Application of Anderson acceleration to the neutron transport equation

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APPLICATION OF ANDERSON ACCELERATION TO THE NEUTRON TRANSPORT EQUATION

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This work investigates the solution of the multigroup neutron transport equation with a discrete ordinates method. More specifically, it focuses on the k-eigenvalue problem of the equation. In this case, the variables of interest are the largest eigenvalue (k_{eff}) and the corresponding eigenmode is called the fundamental mode. Mathematically, this problem is usually solved using the power iteration method [1]. However, the convergence of this algorithm can be very slow, especially if the dominance ratio is high as is the case in some reactor physics applications. Thus, the power iteration method has to be accelerated in some ways to improve its convergence.

One such acceleration is the Chebyshev acceleration method [2] which has been applied to legacy codes. In recent years, nonlinear methods have been applied to solve the k-eigenvalue problem. Nevertheless, these are often compared to the unaccelerated power iteration method. Hence, the goal of this paper is to apply the Anderson acceleration method to the power iteration method, and compare its performance to the Chebyshev acceleration method.

I. MATHEMATICAL BACKGROUND

Neutron transport equation

The multigroup discrete-ordinate transport equation is written in operator form as:

$$\mathcal{H}\psi = \mathcal{F}\psi \tag{1}$$

where

- $\mathcal{H} = \mathbf{\Omega}_n.\nabla\psi_n^g(\mathbf{r}) + \Sigma_t^g\psi_n^g(\mathbf{r}) - \dfrac{1}{2\pi}\sum\limits_{g'=1}^{G}\sum\limits_{n'=1}^{N}\omega_{n'}\Sigma_s^{g'\to g}(\mathbf{r}, \mathbf{\Omega}_{n'}\cdot\mathbf{\Omega}_n)\,\psi_{n'}^{g'}(\mathbf{r})$
- $\mathcal{F} = \dfrac{\chi(E)}{4\pi}\sum\limits_{g'=1}^{G}\sum\limits_{n'=1}^{N}\omega_{n'}\nu\Sigma_f\psi_{n'}^{g'}(\mathbf{r})$

The solution to Equation (1) is physical, *i.e.*, positive, if the characteristics of the problem is such that $\lambda = 1$ is the smallest eigenvalue of the following:

$$\mathcal{H}\psi = \lambda\mathcal{F}\psi \tag{2}$$

Therefore, the critical reactor core is obtained by establishing an equilibrium between fission sources and the removal term, without external sources, and is equivalent to solving for the largest eigenvalue k_{eff} such that (k_{eff}, ψ) is the solution to:

$$\mathcal{H}^{-1}\mathcal{F}\psi = k_{eff}\psi \tag{3}$$

Power Iteration

The Power Iteration (PI) method consists in iterating on the fission sources to solve the eigenvalue problem and is as follows:

Algorithm 1: Power Iteration

while $\dfrac{k_{eff}^{(n+1)} - k_{eff}^{(n)}}{k_{eff}^{(n)}} < \epsilon_{k_{eff}}$ *and* $\dfrac{\|\mathcal{F}\psi^{(n+1)} - \mathcal{F}\psi^{(n)}\|}{\|\mathcal{F}\psi^{(n)}\|} < \epsilon_{\psi}$ **do**

  Apply source iteration for new flux $\mathcal{H}\psi^{(n+1)} = \dfrac{1}{k_{eff}^{(n)}}\mathcal{F}\psi^{(n)}$

  Compute the new eigenvalue $k_{eff}^{(n+1)} = k_{eff}^{(n)}\sqrt{\dfrac{\left\langle \mathcal{F}\psi^{(n+1)}, \mathcal{F}\psi^{(n+1)} \right\rangle}{\left\langle \mathcal{F}\psi^{(n)}, \mathcal{F}\psi^{(n)} \right\rangle}}$

end

The eigenvector $\psi^{(n)}$ can be decomposed on the basis of eigenvectors of matrix $\mathcal{H}^{-1}\mathcal{F}$ as $\psi^{(n)} = \lambda^n\alpha_1\psi_1 + \mathcal{O}(\left(\dfrac{\lambda_2}{\lambda_1}\right)^n)$. For thermal reactors, the dominance ratio is usually above 0.95, and the PI method converges slowly. Thus, over the years, several acceleration methods have been conceived among which are rebalance techniques, Chebyshev acceleration and more recent nonlinear methods [3].

