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ABSTRACT

In this paper, we study the Least-Squares (LS) P_N form of the transport equation compatible with voids [1] in the context of Continuous Finite Element Methods (CFEM). We first derive weakly imposed boundary conditions which make the LS weak formulation equivalent to the Self-Adjoint Angular Flux (SAAF) variational formulation with a void treatment [2], in the particular case of constant cross-sections and a uniform mesh. We then implement this method in Rattlesnake with the Multiphysics Object Oriented Simulation Environment (MOOSE) framework [3] using a spherical harmonics (P_N) expansion to discretize in angle. We test our implementation using the Method of Manufactured Solutions (MMS) and find the expected convergence behavior both in angle and space. Lastly, we investigate the impact of the global non-conservation of LS by comparing the method with SAAF on a heterogeneous test problem.

Key Words: **Least-Squares, boundary conditions, P_N, Transport**

1. INTRODUCTION

The original self-adjoint angular flux (SAAF) formulation [2, 4–7] presents the inconvenience of having a term proportional to the inverse of the total cross-section σ_t and thus of becoming singular if there is a void anywhere in the spatial domain. The SAAF formulation with a void treatment [2] has been developed to eliminate that problem but does so at a cost: the streaming and collision operators are no longer symmetric and positive definite and the solution depends on non-physical parameters such as the elements size. An alternative is to use a LS transport equation compatible with voids [1] whose variational formulation – although fairly close to that of SAAF – does not formally break down if void is present in the problem. It also has the advantage of preserving the intermediate and thick diffusion limits [1]. Nevertheless, unlike for the SAAF formulation, no boundary terms appear in the derivation

of the LS weak formulation so the boundary conditions cannot be naturally weakly imposed. Instead it is common to enforce them either strongly or weakly by adding an additional penalty term. Weakly imposed boundary conditions are preferred from an implementation point of view. However, it is not straightforward to know how to scale this boundary term. In this work, we show that the scaling constant can actually be chosen in such a way that the SAAF and LS weak formulations are equivalent in the particular case of a constant σ_t and a uniform mesh. This derivation is independent of the angular discretization.

Next, we choose to use a truncated spherical harmonics (P_N) expansion to approximate the angular dependency of the solution. This ensures in particular that the numerical scalar flux is immune to ray-effects but – among other flaws – it can potentially become oscillatory and/or negative [8–11]. The odd moments can be simply expressed as a function of the even moments under the condition that σ_t is non-zero. The number of unknowns can then be reduced almost by half but may induce a loss of accuracy.

We refer to the method as a whole as LS-P_N. The detailed equations are given in Section 2. We implement it in the MOOSE-based [3] application named Rattlesnake, the transport solver from the Idaho National Laboratory (INL). In Section 3, the correctness of the implementation is verified first by checking that the SAAF-P_N and LS-P_N implementations give identical results with a uniform mesh and σ_t constant, then using the Method of Manufactured Solutions (MMS) with discontinuous cross-sections and an anisotropic solution. The convergence both in angle and space are then studied. Lastly, we compare the SAAF-P_N and LS-P_N results on a test problem with significant heterogeneity. LS being globally non-convervative, the convergence is slower compared to SAAF. Conclusions are drawn in Section 4.

2. SAAF-CONSISTENT BOUNDARY CONDITIONS FOR LEAST-SQUARES

2.1. Notations

We use the following notations: the spatial domain is noted $\mathcal{D}$ and its boundary $\partial\mathcal{D}$. Besides:

$$(a,b)_{\mathcal{D}} \equiv \int_{\mathcal{D}}\int_{4\pi} a(\vec{r},\vec{\Omega})b(\vec{r},\vec{\Omega})\ \mathrm{d}\Omega\mathrm{d}r \quad , \quad \langle a,b\rangle_{\partial\mathcal{D}} \equiv \int_{\partial\mathcal{D}}\int_{4\pi} a(\vec{r},\vec{\Omega})b(\vec{r},\vec{\Omega})\ \vec{\Omega}\cdot\vec{n}\,\mathrm{d}\Omega\mathrm{d}r,$$

$$\langle a,b\rangle^{+}_{\partial\mathcal{D}} \equiv \int_{\partial\mathcal{D}}\int_{\vec{\Omega}\cdot\vec{n}(\vec{r})>0} a(\vec{r},\vec{\Omega})b(\vec{r},\vec{\Omega})\ |\vec{\Omega}\cdot\vec{n}|\mathrm{d}\Omega\mathrm{d}r\ ,\ \langle a,b\rangle^{-}_{\partial\mathcal{D}} \equiv \int_{\partial\mathcal{D}}\int_{\vec{\Omega}\cdot\vec{n}(\vec{r})<0} a(\vec{r},\vec{\Omega})b(\vec{r},\vec{\Omega})\ |\vec{\Omega}\cdot\vec{n}|\mathrm{d}\Omega\mathrm{d}r,$$

where $\vec{r}$ is the spatial independent variable, $\vec{\Omega}$ is the angular independent variable and $\vec{n}(\vec{r})$ is the outward normal unit vector at a point $\vec{r}\in\partial\mathcal{D}$.

