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The Davidson Method as an Alternative to Power Iterations for Criticality Calculations

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ABSTRACT

The Davidson method is implemented within the neutron transport core solver PARAFISH to solve k-eigenvalue criticality transport problems. The PARAFISH solver is based on domain-decomposition, uses spherical harmonics (P_N method) for angular discretization, and non-conforming finite elements for spatial discretization. The Davidson method is compared to the traditional power iteration method in that context. Encouraging numerical results are obtained with both sequential and parallel calculations.

Key Words: P_N transport, criticality eigenvalue calculations, Davidson method, power iteration, domain decomposition, parallel computing

1. INTRODUCTION

The power iteration method, sometimes accelerated with Chebyshev acceleration, has been up to now the method of choice for solving the k-eigenvalue criticality problem in reactor applications [11]. Several research works have been conducted in the past to find a better alternative to this rather basic method. In this view, several ways have been investigated: the Arnoldi method (IRAM) [1, 23, 24], the Jacobi-Davidson method [8, 22], and, more recently, the Jacobian-Free Newton-Krylov method [5, 6, 10]. These techniques have been up to now applied to the diffusion equation or to the discrete ordinate (S_N) transport approximation.

In this work, we investigate the Davidson method [2, 17], which is in fact an earlier development of the Jacobi-Davidson method [18]. We believe that such an investigation is valuable, since the Jacobi-Davidson is not proved to be better than Davidson in all cases [13].

Our investigation is done within the framework of the PARAFISH solver [21]. This parallel solver is based on a domain-decomposition technique. It uses the traditional multigroup approach for the energy discretization, non-conforming finite elements (FEs) for the spatial discretization, and spherical harmonics (P_N method) for the angular discretization. Moreover, PARAFISH is designed in such a way that each computer core of the parallel platform can handle more than one domain.

2. CRITICALITY CALCULATIONS

The k-eigenvalue criticality problem derived from the time-independent linear Boltzmann transport equation in the angular flux $\psi(\mathbf{r}, \mathbf{\Omega}, E)$, reads

$$\begin{aligned}\Big[\mathbf{\Omega}\cdot\nabla + \sigma(\mathbf{r},E)\Big]\psi(\mathbf{r},\mathbf{\Omega},E) = \\ \int_0^\infty\int_{4\pi}\sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\cdot\mathbf{\Omega})\,\psi(\mathbf{r},\mathbf{\Omega},E)\,d\mathbf{\Omega}'\,dE' \\ +\frac{\chi(E)}{k}\int_0^\infty\int_{4\pi}\nu(E')\,\sigma_f(\mathbf{r},E')\,\psi(\mathbf{r},\mathbf{\Omega},E)\,d\mathbf{\Omega}'\,dE'\end{aligned} \tag{1}$$

where $\sigma(\mathbf{r}, E)$ is the macroscopic total cross-section (assumed strictly positive) $\sigma_s(\mathbf{r}, E' \to E, \mathbf{\Omega}' \cdot \mathbf{\Omega})$ the scattering cross-section and $\sigma_f(\mathbf{r}, E')$ the fission cross-section. Moreover, $\chi(E)$ is the spectrum of emitted fission neutrons and $\nu(E')$ the number of neutrons emitted per fission. In PARAFISH, the linear Boltzmann transport equation is discretized starting from its second-order even-parity formulation [11]. This formulation is obtained using the even- and odd- (angular) parity decomposition reading

$$\psi^{\pm}(\mathbf{r},\mathbf{\Omega}) = \frac{1}{2}\left(\psi(\mathbf{r},\mathbf{\Omega}) \pm \psi(\mathbf{r},-\mathbf{\Omega})\right).$$

From there, some algebraic manipulations [4, 11, 20] enable to eliminate the odd-parity flux, and lead to a criticality problem of the form

$$\mathcal{T}\psi^+ = \mathcal{S}\psi^+ + \frac{1}{k}\mathcal{F}\psi^+ , \tag{2}$$

where the streaming operator $\mathcal{T}$, the scattering operator $\mathcal{S}$ and the fission operator $\mathcal{F}$ all apply to the even-parity flux $\psi^+(\mathbf{r}, \mathbf{\Omega})$. The streaming operator $\mathcal{T}$ can be shown to act as follows

$$\mathcal{T}\,\psi^+(\mathbf{r},\mathbf{\Omega}) = -\mathbf{\Omega}\cdot\nabla\frac{\mathbf{1}}{\sigma(\mathbf{r})}\,\mathbf{\Omega}\cdot\nabla\psi^+(\mathbf{r},\mathbf{\Omega}) + \sigma(\mathbf{r})\,\psi^+(\mathbf{r},\mathbf{\Omega}) ,$$

which legitimates the "second-order" denomination of the formulation. Moreover, this formulation can be shown to be self-adjoint. A detailed description of the weak form and its matrix formulation can be found elsewhere [4, 20].

