the proposed algorithm. A few remarks and conclusions are drawn in Section 6.

2. Problem description. In this section, we first describe the multigroup neutron transport equations in detail, and then present the corresponding spatial and angular discretizations.

2.1. Multigroup neutron transport equations. The fundamental quantity of interest, neutron angular flux $\Psi_g [\text{cm}^{-2}\text{s}^{-1}\text{st}^{-1}]$, is governed by the multigroup neutron transport equations in $D \times S$ as follows:

$$
\vec{\Omega} \cdot \vec{\nabla} \Psi_g + \sum_{s' = 1}^{G} \sum_{g' = 1}^{G} \int_{S} \Sigma_{s' \rightarrow g} \phi_{g'} (\vec{\Omega}' \cdot \vec{\Omega}) \Psi_{g'} (\vec{x}, \vec{\Omega}') d\Omega',
$$

$$
+ \frac{1}{4\pi} \frac{\chi_g}{k} \sum_{s' = 1}^{G} v \Sigma_{s' \rightarrow g} \Phi_{g'}, \text{in } D \times S,
$$

(2.1a)

(2.1b) $\Psi_g = \alpha_s^g \Psi_g (\vec{\Omega}_r) + \alpha_s^d \int_{\{\vec{\Omega}' \cdot \vec{n}_b > 0\}} \left| \frac{\vec{\Omega}' \cdot \vec{n}_b}{\left| \vec{\Omega}' \cdot \vec{n}_b \right|} \right| \Psi_g d\Omega', \text{on } \partial D : \vec{\Omega} \cdot \vec{n}_b < 0,$

where $g = 1, \cdots, G$, and $G$ is the number of energy groups. $D$ is a 3D spatial domain (e.g. shown in Fig. 1) and $S$ is a 2D sphere. $\vec{x} \in D$ is the independent spatial variable [cm], $\vec{\Omega} \in S$ denotes the independent angular variable, $\vec{\Omega}_r = \vec{\Omega} - 2(\vec{\Omega} \cdot \vec{n}_b)\vec{n}_b$, $\partial D$ is the boundary of $D$, $\vec{n}_b$ is the outward unit normal vector on the boundary, $\Sigma_{s' \rightarrow g}$ is the macroscopic total cross section [cm$^{-1}$], $\Sigma_{s' \rightarrow g}^d$ is the macroscopic scattering cross section from group $g'$ to group $g$ [cm$^{-1}$], $\alpha_s^g$ is the specular reflectivity on $\partial D$, $\alpha_s^d$ is the diffusive reflectivity on $\partial D$, $k$ is the eigenvalue (sometimes referred to as...
a multiplication factor), \( \chi_g \) is the prompt fission spectrum, \( \Sigma_{f,g} \) is the macroscopic fission cross section \( [\text{cm}^{-1}] \), and \( \nu \) is the averaged neutron emitted per fission. \( \Phi_g \) is the scalar flux \( [\text{cm}^{-2}\text{s}^{-1}] \) defined as \( \Phi_g \equiv \int_g \Psi_g d\Omega \), and \( f_{g' \rightarrow g} \) is the scattering phase function. In (2.1a), the first term is the streaming term, and the second is the collision term. The first term of (2.1a) on the right hand side is the scattering term, which couples the angular fluxes of all directions and energy groups together. The second term of the right hand side of (2.1a) is the fission term, which also couples the angular fluxes of all directions and energy groups together. For a more detailed description on the neutron transport equations, please see [21, 33].

For convenience, let us define some operators:

\[
\begin{align*}
L \Psi &\equiv [L_1 \Psi_1, L_2 \Psi_2, \ldots, L_G \Psi_G]^T, \quad L_g \Psi_g &\equiv \hat{\nabla} \cdot \hat{\Omega} \Psi_g + \Sigma_{f,g} \Psi_g, \\
S \Psi &\equiv [S_1 \Psi_1, S_2 \Psi_2, \ldots, S_G \Psi_G]^T, \quad S_g \Psi_g &\equiv \sum_{g'}^G \Sigma_{g,g' \rightarrow g} f_{g' \rightarrow g} \Psi_{g'} d\Omega', \\
F \Psi &\equiv [F_1 \Psi_1, F_2 \Psi_2, \ldots, F_G \Psi_G]^T, \quad F_g \Psi_g &\equiv \frac{1}{4\pi} \chi_g \sum_{g'}^G \nu \Sigma_{f,g} \Phi_{g'}. 
\end{align*}
\]

Here \( L \) is the streaming-collision operator, \( S \) is the scattering operator and \( F \) is the fission operator. Similarly, the operator for the boundary condition mapping from \( \partial D \times S^+_{\hat{n}_b} \) to \( \partial D \times S^-_{\hat{n}_b} \) is defined as

\[
B \Psi \equiv [B_1 \Psi_1, B_2 \Psi_2, \ldots, B_G \Psi_G]^T, \quad B_g \Psi_g &\equiv \alpha_s^g \Psi_g(\hat{\Omega}) + \alpha_d^g \int_{\hat{\Omega} \cdot \hat{n}_b > 0} \left| \hat{\Omega}' \cdot \hat{n}_b \right| \Psi_g(\hat{\Omega}') d\Omega' + \int_{\hat{\Omega} \cdot \hat{n}_b < 0} \left| \hat{\Omega}' \cdot \hat{n}_b \right| \Psi_g(\hat{\Omega}') d\Omega'.
\]

where \( S^\pm_{\hat{n}_b} = \{ \hat{\Omega} \in S, \hat{\Omega} \cdot \hat{n}_b \geq 0 \} \) is a half angular space defined with respect to the unit vector \( \hat{n}_b \). Finally, (2.1a) is rewritten as

\[
(2.2) \quad L \Psi = S \Psi + \frac{1}{k} F \Psi,
\]

with the boundary condition \( \Psi = B \Psi \) corresponding to (2.1b).
2.2. Spatial and angular discretizations. Before the weak form of (2.2) is presented, some notations are introduced. An inner product is defined as
\[
\langle a, b \rangle_{D \times S} \equiv \sum_{g=1}^{G} \int d\Omega \int_{D} dx \, a_{g}(\vec{x}, \vec{\Omega}) b_{g}(\vec{x}, \vec{\Omega}),
\]
where \(a\) and \(b\) are generic multigroup functions defined in \(D \times S\). We drop the subscript \(D \times S\) for notation simplicity. We also have a similar definition for the boundary integral as:
\[
\langle a, b \rangle \equiv \langle a, b \rangle^{+} + \langle a, b \rangle^{-}, \quad \langle a, b \rangle^{\pm} \equiv \sum_{g=1}^{G} \int_{\partial D} dx \int_{S_{b}^{\pm}} d\Omega \left| \vec{\Omega} \cdot \vec{n}_{b} \right| a_{g}(\vec{x}, \vec{\Omega}) b_{g}(\vec{x}, \vec{\Omega}).
\]