2.2. Least-Squares Weak Formulation

We consider the steady-state, one-group transport equation with fission and anisotropic scattering:

$$\vec{\Omega}\cdot\vec{\nabla}\Psi+\sigma_t(\vec{r})\Psi(\vec{r},\vec{\Omega})=\int_{4\pi}\sigma_s(\vec{r},\vec{\Omega}'\rightarrow\vec{\Omega})\Psi(\vec{r},\vec{\Omega}')\,\mathrm{d}\vec{\Omega}'+\nu\sigma_f(\vec{r})\Phi(\vec{r})+S(\vec{r},\vec{\Omega}), \tag{1}$$

where Ψ and Φ represent respectively the angular and scalar flux. In addition, σ_t, σ_s and σ_f respectively denote the total, scattering and fission macroscopic cross-sections and ν is the average number of neutrons emitted per fission. S is the volumetric source. We can rewrite Eq. (1) in operator form:

$$L\Psi=H\Psi+S, \tag{2}$$

where L is the streaming plus collision operator and H is the fission plus scattering operator. Using $L\Psi^\star$ as the test function and adding a penalty term to weakly impose the boundary conditions, we obtain the following weak formulation: find $\Psi\in V$ such that for all $\Psi^\star\in V$,

$$(L\Psi^\star,L\Psi)_{\mathcal{D}}+\langle c\Psi^\star,(\Psi-\Psi^{\text{inc}})\rangle^-_{\partial\mathcal{D}}=(L\Psi^\star,H\psi+S)_{\mathcal{D}}\,, \tag{3}$$

where V is the finite element space where the solution is sought and where c is a positive constant [1, 12]. Extending this theory to multigroup would be a minor complication.

2.3. Boundary Conditions

From [2], the weak formulation for SAAF with void treatment is given by: find $\Psi\in V$ such that, for all $\Psi^\star\in V$,

$$\begin{aligned}\left(\vec{\Omega}\cdot\vec{\nabla}\Psi^\star,\tau\,\vec{\Omega}\cdot\vec{\nabla}\Psi\right)_{\mathcal{D}}-\left(\vec{\Omega}\cdot\vec{\nabla}\Psi^\star,(1-\tau\sigma_t)\Psi\right)_{\mathcal{D}}+(\sigma_t\Psi^\star,\Psi)_{\mathcal{D}}\\+\langle\Psi^\star,\Psi\rangle^+_{\partial\mathcal{D}}-\langle\Psi^\star,\Psi^{\text{inc}}\rangle^-_{\partial\mathcal{D}}=\left(\tau\,\vec{\Omega}\cdot\vec{\nabla}\Psi^\star+\Psi^\star,H\Psi+S\right)_{\mathcal{D}}.\end{aligned} \tag{4}$$

The constant τ is defined as follows:

$$\tau=\min\left(\frac{1}{\sigma_t},\frac{h}{\varsigma}\right), \tag{5}$$

where h characterizes the mesh size and ς is a constant, typically chosen to be 2.

In this subsection, we assume that τ is constant and we show that there is only one value for c such that Eqs. (3) and (4) are almost equivalent. We first multiply Eq. (3) with τ and use the divergence theorem to get:

$$\begin{aligned}\left(\vec{\Omega}\cdot\vec{\nabla}\Psi^\star,\tau\vec{\Omega}\cdot\vec{\nabla}\Psi\right)_{\mathcal{D}}+\langle\tau\sigma_t\Psi^\star,\Psi\rangle^+_{\partial\mathcal{D}}-\langle\tau\sigma_t\Psi^\star,\Psi\rangle^-_{\partial\mathcal{D}}+(\tau\sigma_t\Psi^\star,\sigma_t\Psi)_{\mathcal{D}}\\+c\,\langle\Psi^\star,\tau(\Psi-\Psi^{\text{inc}})\rangle^-_{\partial\mathcal{D}}=\left(\tau\vec{\Omega}\cdot\vec{\nabla}\Psi^\star+\tau\sigma_t\Psi^\star,H\Psi+S\right)_{\mathcal{D}}.\end{aligned} \tag{6}$$