Mathematically, the criticality problem (2) is a generalized eigenvalue problem seeking for the largest eigenvalue of

$$\mathcal{F}u = \lambda\mathcal{H}u,$$

where u is the even-parity flux ψ^+ and the streaming and scattering operators have been joined into $\mathcal{H}$.

Note finally that the odd-parity fluxes are not needed to compute reaction rates, which are the primary interest in many reactor applications. However, if needed as in the case neutron currents are required, the odd-parity fluxes can be retrieved from the even-parity ones [11].

Algorithm 1 Davidson method for computing the l largest eigenpairs of $Fu = \lambda Hu$.

1: **function** DAVIDSON(F, H, l, m)
2: Choose an initial orthonormal matrix $V_1 = [v_1, \ldots, v_l]$;
3: **for** $j = 1, 2, \ldots$ **do**
4: Compute matrix $F_j = V_j^{\mathrm{H}} F V_j$;
5: Compute matrix $H_j = V_j^{\mathrm{H}} H V_j$;
6: Compute the l largest eigenpairs $(\lambda_{j,i},\, y_{j,i})_{1 \le i \le l}$ of $F_j y_j = \lambda_j H_j y_j$;
7: Compute Ritz vectors $u_{j,i} = V_j\, y_{j,i}$ for $i = 1, \ldots, l$;
8: Compute residuals $r_{j,i} = F u_{j,i} - \lambda_{j,i} H u_{j,i}$ for $i = 1, \ldots, l$;
9: **if** convergence **then** exit;
10: Compute new directions $t_{j,i} = C_{j,i}\, r_{j,i}$ for $i = 1, \ldots, l$;
11: **if** $\dim(V_j) \le m - l$ **then**
12: $V_{j+1} = \mathrm{MGS}(V_j, t_{j,1}, \ldots, t_{j,l})$;
13: **else**
14: $V_{j+1} = \mathrm{MGS}(u_{j,1}, \ldots, u_{j,l}, t_{j,1}, \ldots, t_{j,l})$;
15: **end if**
16: **end for**
17: **end function**

3. THE DAVIDSON METHOD

The Davidson method is an iterative algorithm to compute few extreme eigenvalues and the corresponding eigenvectors of large sparse matrices. It was originally developed in 1975 by Davidson for real-symmetric matrices in the field of quantum chemistry [3]. Later, this method was also successfully applied to nonsymmetric problems [12, 17]. Its basic idea relies on a projection on a dedicated subspace, which is built iteratively.

The Davidson method for computing the l largest eigenpairs $(\lambda_i, u_i)_{1 \le i \le l}$ of the generalized eigenvalue problem $Fu = \lambda Hu$ is given in Algorithm 1. The integer m refers to restart parameter, i.e. the maximum size of the basis V_j from which the eigenvectors are built. At each iteration j, we compute the Rayleigh projections F_j and H_j of the matrices F and H. Then, in step 6, the projected eigenvalue problem is solved. This problem is of maximum size m and one can apply the QZ algorithm [7] to determine the l largest eigenvalues and the corresponding eigenvectors. In step 12 (and step 14 respectively), new directions $t_{j,i} = C_{j,i}\, r_{j,i}$ are incorporated in the basis V_j. We choose the preconditioning matrices $C_{j,i}$ to be of the form M^{-1} where M is an approximation to H. In our framework, the description of the preconditioner is given in Section 4. MGS stands for the modified Gram-Schmidt orthogonalization procedure.

Note that, besides some basic vector routines, only sparse matrix-vector multiplications Fv and Hv for a given vector v are needed. This can be implemented very efficiently. Since the preconditioning matrices $C_{j,i}$ may vary at each iteration j, these need not to be built actually. Instead, one can use iterative methods in order to determine $t_{j,i}$, i.e. one solves $Ht_{j,i} = r_{j,i}$ in step 10 iteratively. Furthermore, note that the Rayleigh matrices F_j and H_j can be computed only by updating the last l rows and columns.

Algorithm 1 is valid for both symmetric and unsymmetric eigenvalue problems. In the unsymmetric case, the only difference is that complex eigenvalues may occur. However, a complex

arithmetic is easily avoided, by splitting complex vectors in two real vectors: one holding the real part, the other the imaginary part. In order to add a complex vector to the basis V_j, we just append both real and imaginary part as two real vectors. This separation is no restriction. Actually it induces more flexibility, since with more vectors in V_j, there are more ways to combine them. In all our numerical results, the eigenvalues we obtained are real, which complies with the physical assumption.