Following a standard finite element technique, we multiply a test function \(\Psi^{*}\) with (2.2), and then integrate over the phase space, \(D \times S\),
\[
(\Psi^{*}, L \Psi) = (\Psi^{*}, S \Psi) + \frac{1}{k} (\Psi^{*}, F \Psi).
\]

After some manipulations, the weak form reads as
\[
(L^{*} \Psi^{*}, \Psi) + (\Psi^{*}, \Psi)^{+} - (\Psi^{*}, B \Psi)^{-} = (\Psi^{*}, S \Psi) + \frac{1}{k} (\Psi^{*}, F \Psi),
\]
where \(L^{*}\) is the adjoint operator of \(L\). The form (2.4) is usually unstable, and here a stabilizing technique, SAAF (self-adjoint angular flux), is included to remedy this issue. In the SAAF method, the streaming-collision operator \(L\) is split into two parts (the streaming operator \(L_{1}\) and the collision operator \(L_{2}\)),
\[
L \Psi \equiv L_{1} \Psi + L_{2} \Psi,
\]
where
\[
L_{1} \Psi \equiv \begin{bmatrix} \ll_{1,1} \Psi_{1}, \ll_{1,2} \Psi_{2}, \cdots, \ll_{1,G} \Psi_{G} \end{bmatrix}^{T}, \quad \ll_{1,g} \Psi_{g} \equiv \vec{\Omega} \cdot \vec{\nabla} \Psi_{g},
\]
\[
L_{2} \Psi \equiv \begin{bmatrix} \ll_{2,1} \Psi_{1}, \ll_{2,2} \Psi_{2}, \cdots, \ll_{2,G} \Psi_{G} \end{bmatrix}^{T}, \quad \ll_{2,g} \Psi_{g} \equiv \Sigma_{t,g} \Psi_{g}.
\]
The “inverse” of \(L_{2}\) is further defined as
\[
L_{2}^{-1} \Psi \equiv \begin{bmatrix} \ll_{2,1}^{-1} \Psi_{1}, \ll_{2,2}^{-1} \Psi_{2}, \cdots, \ll_{2,G}^{-1} \Psi_{G} \end{bmatrix}^{T}, \quad \ll_{2,g}^{-1} \Psi_{g} \equiv \Psi_{g} / \Sigma_{t,g}.
\]
It is easy to verify that \(L_{2}^{-1} L_{2} = I\), \(L_{2}^{-1} L_{2} = L_{2}\), \(L_{1}^{*} = -L_{1}\) and \(L_{1} L_{2} = L_{2} L_{1}\). With rearranging (2.2), we have
\[
\Psi = L_{2}^{-1} \left( \frac{1}{k} F \Psi + S \Psi - L_{1} \Psi \right),
\]
which is called the angular flux equation (AFE). We substitute (2.6) into the streaming kernel of (2.4),
\[
(L_{1}^{*} \Psi^{*}, \Psi) + (L_{2}^{*} \Psi^{*}, \Psi) + (\Psi^{*}, \Psi)^{+} - (\Psi^{*}, B \Psi)^{-} = (\Psi^{*}, S \Psi) + \frac{1}{k} (\Psi^{*}, F \Psi),
\]
and obtain the following form after a few manipulations
\[
\left( L_1 \Psi^*, L_2^{-1} L_1 \Psi \right) + \left( L_2 \Psi^*, \Psi \right) + \left( \Psi^*, \Psi^* \right) - \left( \Psi^*, B \Psi \right) = \left( L_2^{-1} L \Psi^*, S \Psi \right) + \frac{1}{k} \left( L_2^{-1} L \Psi^*, F \Psi \right).
\]

We noticed that the boxed kernels are symmetric positive definite (SPD), and the calculation of the SPD system is possible using the multilevel method equipped with algebraic coarse spaces. SAAF is equivalent to SUPG (Streamline upwind/Petrov-Galerkin) [3] with the inverse of group-wise total cross sections as the stabilization parameter. Finally, we denote the weak form obtained using the SAAF method as
\[
(2.7) \quad a(\Psi^*, \Psi) = \frac{1}{k} \mathbb{H}(\Psi^*, \Psi),
\]
with
\[
a(\Psi^*, \Psi) \equiv \left( L_1 \Psi^*, L_2^{-1} L_1 \Psi \right) + \left( L_2 \Psi^*, \Psi \right) + \left( \Psi^*, \Psi^* \right) - \left( \Psi^*, B \Psi \right),
\]
\[
\mathbb{H}(\Psi^*, \Psi) \equiv \left( L_2^{-1} L \Psi^*, F \Psi \right).
\]

The $S_N$ (discrete ordinates) method that can be thought of as a collocation method is considered for the angular discretization. Given an angular quadrature set \{\$d, w_d, d = 1, \cdots, N_d\} consisting of $N_d$ directions $d$ and weights $w_d$, the multigroup transport equations is solved along these directions and all angular integrations in the kernels are numerically evaluated with the angular quadrature. With the $S_N$ method, an integral of general functions over $S$ is represented as a weighted summation, that is,
\[
\int_S \Psi g d\Omega' = \sum_{d=1}^{N_d} w_d \Psi g d.
\]

It is straightforward to apply the technique to (2.7). Take the collision term as an example, we have
\[
(2.8) \quad (L_2 \Psi^*, \Psi) = \sum_{g=1}^{G} \int_{S} d\Omega' \left( \Sigma_{t,g} \Psi_{g}^*, \Psi_{g}^* \right)_{D} = \sum_{g=1}^{G} \sum_{d=1}^{N_d} w_d \left( \Sigma_{t,g} \Psi_{g,d}^*, \Psi_{g,d}^* \right)_{D},
\]
where $(\cdot, \cdot)_D$ denotes that the integral is taken over $D$ only. For the spatial discretization, the first-order Lagrange finite element is applied to $(\cdot, \cdot)_D$. For more details on the angular and spatial discretization of the neutron transport equations used in this work, please see [33]. After the angular and spatial discretization, a large eigenvalue system with the dense coupling block matrices in the energy and angle is produced. The potential dense matrix in energy is generated because a high energy neutron can be scattered down to a low energy group (down-scattering) and a low energy neutron can be also scattered up to a high energy group (up-scattering). The equation is fully coupled in the angle. We will introduce a scalable eigenvalue solver in next Section to handle the large system of eigenvalue equations.
3. Scalable parallel algorithm framework. In this Section, we describe the parallel algorithm framework consisting of the Newton method for calculating the non-linear system of equations, the Krylov subspace method for solving the Jacobian system and the Schwarz preconditioner for accelerating the linear solver.

The corresponding algebraic system of equations for (2.7) reads as

\[ A \Psi = \frac{1}{k} B \Psi, \]

where \( \Psi \) is also used to represent the solution vector that corresponds to the nodal values of the neutron flux at the mesh vertices, \( A \) is the corresponding matrix of \( a \), and \( B \) is the corresponding matrix of \( f \). Note that the matrices \( A \) and \( B \) are not necessary to be formed explicitly, and we will have a detailed discussion on this shortly.