Subtracting (4) from (6) and looking for the value of c such that this equation is satisfied for all $\Psi^\star \in V$, it yields:

$$\begin{aligned}(1-\tau\sigma_t)\left[-\langle\Psi^\star,\Psi\rangle^-_{\partial\mathcal{D}}-\left(\Psi^\star,\vec{\Omega}\cdot\vec{\nabla}\Psi\right)_{\mathcal{D}}\right]+(\tau\sigma_t-1)\left(\tau\sigma_t\Psi^\star,\sigma_t\Psi\right)_{\mathcal{D}}\\ +(c\tau-\tau\sigma_t)\left\langle\Psi^\star,\Psi\right\rangle^-_{\partial\mathcal{D}}+(1-c\tau)\langle\Psi^\star,\Psi^{\text{inc}}\rangle^-_{\partial\mathcal{D}}=(\tau\sigma_t-1)\left(\Psi^\star,H\Psi+S\right)_{\mathcal{D}}.\end{aligned} \tag{7}$$

Besides, since Ψ is the solution of the transport equation in a weak sense we have, neglecting the discretization error:

$$\left(\Psi^\star,\vec{\Omega}\cdot\vec{\nabla}\Psi+\sigma_t\Psi\right)_{\mathcal{D}}\approx\left(\Psi^\star,H\Psi+S\right)_{\mathcal{D}}. \tag{8}$$

The previous terms then reduce to:

$$(c\tau-1)\left\langle\Psi^\star,(\Psi-\Psi^{\text{inc}})\right\rangle^-_{\partial\mathcal{D}}=0. \tag{9}$$

Therefore, under the assumption that τ is constant, the LS and SAAF formulations are equivalent if and only if:

$$c=\frac{1}{\tau}=\max\left(\sigma_t,\frac{\varsigma}{h}\right). \tag{10}$$

2.4. Spherical Harmonics Expansion

The P_N approximation consists of using a truncated spherical harmonics expansion for Ψ:

$$\Psi(\vec{r},\vec{\Omega})=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\Phi_\ell^m(\vec{r})R_\ell^m(\vec{\Omega})\approx\sum_{\ell=0}^{N}\sum_{m=-\ell}^{\ell}\Phi_\ell^m R_\ell^m, \tag{11}$$

given $\vec{\Omega}=\sqrt{1-\mu^2}\cos\varphi\,\vec{e}_x+\sqrt{1-\mu^2}\sin\varphi\;\vec{e}_y+\mu\,\vec{e}_z$. The real-form spherical harmonics are defined as:

$$R_\ell^m(\vec{\Omega})=\begin{cases}\sqrt{2}\,C_\ell^m\,P_\ell^m(\mu)\cos(m\varphi), & 0<m\leq\ell\leq N\\ C_\ell^0\,P_\ell^0(\mu), & 0\leq\ell\leq N\\ \sqrt{2}\,C_\ell^{|m|}\,P_\ell^{|m|}(\mu)\sin(|m|\varphi), & 0<-m\leq\ell\leq N\end{cases}, \tag{12}$$

where $C_\ell^m=(\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!})^{1/2}$ are normalization constants and P_ℓ^m designates the associated Legendre polynomial of degree l and order m. The Φ_ℓ^m are called the *moments* of Ψ.

2.5. Even-parity

Solving solely for the even-parity component of Ψ can be beneficial in an effort to significantly reduce the number of unknowns [13]. This can be done by defining the new variables $\Psi_e=(\Psi(\vec{\Omega})+$

$\Psi(-\vec{\Omega}))/2$ and $\Psi_o = (\Psi(\vec{\Omega}) - \Psi(-\vec{\Omega}))/2$. The 'even' LS-P$_N$ weak formulation is then obtained by keeping only the terms associated to even test functions and is given by: find $\Psi_e \in V$ such that for all $\Psi_e^\star \in V$,

$$\left(\vec{\Omega}\cdot\vec{\nabla}\Psi_e^*, \vec{\Omega}\cdot\vec{\nabla}\Psi_e\right)_{\mathcal{D}} + \left(\sigma_t\Psi_e^*, \vec{\Omega}\cdot\vec{\nabla}\Psi_o\right)_{\mathcal{D}} + \left(\vec{\Omega}\cdot\vec{\nabla}\Psi_e^*, \sigma_t\Psi_o\right)_{\mathcal{D}} + (\sigma_t\Psi_e^*, \sigma_t\Psi_e)_{\mathcal{D}} + \langle\sigma_t\Psi_e^*, (\Psi - \Psi^{\text{inc}})\rangle^-_{\partial\mathcal{D}} = \left(\vec{\Omega}\cdot\vec{\nabla}\Psi_e^*, H\Psi_o + S_o\right)_{\mathcal{D}} + (\sigma_t\Psi_e^*, H\Psi_e + S_e)_{\mathcal{D}}\,, \tag{13}$$