Chebyshev acceleration

This consists of modifying the initial problem into an equivalent one with a smaller dominance ratio to improve the convergence of the PI algorithm. The Chebyshev acceleration consists in applying PI method on a polynomial of $\mathcal{H}^{-1}\mathcal{F}$ such that the dominance ratio $\kappa = \lambda_2/\lambda_1$ is as small as possible without changing the eigenvectors of the latter. Thus, the starting point is to expand $\psi^{(n)}$ on the basis of eigenvectors of $A = \dfrac{\mathcal{H}^{-1}\mathcal{F}}{k_{eff}^{(n)}}$ as a polynomial P_l

Given that $P_l(A)\psi = \sum_{i=1}^{m}\alpha_i P_l(A)\psi_i$ and that $A^l\psi = \sum_{i=1}^{l}\alpha_i\lambda^i\psi_i$:

$$P_l(A)\psi = \alpha_1 P_l(\lambda_1)\psi_1 + P_l(\lambda_1)(\alpha_2\frac{P_l(\lambda_2)}{P_l(\lambda_1)}\psi_2 + \cdots + \alpha_m\frac{P_l(\lambda_m)}{P_l(\lambda_1)}\psi_m) \tag{4}$$

and by minimising the fractional part of the former expression, the polynomial P_l obtained may be applied to accelerate the PI [2]. One such polynomial is obtained from the Chebyshev polynomial defined

as $P_n(x) = \dfrac{C_n(\frac{2x}{\kappa} - 1)}{C_n(\frac{2}{\kappa} - 1)}$ where $C_n(x) = \cos(n \arccos(x))$ if $|x| < 1$ or $C_n(x) = \cosh(n\text{arccosh}(x))$ otherwise. Following the recurrence property of the Chebyshev polynomials, the acceleration step is hence expressed as:

$$\mathcal{F}\psi^{(n+1)} = \frac{\rho^{(n+1)}\gamma}{\lambda_1}\mathcal{F}\psi^{(n+1)} - \rho^{(n+1)}(1-\gamma)\mathcal{F}\psi^{(n)} + (1-\rho^{(n+1)})\mathcal{F}\psi^{(n-1)} \tag{5}$$

with $\gamma = \dfrac{2}{2-\kappa}$, $\sigma = \dfrac{\kappa}{2-\kappa}$, $\rho^{(1)} = 1$, $\rho^{(2)} = \dfrac{2}{2-\sigma^2\rho^{(1)}}$, and $\rho^{(n+1)} = \dfrac{2}{2-\sigma^2\rho^{(n)}}$. The main drawback of this method is that it requires *a priori* knowledge of λ_1 and the dominance ratio κ; its efficiency depends on an appropriate estimate for these. Algorithm 2 describes the Chebyshev acceleration as applied.