The simplest algorithm for the eigenvalue calculation of (3.1) is the inverse power iteration, shown in Alg. 3.1, that works well only when the ratio of the minimum eigenvalue to the second smallest eigenvalue is sufficient small, but it converges slow or even fails to converge when the ratio is close to “1”. The difficulty is overcome by a Newton method that accelerates the convergence. To take the advantage of Newton, lines 5 and 6 of Alg. 3.1 are rewritten as follows:

\[ F(\Psi) = A \Psi - \frac{1}{\|B\Psi\|} B \Psi. \]

And then an inexact Newton is applied to (3.2). More precisely, for a given \( \Psi_n \), the new solution is updated as follows:

\[ \Psi_{n+1} = \Psi_n + \bar{\Psi}_n. \]

Here \( \bar{\Psi}_n \) is the Newton update direction obtained by solving the following Jacobian system of equations

\[ J(\Psi_n) \bar{\Psi}_n = -F(\Psi_n), \]
where $\mathcal{J}(\Psi_n)$ is the Jacobian matrix at $\Psi_n$, and $\mathcal{F}(\Psi_n)$ is the nonlinear function residual evaluated at $\Psi_n$. To save the memory, $\mathcal{J}(\Psi_n)$ is not explicitly formed, instead, it is carried out in a matrix-free manner. The corresponding Newton is referred to as “Jacobian-free Newton” method [11]. That is, a matrix-vector product, $\mathcal{J}(\Psi_n)\bar{\Psi}_n$, is approximated by

$$\mathcal{J}(\Psi_n)\bar{\Psi}_n = \frac{\mathcal{F}(\Psi_n + \delta\bar{\Psi}_n) - \mathcal{F}(\Psi_n)}{\delta},$$

where $\delta$ is a small permutation that is a square root of the machine epsilon in this paper. (3.4) is solved using an iterative method such as GMRES [24], and a preconditioner is required to construct a scalable and efficient parallel solver. Let us rewrite (3.4) as a preconditioned form

$$\mathcal{J}\mathcal{P}^{-1}\mathcal{P}\Psi = -\mathcal{F},$$

where $\mathcal{P}$ is the preconditioning matrix that is often an approximation to $\mathcal{J}$, and $\mathcal{P}^{-1}$ is a preconditioning process. The Jacobian $\mathcal{J}$ is carried out in a matrix-free manner since it has dense diagonal blocks since all groups and all directions are coupled through the fission term and the scattering term. The preconditioning matrix $\mathcal{P}$ is formed explicitly by only taking into consideration the first three terms of (2.7) since they form a SPD matrix that can be calculated using the multilevel method with algebraic coarse spaces. In fact, the angular fluxes in the energy and angle are independent in the first three terms of (2.7). If the variables were ordered group-by-group and direction-by-direction, $\mathcal{P}$ is written as

$$\mathcal{P} = \begin{bmatrix} \mathcal{P}_{0,0} & \mathcal{P}_{1,1} & \cdots & \mathcal{P}_{G,G} \\ \end{bmatrix},$$

where $\mathcal{P}_{g,g}$ is a block diagonal matrix for the $g$th energy group expressed as

$$\mathcal{P}_{g,g} = \begin{bmatrix} \mathcal{P}_{g,g}^{(0,0)} & \mathcal{P}_{g,g}^{(1,1)} & \cdots & \mathcal{P}_{g,g}^{(N_d,N_d)} \\ \end{bmatrix}.$$
Generally speaking, a preconditioning procedure is designed to find the solution of the following residual equations,

\[ P e = r, \]

where \( r \) is the residual vector from the outer solver (GMRES). To carry out the simulation in parallel, the mesh \( D_h \), corresponding to a triangulation of \( D \), is partitioned into \( np \) (\( np \) is the number of processor cores) submeshes \( D_{h,i}, i = 1, 2, \ldots, np \). This is accomplished by a hierarchical partitioning method since most existing partitioners such as ParMETIS [9] do not work well when the number of processor cores is close to or more than 10,000. The basic idea of the hierarchical partitioning is to apply an existing partitioner such as ParMETIS or PT-Scotch [5] twice. The computational mesh \( D_h \) is first partitioned into \( np_1 \) “big” submeshes (\( np_1 \) often is the number of compute nodes), and each “big” submesh is further divided into \( np_2 \) (\( np_2 \) is the number of processor cores per compute node) small submeshes. A 2D example with assuming that each compute node has 4 processor cores is shown in Fig. 2, where the mesh is partitioned into 2 “big” submeshes, and then each “big” submesh is further divided into 4 small submeshes, and finally we have 8 small submeshes in total.

Note that the hierarchical partitioning works for 3D meshes, and the 2D example is shown for the demonstration. Using the hierarchical partitioning method, we are able to not only produce a large number of submeshes, but also minimize the off-node communication since \( np_2 \) small submeshes on a compute node are physically connected and the communication between them is cheap. Interested readers are referred to our previous works [13, 18] for more details of the hierarchical partitioning.

Let us denote the submatrix and the subvectors associated with a submesh \( D_{h,i} \) as \( P_i, e_i \) and \( r_i \), respectively. We define a restriction operator, \( R_i \), that restricts a global vector \( r \) to a nonoverlapping submesh, that is, \( r_i = R_i r \). With those notations, the one-level nonoverlapping Schwarz preconditioner is expressed as

\[ P_{\text{one}}^{-1} = \sum_{i=1}^{np} R_i^T P_i^{-1} R_i, \quad P_i = R_i P R_i^T \]

where \( P_i^{-1} \) is a subdomain solver that is a successive over-relaxation (SOR) algorithm in this paper. The subdomain restriction \( R_i \) does not extract any overlapping
values. The overlapping version of (3.9) has been successfully employed in our previous works [13, 14, 16, 17] for elasticity equations, incompressible flows and fluid-structure interactions. Interested readers are referred to [27, 29] for more details on the Schwarz methods. After many experiments, we find that the nonoverlapping Schwarz preconditioner is able to maintain a strong scalability for the targeting applications when it is equipped with the subspace-based coarse spaces to be introduced shortly, and meanwhile the nonoverlapping Schwarz preconditioner uses less memory and communication compared with the overlapping version since no ghosting matrix entries need to be stored and exchanged. Coarse spaces need to be investigated for $P_{one}^{-1}$ to form its multilevel version when the number of processor cores is large, the materials are heterogeneous and the computational domain is complex. Let us denote $L$ spaces as $D^{(1)}_h, D^{(2)}_h, ..., D^{(L)}_h$, and the associated operators as $P^{(1)}, P^{(2)}, ..., P^{(L)}$. Here $D^{(1)}_h = D_h$ and $P^{(1)} = P$. The interpolation operator from $D^{(l+1)}_h$ to $D^{(l)}_h$ is denoted as $I^{l+1}_{l+1}$, and the corresponding restriction operator from $D^{(l)}_h$ to $D^{(l-1)}_h$ is $(I^{l}_{l+1})^T$. A multilevel additive Schwarz preconditioner (abbreviated as “MASM”) is summarized as Alg. 3.2. The fundamental motivation behind