S_e and S_o being respectively the even and odd components of S. This weak formulation is only solved for Ψ_e, the value of Ψ_o being computed directly using:

$$\Psi_o = (\sigma_t - H)^{-1}\left(S_o - \vec{\Omega}\cdot\vec{\nabla}\Psi_e\right). \tag{14}$$

While this method reduces the number of unknowns almost by half and can therefore be fairly attractive, it also induces a loss of accuracy because of the gradient operation in Eq. (14): in particular, if V is the space of the piecewise polynomials of order 1, the second term in Eq. (13) simply vanishes. In practice, we observe that the spatial convergence is then only first order. The other disadvantage is that Eq. (14) cannot be used in void or purely scattering regions.

3. RESULTS AND CODE VERIFICATION

3.1. Method of Manufactured Solution

We consider the following pure-absorber problem:

$$\mu\frac{\partial\Psi}{\partial x} + \sigma_t(x)\Psi(x,\mu) = q \quad , \quad 0 \le x \le L \quad , \quad -1 \le \mu \le 1, \tag{15}$$

where $\sigma_t = \sigma_1$ for $L/4 < x < 3L/4$ and $\sigma_t = \sigma_0$ otherwise, with reflecting boundaries at $x = 0$ and $x = L$. We choose our solution in the following form:

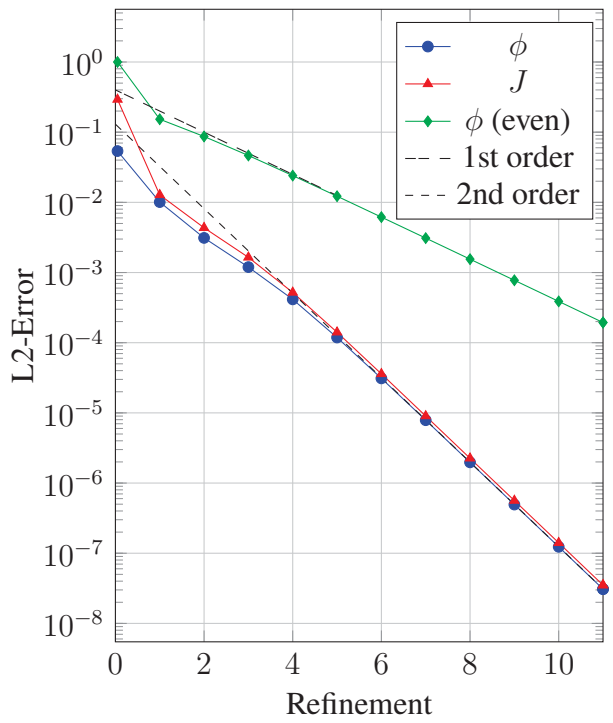
$$\tilde{\Psi} = f(x)\,g(\mu) \quad , \quad 0 \le x \le L \quad , \quad -1 \le \mu \le 1, \tag{16}$$

where:

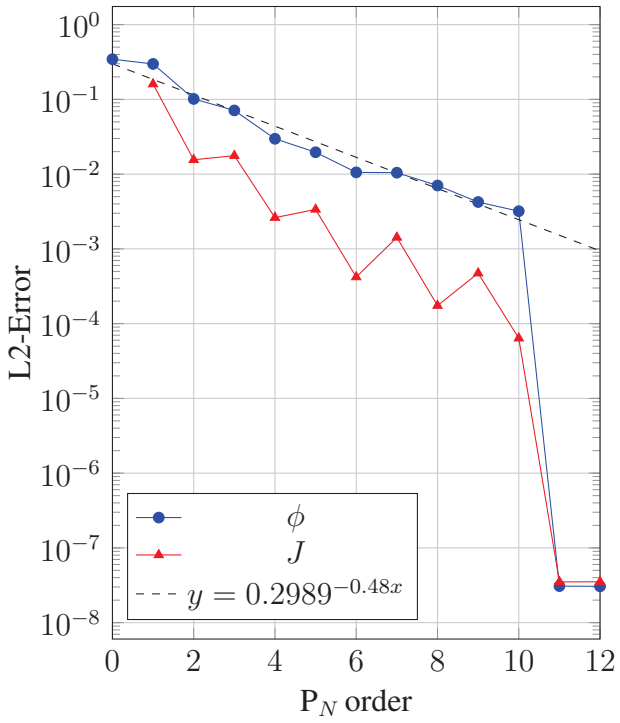
$$f(x) = \phi_0\left(\cos\left(\frac{\pi x}{L}\right) + a\right), \tag{17}$$

$$g(\mu) = R_0^0 + 0.5R_2^0(\mu) + 0.25R_4^0(\mu) + 0.125R_6^0(\mu) + 0.1R_8^0(\mu) + 0.05R_{10}^0(\mu). \tag{18}$$

The convergence results are shown on Figs. 1a and 1b. In particular, if we choose to express the odd-parity moments as a function of the even moments, we can reduce the number of unknowns but we lose one order of spatial of convergence, as shown on Fig. 1a.