4. THE PARAFISH CALCULATION SCHEME

The Davidson method appears to be a robust method to compute eigenvalues and the corresponding eigenvectors, since the residuals are computed accurately [9]. Moreover, the Davidson method builds a full basis of adequate vectors, whereas the power iteration method projects only onto the space spanned by the last built vector $(H^{-1}F)^j v$ at each iteration j. Hence the Davidson method keeps track of more information and needs less iterations than the power iteration method. Both methods require solving linear systems of the form $Hx = y$. The Davidson method is more robust in practice in the sense that the choice of preconditioner is less restrictive than in the power method. That means, solving the linear system $Ht_{j,i} = r_{j,i}$ in step 10 can be done very roughly, while the power iteration method needs a more precise solving in order to converge.

In PARAFISH, the order of discretization is as follows: first the energy, then the space, and finally the angle. At the energy level, we use a block version of the Gauss-Seidel method given the quasi-block triangular shape obtained with the multigroup discretization. If no upscattering is present, block triangularity is fully achieved, and only one Gauss-Seidel iteration is sufficient.

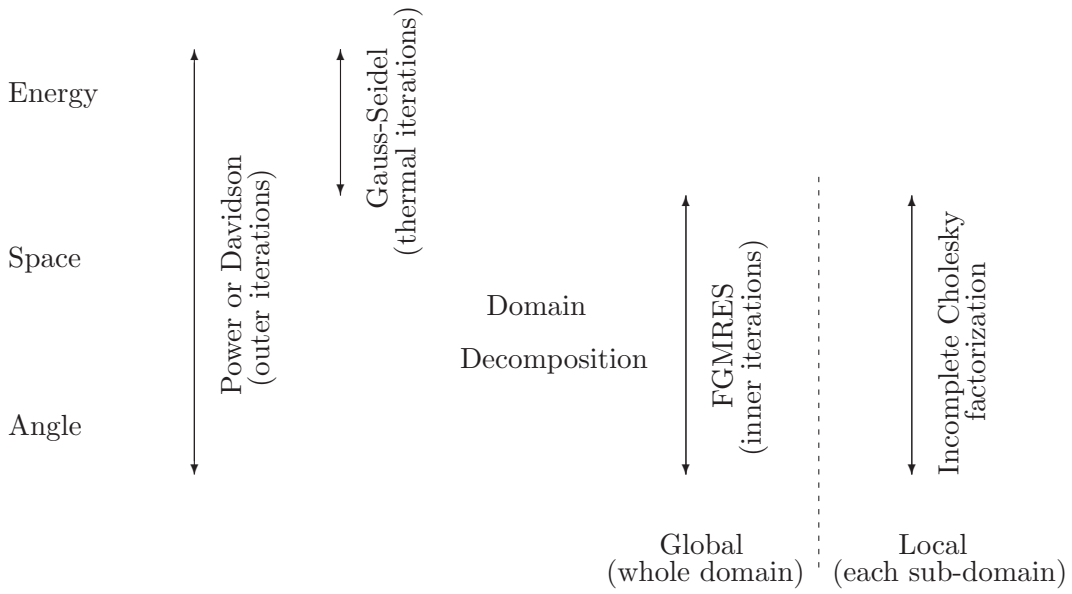

Figure 1: Parafish calculation scheme

Each diagonal block of the energy discretization corresponds to a spatio-angular problem (within a given energy group). At this spatio-angular level, domain-decomposition is applied [21], yielding an interior block shape such that each interior diagonal block is symmetric and corresponds to one domain in the domain decomposition. Therefore, these blocks can be treated in parallel on different cores. A block-diagonally preconditioned version of the GMRES method [16] is then applied: each interior diagonal block is factorized by the incomplete Cholesky method. The matrix-vector multiplications involving these factorized interior blocks are done locally on each core.

The different iteration loops are schematically displayed in Fig. 1.

5. NUMERICAL RESULTS

5.1 The Takeda 1 benchmark

The 3-D Takeda 1 benchmark consists of a small LWR quarter-core of cubic shape as depicted in Fig. 5.1. Three zones appear in the geometry: the core zone, the reflector zone and the guide tube zone. The 2-group cross-section values can be found in [19]. No upscattering is present. Here we consider the 'case 2' of the benchmark, i.e. the control rods are in the core.