| Algorithm 3.2 MASM($P^{(l)}$, $e^{(l)}$, $r^{(l)}$) |
|---|
| 1: if $l = L$ then |
| 2:  Solve $P^{(L)}e^{(L)} = r^{(L)}$ with a redundant direct solver on each compute node |
| 3: else |
| 4:  Pre-solve $P^{(l)}e^{(l)} = r^{(l)}$ using an iterative solver preconditioned by $(P^{(l)}_{one})^{-1}$ |
| 5:  Set $\bar{r}^{(l)} = r^{(l)} - P^{(l)}e^{(l)}$ |
| 6:  Apply the restriction: $\bar{r}^{(l+1)} = (I^{l+1}_{l+1})^T\bar{r}^{(l)}$ |
| 7:  $z^{(l+1)} = \text{MASM}(P^{(l+1)}e^{(l+1)}, z^{(l+1)}, r^{(l+1)})$ |
| 8:  Apply the interpolation: $z^{(l)} = I^{l}_{l+1}z^{(l+1)}$ |
| 9:  Correct the solution: $e^{(l)} = e^{(l)} + z^{(l)}$ |
| 10: Post-solve $P^{(l)}e^{(l)} = r^{(l)}$ using an iterative solver preconditioned by $(P^{(l)}_{one})^{-1}$ |
| 11: end if |
| 12: Return $e^{(l)}$ |

Alg. 3.2 is that the high frequency mode of the solution is efficiently resolved using an iterative method together with the preconditioner $P_{one}^{-1}$, and then the remaining low high frequencies will be handled in the coarse levels. The performance of Alg. 3.2 is largely affected by how to construct coarse spaces and their associated interpolations. Generally speaking, there are two ways to construct a set of coarse spaces. The first approach is to geometrically coarsen the fine mesh $D_h$ to generate coarse meshes, which has been shown to be powerful in our previous works [13] for elasticity problems and [12, 14, 15] for fluid-structure interactions. However, the geometry of the targeting application is complex so that it is nontrivial to setup a geometric mesh coarsening algorithm. The second one is to construct coarse spaces without querying any mesh information, instead, the coarse spaces and their interpolations are derived based on the matrix information only. The second approach has been successfully applied for different applications [7, 32, 34]. However, it is well known that the setup phase of the algebraic-version preconditioner is not strongly scalable in terms of the compute time since the matrix coarsening and the interpolation construction are expensive [34]. Fortunately, the overall algorithm can be still scalable if
the preconditioner setup phase accounts for a reasonably small portion of the total compute time. We will introduce such a new subspace-based coarsening algorithm that the preconditioner setup time is significantly reduced and the overall algorithm is able to maintain a good scalability with more than 10,000 processor cores. We will give a detailed description of the proposed coarsening algorithm in next Section.

4. Coarse spaces. In this section, we discuss a coarse space construction for Alg. 3.2. First, a matrix coarsening algorithm based on subspace is introduced, where the “grid” point selection is accomplished using a submatrix instead of the global matrix. A subinterpolation is constructed based on the splitting of the coarse points and the fine points, and the global interpolation is built from the subinterpolation.

4.1. Matrix coarsening based on subspace. According to (3.6) and (3.7), it is easily found that $P$ is a block diagonal matrix and each block corresponds to the spatial discretization of (2.2) for a given energy group and angular direction. Furthermore, there is no coupling between a block and the other blocks since we ignore the scattering and the fission terms in the preconditioning matrix. The individual matrix blocks are similar to each other in the sense that they correspond to the same continuous operators and share the same computational mesh $D_h$. The differences between them come from different materials (i.e. cross sections) being used by different energy groups. Our motivation here is to coarsen a block of $P$ instead of the entire matrix to generate subinterpolations, and then the subinterpolations are expanded to covered the entire space by defining an expanding operator. The benefit of this approach is potentially save a lot of the setup time and also the memory usage since the coarsening phase operates on a much smaller data set. Let us define a restriction $R_{s,i}$ that extracts the corresponding components from the entire vector $r$ for a given angular direction and energy group to form a subspace vector $r_{s,i}$, that is,

$$r_{s,i} = R_{s,i}r \equiv (\begin{bmatrix} I & 0 \end{bmatrix} \begin{bmatrix} r_{s,i} \\ r/r_{s,i} \end{bmatrix}),$$

where “/” denotes the components in $r$ but not in $r_{s,i}$. The choice of energy groups and angular directions is arbitrary in this paper, and we use the first energy group and angular direction, that is, $i = 1$. Without any confusion, we drop the second subscript of $r_{s,1}$ and $R_{s,1}$, and denote them as $r_s$ and $R_s$, respectively, for the simplicity of notations. With these notations, a subspace preconditioning matrix (for the first energy group and angular direction) is formed as

$$P_s = R_s P R_s^T.$$

Here $P_s$ can be coarsened using one of the existing matrix coarsening algorithms. We use a hybrid method of the Ruge-Stüben (RS) coarsening [28] and the Cleary-Luby-Jones-Plassman (CLJP) coarsening method [32]. For completeness, we briefly describe these methods here, and interested readers are referred to [22, 23, 34] for more details. Before starting a coarsening process, a “strength” matrix (graph), $G = (V, E)$, need to be constructed from $P_s$ since not all coefficients are equally important to determine the coarse spaces (grids) and we should consider the important coefficients only. Here $V$ is a set of all points in $P_s$, that is, $V = \{v_i\}$, and the size of $V$ is the number of rows of $P_s$. $E$ is a set of the corresponding edges, that is, $E = \{\tilde{e}_{ij}\}$. An edge $\tilde{e}_{ij}$ is formed when $v_i$ strongly depends on $v_j$ or $v_j$ strongly influences $v_i$ according to the following formula

$$-p_{ij} \geq \theta \max_{k \neq i}(-p_{ik}),$$
where \( p_{ij} \) is an entity of \( P_s \), and \( \theta \) is the strength threshold that sometimes has an important impact on the overall algorithm performance because it changes the matrix complexities, the stencil sizes, and the solver convergence rate. A coarsening algorithm tries to split \( V \) into either coarse points (C-point), denoted as \( C \), which will be taken into the next level, or fine points (F-points), denoted as \( F \), which will be interpolated by C-points.

The RS coarsening algorithm (also referred to as “classical” coarsening in some literatures) has two targets:

A1 For each point \( v_j \) that strongly influences an F-point \( v_i \), \( v_j \) is either a C-point or it shares a common C-point \( v_k \) with \( v_i \).