Algorithm 2: Chebyshev acceleration

while $\dfrac{k_{\mathit{eff}}^{(n+1)} - k_{\mathit{eff}}^{(n)}}{k_{\mathit{eff}}^{(n)}} < \epsilon_{k_{\mathit{eff}}}$ *and* $\dfrac{\|\mathcal{F}\psi^{(n+1)} - \mathcal{F}\psi^{(n)}\|}{\|\mathcal{F}\psi^{(n)}\|} < \epsilon_\psi$ **do**
- Apply Power Iteration as in Algorithm 1
- Compute an estimation of κ as $\tau^{(n+1)} = \dfrac{\epsilon^{(n+1)}}{\epsilon^{(n)}}$, $\epsilon^{(n)}$ = relative error at iteration n
- Accelerate source vector
- **if** $\tau^{(n+1)} < 1$ & $\|\tau^{(n+1)} - \tau^{(n)}\| < 0.01$ & *accelerate* = *False* **then**
  - $accelerate = True$ (flag to control acceleration phase)
  - $\alpha = \dfrac{2}{\tau^{(n+1)}}$, $\rho^{(n+1)} = \dfrac{1}{\alpha - 1}$
  - $\mathcal{F}\psi^{(n+1)} = \alpha\rho^{(n+1)}\mathcal{F}\psi^{(n+1)} - \rho^{(n+1)}\mathcal{F}\psi^{(n)}$
- **end**
- **if** $accelerate = True$ **then**
  - $\rho^{(n+1)} = \dfrac{4}{4(\alpha-1) - \rho^{(n)}}$
  - $\mathcal{F}\psi^{(n+1)} = \alpha\rho^{(n+1)}\mathcal{F}\psi^{(n+1)} - \rho^{(n+1)}\mathcal{F}\psi^{(n)} + (1 - \alpha\rho^{(n+1)} + \rho^{(n+1)})\mathcal{F}\psi^{(n-1)}$
- **end**

end

Anderson acceleration

In this research effort, the Anderson acceleration [4] is applied to the PI algorithm. This method has been successfully applied recently for accelerating the eigenvalue problem by [3, 5] and is described by Algorithm 3. It ressembles a GMRES method, except that the subspace projection is orthogonalised using only the number of vectors prescribed by the history length of the method. Thus, the subspace spanned does not guarantee a theoretical convergence of the method but past works [3, 5] have shown that it converges in practical situations where the PI converges.

The application to the PI method is implemented in our case by substituting the function f in Algorithm 3 by the Algorithm 1. Successive iterations of the Anderson algorithm evaluates the PI only once. Unlike

past works, this investigation differs in its application of the Anderson acceleration to the source vector, and not the flux, similar to the Chebyshev acceleration described previously. Furthermore, the history length is arbitrarily set to 2 to compare to the amount of data required by the Chebyshev acceleration method.

Algorithm 3: Anderson acceleration

Given $\mathbf{u}^{(0)}$ and a history length of $m \geq 1$
$\mathbf{u}^{(1)} = f(\mathbf{u}^{(0)})$
while $\dfrac{\|\mathbf{u}^{(n+1)} - f(\mathbf{u}^{(n)})\|}{\|f(\mathbf{u}^{(n)})\|} < \epsilon_{\mathbf{u}}$ **do**
  $m_n = min(m, n)$
  Compute current residual
  $\mathcal{G}^{(n)} = (\mathbf{g}_{n-m}, \ldots, \mathbf{g}_k)$ with $\mathbf{g}_n = f(\mathbf{u}^{(n)}) - \mathbf{u}^{(n)}$
  Determine $\alpha^{(n)} = (\alpha_0^{(n)}, \ldots, \alpha_{m_n}^{(n)})$ which solves the following minimisation problem
  $min_\alpha \|\mathcal{G}^{(n)}\alpha\|$ such that $\sum_{i=0}^{m_n} \alpha_i = 1$
  Compute new estimate for unknown vector
  $\mathbf{u}^{(n+1)} = \sum_{i=0}^{m_n} \alpha_i^{(n)} f(\mathbf{u}^{(n-m_n+i)})$
end

II. SLAB PROBLEM

The case considered for the numerical test is monogroup 1D slab problem, with a fuel zone of 200 cm enclosed between two reflector regions of 5 cm each. The problem is solved using the unaccelerated PI, and PI accelerated by the previously described acceleration methods. The stopping criteria for the iterative schemes are set to 1.e-6.

Table I. Results for 1D problem

Method	No. of iterations	Residual Error
PI	4008	9.9e-7
PI + Chebychev	340	5.1e-7
PI + Anderson	236	9.5e-7

III. CONCLUDING REMARKS

The Anderson acceleration method has been successfully applied to the 1D problem considered in this work. During this work, multigroup cases have also been tested, and the results remain still very similar to the observations made with the monogroup case. The aim is to extend it to further multidimensional problems and compare its behaviour with respect to the Chebyshev acceleration.

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