For the angular discretization, we use the P_N method, with N ranging from 3 to 7 as indicated. For the spatial discretization, we use a $25 \times 25 \times 25$ mesh of the cubic NC_6 non-conforming FEs. The capacity of these FEs to accurately solve the Takeda 1 benchmark has been assessed previously [20]. The FE nodes are distributed among $5 \times 5 \times 5$ domains, with domain interfaces parallel to the cube faces.

Our computations were performed on the HP XC3000 at the Steinbuch Centre for Computing (SCC) in Karlsruhe, Germany. The CPUs (Quad-core Intel Xeon processors) run at a clock speed of 2.53 GHz.

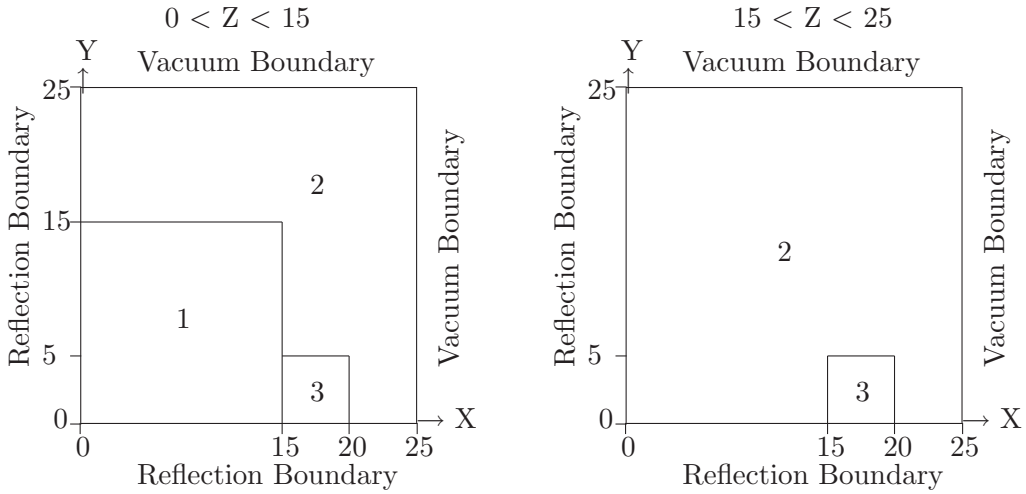

Figure 2: Geometry of the 3-D Takeda 1 benchmark. Zone 1 = core, zone 2 = reflector, zone 3 = guide-tube zone (low-density in case 1, control rod in case 2)

The run times and the speedups for the strong scalability with spherical harmonic approximations P_3, P_5 and P_7 are given in Tables I, II and III. Please note, that we listed only the times for solving the eigenvalue problem including the time for setting up the preconditioner. We excluded the time for building the matrices. For the case P_3 (P_5 and P_7) we obtained for critical eigenvalue $k_{eff} = 0.96122$ (0.96222 and 0.96241 respectively) which agrees decently with the reference values of [19] (0.96230 ± 48 pcm with the Monte-Carlo method).

The computation of the critical eigenvalue and the corresponding eigenfunction using Davidson method consumes roughly 50% of the time which is used by applying the power iteration method to gain comparable results. According to the number of iterations, we have similar results: for the case P_3 (P_5 and P_7) the Davidson method needs 6 (6 and 5 respectively) iterations to convergence, whereas the power iteration method requires 12 (13 and 14 respectively) iterations. For the speedup, we obtain similar results for both the Davidson and the power iteration method. This is due to the fact that the same basic linear algebra operations are used in both methods. The efficiency is computed as the ratio between the speedup and the number of cores.

Table I: Results with P_3 approximation (675,000 unknowns)

	Davidson method			power iteration method		
number cores	time (s)	speedup	efficiency	time (s)	speedup	efficiency
1	21.8	1.	1.	41.0	1.	1.
5	5.6	3.88	0.78	11.2	3.66	0.73
25	1.6	14.03	0.56	3.1	13.14	0.53
125	1.1	20.02	0.16	1.2	33.20	0.27

Table II: Results with P_5 approximation (1,687,500 unknowns)

	Davidson method			power iteration method		
number cores	time (s)	speedup	efficiency	time (s)	speedup	efficiency
1	98.5	1.	1.	182.8	1.	1.
5	24.1	4.08	0.82	46.67	3.92	0.78
25	6.9	14.23	0.57	12.1	15.10	0.60
125	2.4	41.25	0.33	4.0	45.53	0.36

5.2 The NEA "C5G7" benchmark

We now consider the 2-D MOX fuel assembly benchmark issued by the NEA [14]. This benchmark uses C5 MOX fuel and 7 energy groups, hence its "C5G7" nickname. As depicted in Fig. 3, its geometry is a quarter core containing 4 fuel assemblies and the surrounding moderator. Each fuel assembly is made out of a 17×17 lattice of square pin cells. Each of these pin cells contains a fuel-clad mix cylindrical section surrounded by moderator.