A2 C should be a maximal independent set

“A1” is designed to insure the quality of interpolation, while “A2” controls the size of the coarse space and the complexity of the operator. In practice, it is hardly to satisfy both conditions at the same time. The RS coarsening tries to meet A1 while uses A2 as a guideline and it is carried out in two passes. In the first pass, each point \( v_i \) is assigned by a measure \( m_i \) that equals the number of the points strongly influenced by \( v_i \), and the point with the maximum measure is selected as C-point, \( v_c \). All the points strongly influenced by \( v_c \) are chosen as new F-points, \( \{v_f\} \). For each unmarked point that strongly influences any point in \( \{v_f\} \), its measure is increased by the number of F-points it influences. This procedure is repeated until all points are chosen as either C-points or F-points. In the second pass, the algorithm checks every strong F-F connection if two F-points have a common C-point. If there is no a common C-point, and then one of the two F-points is chosen as a C-point. The approach is summarized in Alg. 4.1. It is easily seen that the RS algorithm is inherently sequential. A completely parallel coarsening approach is suggested in [6, 32]. It is based on a parallel maximal independent set (MIS) algorithm as described in [22], and is often denoted as “CLJP” (Cleary-Luby-Jones-Plassman) in other literatures. The CLJP coarsening algorithm starts with adding a measure \( m_i \) for each point \( v_i \in V \) just like the RS coarsening algorithm. Each \( m_i \) is added by a small random value between 0 and 1 so that the points are distinctive even if the original measures are the same. It is now possible to find a local maximum of all the point measures independently in parallel. A point \( v_i \) with the local maximal measure is selected as a C-point, and the measures of the neighboring points strongly influenced by \( v_i \) are decreased by 1. Furthermore, for all the points \( \{v_j\} \) that strongly depend on \( v_i \), remove their connections to \( v_i \). Examine all the points \( \{v_k\} \) that depend on \( v_j \in \{v_j\} \) whether or not they also depend on \( v_i \). If \( v_i \) is a common C-point of \( v_k \) and \( v_j \), remove the connection from \( v_k \) to \( v_j \) and decrease the measure of \( v_j \) by 1. If the measure of \( v_j \in \{v_j\} \) is smaller than 1, it is chosen as a F-point. This procedure is repeated until all points are selected as either C-points or F-points. The algorithm is summarized in Alg. 4.2.
Algorithm 4.1 Subspace based RS coarsening

1: Input: \( \mathcal{P} \)  \( \triangleright \) Submatrix extraction
2: Extract a submatrix: \( \mathcal{P}_s = R_s \mathcal{P} R_s^T \)
3: Construct a strength matrix of \( \mathcal{P}_s, \mathcal{G} = (V, E) \), according to (4.2)
4: Compute measures \( \{m_i\} \) for all points in \( V = \{v_i\} \)
5: Set \( C = \emptyset, F = \emptyset \)
6: while \( V \neq \emptyset \) do  \( \triangleright \) Pass 1
7: Find a point \( v \in V \) that has the maximum measure
8: \( C = C + v \)
9: Find the neighbors of \( v \) (denoted as \( V_n \subset V \)) that strongly depend on \( v \)
10: \( V = V - v \)
11: \( F = F + V_n \)
12: for \( v_n \in V_n \) do
13: Find the neighbors of \( v_n \) (denoted as \( V_{nn} \subset V \)) that strongly influence \( v_n \)
14: for \( v_{nn} \in V_{nn} \) do
15: \( m_{nn} = m_{nn} + 1 \)
16: end for
17: end for
18: \( V = V - V_n \)
19: end while
20: for \( v_i \in F \) do  \( \triangleright \) Pass 2
21: Find the neighbors of \( v_i \) (denoted as \( F_n \subset F \)) that strongly influence \( v_i \)
22: for \( v_n \in F_n \) do
23: \( v_n \) and \( v_i \) do not share a common C-point then
24: \( F = F - v_n \)
25: \( C = C + v_n \)
26: end if
27: end for
28: end for
29: Output: \( C, F \)

issues. The first one is to loose A1 as: A F-point should strongly depends on at least one C-point. This approach often decreases the complexity, but the complexity can be still high and require more memory than desired. This is further improved by an aggressive coarsening algorithm that is most efficiently implemented by applying the coarsening algorithms twice, The resulting aggressive coarsening algorithm is briefly described in Alg. 4.4.

4.2. Interpolation construction based on subspace. With a splitting \((C,F)\), we consider the construction of interpolation. For a given F-point \( v_i \), its interpolation takes the form as follows:

\[
e_i = \sum_{j \in C_i} w_{ji} e_j
\]

where \( C_i \) is the coarse interpolatory set of \( v_i \), and \( w_{ji} \) is an interpolation weight determining the contribution of \( e_j \) to \( e_i \). We assume that an algebraically smooth error corresponds to a small residual, that is, \( \mathcal{P}_s e \approx 0 \) when \( e \) is algebraically smooth. Let \( V_{n,i} \) be the neighboring points of \( v_i \), which strongly or weakly influence \( v_i \), and then
Algorithm 4.2 Subspace based CIJP coarsening

1: Input: $\mathcal{P}$  \hspace{1cm} \triangleright \text{Submatrix extraction}
2: Extract a submatrix: $\mathcal{P}_s = R_s \mathcal{P} R_s^T$
3: Construct a strength matrix of $\mathcal{P}_s$, $\mathcal{G} = (V, E)$, according to (4.2)
4: Compute measure $\{m_i\}$ for all point in $V = \{v_i\}$
5: Set $C = \emptyset$, and $F = \emptyset$
6: Add a random between 0 and 1 to each $m_i \in \{m_i\}$ \hspace{1cm} \triangleright \text{Pass 1}
7: while $V \neq \emptyset$ do
8: Find a point $\nu \in V$ that has the local maximum measure
9: $C = C + \nu$
10: Find the neighbors of $\nu$ (denoted as $V_n \subset V$) that strongly depend on $\nu$
11: for $v_n \in V_n$ do
12: $m_n = m_n - 1$
13: Find the neighbors of $v_n$ (denoted as $V_{nn} \subset V_n$) that strongly depends on $v_n$
14: for $v_{nn} \in V_{nn}$ do
15: if $v_{nn}$ also depends on $v_n$ then
16: $m_{nn} = m_{nn} - 1$
17: end if
18: end for
19: end for
20: if $m_n < 1$ then
21: $F = F + v_n$
22: $V = V - v_n$
23: end if
24: end for
25: $V = V - \nu$
26: end while
27: Output: $C$, $F$

Algorithm 4.3 Subspace based HCIJP coarsening

1: Input: $\mathcal{P}$  \hspace{1cm} \triangleright \text{Submatrix extraction}
2: Extract a submatrix: $\mathcal{P}_s = R_s \mathcal{P} R_s^T$
3: Construct a strength matrix of $\mathcal{P}_s$, $\mathcal{G} = (V, E)$, according to (4.2)
4: Compute measure $\{m_i\}$ for all point in $V = \{v_i\}$
5: Set $C = \emptyset$, and $F = \emptyset$
6: Apply the first pass of Alg. 4.1
7: Apply the first pass of Alg. 4.2
8: Output: $C$, $F$

the $i$th equation of $\mathcal{P}_s \epsilon \approx 0$ reads as

\begin{equation}
\sum_{j \in V_{n,j}} p_{ij} \epsilon_j + \sum_{j \in V_{n,j}} p_{ij} \epsilon_j \approx 0.
\end{equation}

Here $V_{n,j}$ comprises three sets: $C_i$ (coarse neighbors), $F_i^w$ (weakly influencing neighbors) and $F_i^s$ (strongly influencing neighbors). A “classical” interpolation, as de-
Algorithm 4.4 Subspace based aggressive HCJJP coarsening

1: Input: $\mathcal{P}$  \hspace{1cm} \triangleright \ Submatrix extraction  
2: Extract a submatrix: $\mathcal{P}_s = R_s \mathcal{P} R_s^T$  
3: Construct a strength matrix of $\mathcal{P}_s$, $\mathcal{G} = (V, E)$, according to (4.2)  
4: Compute measure $\{m_i\}$ for all point in $V = \{v_i\}$  
5: Set $C = \emptyset$, and $F = \emptyset$  
6: Apply the first pass of Alg. 4.3 to $\mathcal{G}$  
7: Apply the first pass of Alg. 4.3 to $C$  
8: Output: $C, F$

scribed in [23], is constructed as

$$(4.4) \quad w_{ij} = -\frac{1}{p_{ii} + \sum_{k \in F_i} p_{ik}} (p_{ij} + \sum_{k \in F_i} \frac{p_{ik} p_{kj}}{\sum_{m \in C_i} p_{km}}).$$

Eq. (4.4) is easy to implement in parallel since it only involves immediate neighbors and only requires one layer of the ghosting points. This method is invalid if A1 is not met. Another interpolation scheme, often referred as “direction interpolation”, which only needs immediate neighbors and can be used when A1 is violated, is expressed as

$$(4.5) \quad w_{ij} = -\frac{p_{ij}}{p_{ii}} (\sum_{k \in V, i} p_{ik} \sum_{l \in C_i} p_{il}).$$

If an aggressive coarsening scheme such as Alg. 4.4 is adopted, it is necessary to use a long range interpolation, such as a “multipass interpolation” as described in [28], in order to achieve a reasonable convergence. The “multipass” interpolation scheme starts with computing interpolating weights using (4.5) for the $F$-points immediately influenced by at least one $C$-point. In the second pass, for each $F$-point $v_i$ that have not been interpolated yet, find its neighboring interpolated $F$-points $v_j$ and then replace $e_j$ with $\sum_{k \in C_j} w_{jk} e_k$ in Eq. (4.3). A direct interpolation is then applied to the modified equation. We would like to refer interested readers to [7] for more details on different interpolation approaches. Let us denote the subinterpolation constructed using the submatrix $\mathcal{P}_s$ as $I_{1,2}^1$ from the second level to first level. And the full interpolation $I_{1/2}^2$ is expanded using the subinterpolation as follows

$$(4.6) \quad I_{1,2}^1 = \sum_{i=1}^{G \times N_1} (R_i^{(1)})^T I_{1,2}^1 R_i^{(2)}$$

where $R_i^{(l)}$ is the restriction operator defined on the $l$th level for the $i$th variable. The full coarse operator is computed using a Galerkin method

$$(4.7) \quad I_{1/2}^2 = (I_{1/2}^1)^T I_{1/2}^1.$$
5. Numerical results. In this section, we report the algorithm’s performance in terms of the compute time and the strong scalability for the eigenvalue calculation of the multigroup neutron transport equations for a realistic application, namely Advanced Test Reactor (ATR) that is located at the Reactor Technology Complex of the Idaho National Laboratory (INL) and is a 250-MW high flux test reactor. The ATR core, as shown in Fig 1, contains 40 fuel elements arranging in a serpentine annulus between and around nine flux traps. The algorithms are implemented based on PETSc [2] and hypre [20]. The numerical experiments are carried out on a supercomputer at INL, where each compute node has 36 processor cores (2.10 GHz per core) and the compute nodes are connected by a FDR InfiniBand Network of 56 Gbit/s. The problems are solved with an inexact Newton (3.3) together with GMRES preconditioned by Alg. 3.2, where 4 iterations of the inverse power, as shown in Alg. 3.1, is used to generate an initial guess for Newton. In the Newton eigenvalue solver, a relative tolerance of $10^{-6}$ is enforced for the nonlinear solver, and an inexact linear solver with a relative tolerance of 0.5 is adopted. In the inverse power, one iteration of Newton together with a linear solver with a relative tolerance of $10^{-2}$ is employed. The eigenvalue functions for 1st, 8th and 12th are shown in Fig 3. For convenience, let us define some notations that will be used in the rest of discussions. “np” represents the number of processor cores, “NI” is the total number of Newton iterations, “LI” denotes the total number of GMRES iterations, “Newton” is the total compute time spent on the nonlinear solvers and the inverse power iteration, “LSolver” is the compute time on the linear solver, “MF” is the compute time of the matrix-free operations, “PCSetup” is the compute time of the preconditioner setup, “PCApply” is the compute time of the preconditioner apply, “EFF” is the parallel efficiency, and “NR” is the ratio of the maximum number of mesh nodes to the minimum number of mesh nodes. “LSolver” is part of “Newton”, and it consists of “MF” and the preconditioner. The preconditioner time is split into “PCSetup” and “PCApply”.

5.1. Comparison with traditional MASM. We compare the proposed algorithm (denoted as “MASM_{sub}”) with the traditional MASM. We use a mesh with 4,207,728 elements and 4,352,085 nodes, where, at each node, there are 96 unknowns consisting of 12 energy groups and 8 angular directions. That is, the angle is discretized by Level-Symmetric 2 with 8 angular directions. The resulting system of nonlinear equations with 417,800,160 unknowns is solved using 1,152, 2,304, 4,608, and 8,208 processor cores, respectively. The performance comparison with the traditional MASM is summarized in Table 1 and Fig. 4. The nonlinear eigenvalue solver consists of Jacobian evaluation, function evaluation, matrix-vector multiplication, preconditioner setup and preconditioner apply, and where most components except the preconditioner setup are mathematically scalable. As we discussed earlier, the preconditioner setup including the matrix coarsening and the interpolation construction...
is challenging to parallel, and its compute time sometimes increases significantly when we increase the number of processor cores, which deteriorates the overall algorithm. From Fig. 4, we observed that the preconditioner setup for the traditional MASM is not scalable, and the ratio of the preconditioner setup time to the total compute time is increased significantly when we increase the number of processor cores. The ratio is only 6% when the number of processor cores is 1,152, but it jumps to 28% when we use 8,208 processor cores. For the preconditioner setup time, it is 161 s at 1,152 cores and increased to 261 s when 8,208 processor cores is used. In the traditional MASM, the preconditioner setup not only is unscalable, but also takes a big chunk of the total compute time so that the overall algorithm performance is deteriorated and the parallel efficiency is reduced to 30% at 8,208 processor cores. On the other hand, the preconditioner setup of MASM_{sub} performs better since it accounts for only 3% (26 s) of the total compute time at 1,152 cores and it slightly increases to 6% (22 s) when we use 8,208 processor cores. An interesting thing is that the preconditioner setup time of MASM_{sub} does not increase much and stays close to a constant. That makes the overall algorithm scale much better, and the parallel efficiency is about 64% even when the number of processor cores is large, i.e., 8,208.
The compute time comparison on different phases for the problem with 417,800,160 unknowns. Left: preconditioner setup time; middle: preconditioner apply time; right: total compute time.