Table III: Results with P_7 approximation (3,150,000 unknowns)

	Davidson method			power iteration method		
number cores	time (s)	speedup	efficiency	time (s)	speedup	efficiency
1	239.8	1.	1.	479.7	1.	1.
5	69.8	3.43	0.69	141.0	3.40	0.68
25	19.2	12.46	0.50	35.1	13.68	0.55
125	5.0	47.57	0.38	9.5	50.67	0.41

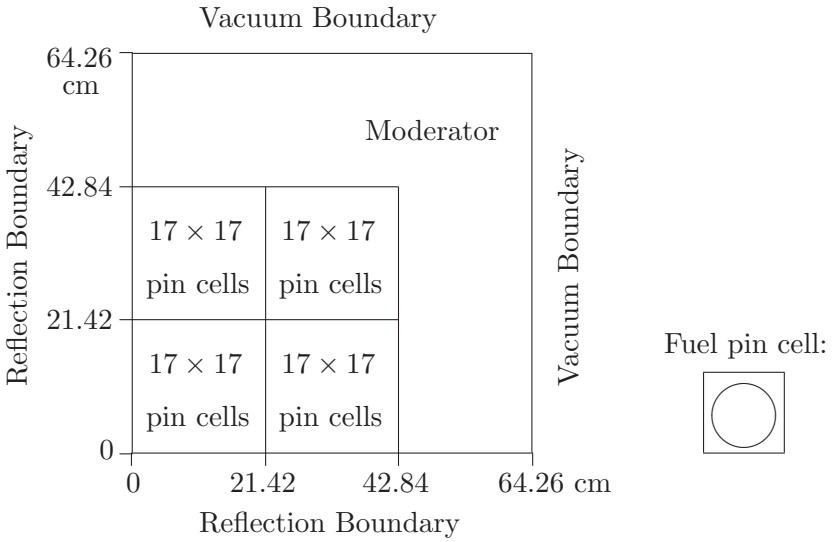

Figure 3: Geometry of the C5G7 benchmark.

The PARAFISH model was done using a finite element mesh of square elements such that each pin cell is discretized into 14×14 elements. This approximation of the cylindrical section by a Cartesian mesh was shown [20] to be appropriate, because it preserves not only the volume ratio between the two pin components, but also the "density" of the meshing in both these components. As for the domain decomposition, good results were obtained by grouping 4 or 9 pin cells into one domain, while grouping the surrounding moderator (outside the fuel assemblies) into 3 larger domains. This yields a total number of 289 domains, that were spread among 16 cores on the JuRoPA (Jülich Research on Petaflop Architectures) supercomputer installed at the Forschungszentrum Jülich (Germany). The total number of unknowns for the 7 groups is 3,719,352.

With the P_1 (i.e. diffusion) approximation, we have k-effective reference values of 1.18323 obtained by the Cronos2 code, and 1.18325 by the Variant code [14]. With the Davidson method used as above, we computed a satisfying k-effective of 1.18396. The eigenvalue solving requires 95 seconds, uses 23 outer (Davidson) iterations and 1 thermal iteration per outer iteration, for a total of 565 inner (GMRES) iterations. With the power method however, no convergence could be obtained with the above settings. To obtain convergence with the power method, it is necessary to perform some additional conjugate gradient iterations at the inner-most level of the calculation scheme, that is, with the incomplete Cholesky factorization computed locally on each

sub-domain. Moreover, since these additional CG iterations are part of the global spatio-angular preconditioner, the GMRES method must then be replaced by its flexible variant FGMRES [15] to allow non-constant preconditioning. With such adaptations, a k-effective of 1.18336 could be obtained, with an eigenvalue solving requiring 875 secs, 29 outer (power) iterations and 2 thermal iterations per outer iteration, for a total of 8549 inner (FGMRES) iterations. Further computational tests, also with higher-order P_N approximations, will be performed in the near future.

6. CONCLUSIONS

The Davidson method was shown to be a valuable alternative to the power iteration for neutronic criticality calculations. This is due to the fact that the Davidson method keeps track of more information along the iterative procedure, the extra storage cost being outweighted by the reduction of number of iterations. Moreover, this storage cost can be controlled by the restart parameter. Furthermore, as particularly visible in the C5G7 benchmark, the Davidson method requires a less accurate solving of the spatio-angular problem (inner iterations) at each eigenvalue (i.e. outer) iteration.

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