The coarsening algorithm affects not only the preconditioner setup time but also the preconditioner apply time. In the traditional MASM, we observed that the preconditioner apply is not ideally scalable since while it accounts for 16% of the total compute time for 1,152 processor cores, the ratio is increased to 39% at 8,208 cores. The corresponding preconditioner apply time is 476 s for 1,152 processor cores, and it is decreased to 298 s by 37 s when we double the number of processor cores. Ideally, the preconditioner apply time should be reduced by 50% when the core count is doubled. The preconditioner apply of MASM\textsubscript{sub} is scalable in the sense that the compute time is decreased from 289 s to 154 s by 47% when we double the number of processor cores from 1,152 to 2,304, and it is further decreased to 89 s when we use 4,608 processor cores. The traditional MASM does not preserve this property, and its preconditioner apply time is actually increased to 327 s from 298 s when the core count is doubled from 2,304 to 4,608. The coarsening algorithm based on subspace make MASM\textsubscript{sub} scalable for the ATR simulation while the traditional MASM does not perform well. At 8,208 core, MASM\textsubscript{sub} is twice faster than MASM. These behaviors can be observed from Table 1 as well, where the number of Newton iterations is similar for both MASM and MASM\textsubscript{sub}, and the GMRES iteration of MASM\textsubscript{sub} is slightly more than that of MASM at 4,608 and 8,208 cores. The impact of the slight increase of GMRES iteration is negligible since the preconditioner apply per iteration is scalable for MASM\textsubscript{sub}. “LSolver” accounts for the most of the overall compute time, and the overall algorithm is scalable as long as the linear solver performs well. The performance of the linear solver is almost completely determined by the preconditioner since “MF” is well-known to be scalable mathematically. In summary, the eigenvalue solver together with MASM is not scalable, while the MASM\textsubscript{sub} equipped eigenvalue solver performs well since the setup phase of MASM\textsubscript{sub} is optimized and the apply phase of MASM\textsubscript{sub} scales well. The same performance comparison is observed in Fig. 5 as well, where the preconditioner setup of MASM\textsubscript{sub} is almost 10 times faster than MASM for all processor counts. The preconditioner apply for MASM\textsubscript{sub} is 2 or 3 times more efficient than MASM when the number of processor cores is small, and 5 times faster at 8,208 cores. Due to these behaviors, the overall algorithm based on MASM\textsubscript{sub} is much better than that with MASM. Note that the total compute time in Fig. 4 is slightly more than that in Table 1 since it is calculated by summing up all the individual components that have some overlap.

To further verify the effectiveness of the proposed algorithm, we add more angular directions for each mesh node, which leads to 288 variables (24 angular directions $\times$ 12 energy groups) one each mesh node. The same mesh as before is used, but the resulting system is much larger than the previous test, having 1,253,400,480 unknowns, since more angular directions are added for each mesh node. The numer-
Performance comparison with MASM for a problem with 1,253,400,480 unknowns. The resulting system of nonlinear equations with 1,253,400,480 unknowns is solved by an inexact Newton with MASM$_{\text{sub}}$ and MASM on 2,304, 4,608, 8,208, and 10,008 processor cores, respectively.

| $n_p$ | scheme | NI | LI | Newton | LSolver | MF | PCSetup | PCApply | EFF |
|-------|--------|----|----|--------|---------|----|---------|---------|-----|
| 2,304 | MASM$_{\text{sub}}$ | 13 | 191 | 2202 | 2027 | 1566 | 54 | 452 | 100% |
| 2,304 | MASM | 12 | 147 | 2466 | 2302 | 1176 | 535 | 635 | – |
| 4,608 | MASM$_{\text{sub}}$ | 13 | 183 | 1199 | 1096 | 860 | 41 | 232 | 92% |
| 4,608 | MASM | 12 | 139 | 1791 | 1694 | 641 | 496 | 589 | 61% |
| 8,208 | MASM$_{\text{sub}}$ | 13 | 183 | 828 | 763 | 552 | 68 | 176 | 75% |
| 8,208 | MASM | 12 | 135 | 1474 | 1412 | 391 | 489 | 554 | 42% |
| 10,008 | MASM$_{\text{sub}}$ | 14 | 184 | 672 | 617 | 447 | 65 | 127 | 76% |
| 10,008 | MASM | 12 | 134 | 1369 | 1317 | 322 | 480 | 531 | 37% |

![Graph showing performance comparison with MASM](image)

Fig. 6. Performance comparison with MASM for the problem with 1,253,400,480 unknowns. The figure shows the compute time spent on Jacobian evaluations (“JacEval”), function evaluations (“FuncEval”), matrix vector multiplications via matrix-free (“MatMultMF”), preconditioner setup (“PCSetUp”) and preconditioner apply (“PCApply”), respectively.

A list of the principal results is summarized in Table 2, Fig. 6 and 7. In Table 2, it is easily seen that the number of Newton iterations stays close to a constant as we increase the number of processor cores from 2,304 to 10,008, and the number of GMRES iterations also keeps as a constant for both MASM and MASM$_{\text{sub}}$. The number of GMRES iterations for MASM$_{\text{sub}}$ is more than that obtained via MASM, but the performance of MASM$_{\text{sub}}$ is not affected much and it is still much better than MASM. The overall algorithm based on MASM$_{\text{sub}}$ has the parallel efficiency of 76% at 10,008 cores while that for MASM is only 37%. Similarly, from Fig. 6 and 7, we observed that the compute time of the preconditioner for MASM$_{\text{sub}}$ is much smaller than that for MASM.

5.2. Node balance improvement. Typically, before a finite element simulation starts, a dual graph of mesh (where each graph vertex corresponds to a mesh element) is partitioned into $n_p$ submeshes that have nearly equal number of elements. While the number of elements assigned to each processor core is nearly equivalent, some processor cores may have more mesh nodes since the shared mesh nodes along the processor boundaries are simply assigned to the cores with lower MPI rank. A scalable calculation requires to balance both mesh elements and mesh nodes. We
The compute time comparison on different phases for the problem with 1,253,400,480 unknowns. Left: preconditioner setup time; middle: preconditioner apply time; right: total compute time.

TABLE 3
Mesh node assignment for the problems with 417,800,160 unknowns.

| np     | scheme       | NI | LI | Newton | LSolver | MF | PCSetup | PCApply | EFF  |
|--------|--------------|----|----|--------|---------|----|---------|---------|------|
| 1,152  | MASM_{sub}   | 13 | 191| 1855   | 1701    | 1418| 26      | 290     | –    |
| 1,152  | MASM_{sub}+NB| 13 | 199| 1821   | 1674    | 1407| 26      | 270     | 100% |
| 2,304  | MASM_{sub}   | 13 | 193| 989    | 908     | 749 | 21      | 154     | 92%  |
| 2,304  | MASM_{sub}+NB| 13 | 207| 1005   | 928     | 769 | 19      | 158     | 91%  |
| 4,608  | MASM_{sub}   | 13 | 202| 581    | 535     | 440 | 18      | 90      | 78%  |
| 4,608  | MASM_{sub}+NB| 13 | 216| 579    | 534     | 436 | 18      | 89      | 79%  |
| 8,208  | MASM_{sub}   | 14 | 216| 404    | 372     | 294 | 22      | 66      | 63%  |
| 8,208  | MASM_{sub}+NB| 14 | 217| 379    | 348     | 272 | 21      | 62      | 67%  |

use a partition-based node assignment, as discussed in our previous work [18], to balance the overall calculation. The basic idea of the partition-based node assignment is that the processor boundary mesh is partitioned into two parts, and each part is assigned to a processor core who shares the processor boundary mesh with the other processor core. Interested readers are referred to [18] for more details. The same configuration as before is used, and the numerical results are shown in Table 3 and 4, and Fig. 8. From Table 3, we observed that the compute time for different components is further improved using the node assignment strategy. The improvement becomes more obvious when the number of variables for each mesh node is increased. In Table 4, the preconditioner setup time is significantly reduced, for example, it is reduced to 37 s from 65 s at 10,008 processor cores, which leads to the parallel efficiency increased from 76% from 83%. The same observation is found in Fig. 8 as well.

5.3. Aggressive coarsening. The numerical results shown earlier are obtained using 10 levels of aggressive coarsening. The aggressive coarsening, Alg. 4.4, is used to reduce the complexities of the operators and the interpolations. More levels are applied by the aggressive coarsening, and the complexities of the operators and the interpolations become lower, but at the same time the convergence may be deteriorated. In this test, different numbers of levels of aggressive coarsening are applied in MASM_{sub}, and the results are summarized in Table 5, where “Agg” denotes the number of levels of aggressive coarsening, and “Agg=0” corresponds to no aggressive coarsening. From Table 5, we observed that both Newton iteration and GMRES iteration do not change much when we apply different numbers of levels of the aggressive coarsening in MASM_{sub}. The preconditioner time including the setup and apply is reduced significantly when the number of levels of aggressive coarsening is increased from 0 to 2, and then it slightly decreases when we increase “Agg”
5.4. Strong scalability. In this test, we study the strong scalability using a “fine” mesh with 25,856,505 nodes and 26,298,300 elements. The resulting eigenvalue system of equations with 2,482,224,480 unknowns is solved by an inexact Newton preconditioned by MASM sub. At the beginning of the strong scaling study, we also test the impact of the number of levels of aggressive coarsening on the overall algorithm for the “fine” mesh case. 4 and 10 levels of aggressive coarsening are tested, and the results are summarized in Table 6. The case with 10 levels of aggressive coarsening has slightly better results than that obtained with “Agg=4”. We therefore use 10 levels of aggressive coarsening in the following scaling study. The numerical results are shown in Table 7. The performance of the node balancing strategy is also reported, and the corresponding algorithm is denoted as “MASM sub+NB”. Again, for MASM sub, the numbers of Newton iterations and GMRES iterations stay as constants when we increase the number of processor cores, which indicates that the algorithm is mathematically scalable. The total compute time (“Newton”) is decreased proportionally when we increase the number of processor cores from 4,608 to 10,008. For instance, the total compute is reduced from 2808 s to 2084 s, when we increase the number of processor cores from 4,608 to 6,048, and it further is reduced to 1707 s and 1423 s when the number of processor cores is 8,208 and 10,008. The preconditioner setup is not scalable, but it does not affect the overall performance much since it ac-
counts for only a small portion of the total compute time. A good parallel efficiency of 77% is achieved at 10,008. While the performance of MASM\textsubscript{sub} is already good, it can be further enhanced by applying the node balancing strategy to make the overall distribution more balanced. In the odd rows of Table 7, the node balancing strategy is able to improve the overall algorithm performance, especially, the preconditioner setup time is significantly reduced. For example, at 8,208 cores, the compute time is reduced by 200 s when the node balancing strategy is used, most of the time reduction results from the improvement of the preconditioner setup. At 10,008 cores, the preconditioner setup time is reduced to 82 s from 138 s. The preconditioner apply also benefits from a more balanced workload, for example, the preconditioner apply time is reduced from 274 s to 208 s at 10,008 processor cores. We have almost-perfect parallel efficiencies when we use MASM\textsubscript{sub}+NB. The parallel efficiency is as high as 87%, even when the number of processor cores is more than 10,000. The Schwarz preconditioner together with both the subspace-based coarsening and the partition-based node balancing offers a highly scalable solver for the eigenvalue calculations for the targeting application. The corresponding parallel efficiency and speedup are plotted in Fig. 9.

6. Conclusions. A parallel Newton-Kyrlov-Schwarz method is studied for the numerical simulation of the multigroup neutron transport equations on 3D unstruc-
TABLE 7

| np   | Scheme       | NI | LI | Newton | LSolver | MF | PCSetup | PCApply | NR | EFF |
|------|--------------|----|----|--------|---------|----|---------|---------|----|-----|
| 4,608| MASM[sub]+NB | 12 | 160| 2398   | 2182    | 1743| 94      | 396     | 1.8| 100%|
|      | MASM[sub]    | 13 | 171| 2808   | 2567    | 2002| 131     | 511     | 2.2| –   |
| 6,048| MASM[sub]+NB | 13 | 176| 2035   | 1858    | 1470| 87      | 337     | 1.8| 90% |
|      | MASM[sub]    | 13 | 171| 2084   | 1898    | 1510| 84      | 352     | 2.7| 89% |
| 8,208| MASM[sub]+NB | 12 | 167| 1504   | 1373    | 1081| 76      | 244     | 2  | 90% |
|      | MASM[sub]    | 12 | 161| 1707   | 1570    | 1139| 142     | 364     | 2.8| 79% |
| 10,008| MASM[sub]+NB| 13 | 168| 1275   | 1160    | 896 | 82      | 208     | 2  | 87% |
|      | MASM[sub]    | 12 | 160| 1423   | 1307    | 951 | 138     | 274     | 2.9| 77% |

Fig. 9. Parallel efficiency and speedup for the problem with 2,482,224,480 unknowns. Left: speedup, right: parallel efficiency.

- A hierarchal partitioning is used to divide the computational domain into a large number of subdomains while the existing partitioners are from ideal. Two novel components including the subspace-based coarsening and the partition-based workload balancing are introduced and carefully studied. The total compute time using the subspace-based coarsening is halved compared with the traditional approach, and therefore the corresponding parallel efficiency is doubled to 76% when more than 10,000 processor cores are used. In addition, the partition-based workload balancing is able to assign a nearly equal amount of work to each processor core, and the parallel efficiency at 10,000 is further increased to 87%. The scalability of the overall algorithm is studied for a realistic application with 2,482,224,480 unknowns on a supercomputer with up to 10,008 processor cores.

While this paper focuses on the multilevel Schwarz preconditioner, other popular methods such as DSA [1] and NDA (nonlinear diffusion acceleration method) [25] will be explored in the future.

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