(a) L2-Error for ϕ and J for $N = 11$ (4 cells for ref = 0).



(b) L2-Error for ϕ and J for a refinement of 11. The dashed line is the interpolation of ϕ for N in [0,10].

3.2. Comparison between SAAF-P$_N$ and LS-P$_N$ with significant heterogeneity

We consider the test problem described in Fig. (2) which consists of 8 pin cells surrounding a void region. The material properties of the fuel and moderator (respectively shown in blue and yellow on the figure) are chosen to be the same as the "UO_2 Fuel-Clad mix" and "Moderator" materials from the C5G7 benchmark [14]. All boundary conditions are chosen to be reflective. The goal of this test problem is to test our methods on a multigroup heterogeneous test problem involving a void region. As mentioned above, we do not consider solving only for Ψ_e in this problem because of the void region.

Table I shows some of the values for the multiplication factor k_{eff} obtained on this particular test problem. The first column designates the level of uniform refinement of the mesh (see Fig. 2). The second column shows the P$_N$ order for the LS-P$_N$ calculations while the forth column indicates the Level-Symmetric quadrature order for the LS-S$_N$ and SAAF-S$_N$ calculations. The results for SAAF-S$_N$ with void treatment are considered to be more reliable because this method has global conservation which is what matters most to get a good k-eigenvalue estimation. The fact that SAAF is globally conservative while LS is not can be seen in Eqs. (4) and (3) with a constant test function over the entire domain [15]. In this heterogeneous example, the convergence for LS is much slower. A very fine refinement in both angle and space is indeed necessary to achieve good convergence in k_{eff}. In particular, the LS-P$_{39}$ calculation with the most refined mesh has over 500 million unknowns and still differs from the most refined SAAF calculation by more than 650 pcm.

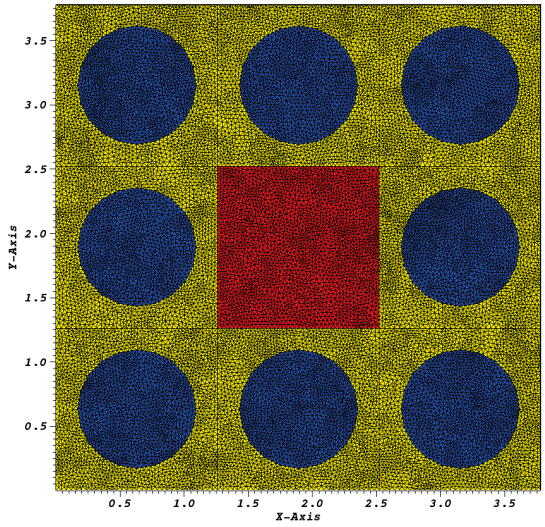


Figure 2: Geometry of a 3x3 pin cell test problem. The regions in blue, yellow and red respectively correspond to the fuel, moderator and void. The former two use the cross-sections of the C5G7 benchmark [14]. The latter is in practice chosen such that $\sigma_t = 10^{-10}$ cm^{-1}. The fuel boundary is approximated with a 20-side polygon. The meshes with a refinement of 0, 1, 2 (shown) and 3 have respectively 1116, 4829, 21090 and 92912 nodes. Besides, they respectively have 2134, 9455, 41776 and 184962 elements and 3249, 14283, 62865 and 277873 sides.

In summary, although the SAAF and LS methods are equivalent for a uniform σ_t with the boundary conditions given in Section 2.3, the results are quite different with large variations of σ_t. We attribute this difference to the fact that LS is globally non-conservative. We observe that the convergence upon angular and spatial discretization on this particular test problem is fairly slow. Future work will include comparing these results with the PDT code, a first-order S_N solver developed at Texas A&M, which was previously used to run the C5G7 test problem [15]. Further, we wish to look at the LS results obtained using conservative Nonlinear Diffusion Acceleration (NDA) which would help recover the global conservation of the scheme [2]. Some work will be necessary to make sure that the low-order diffusion scheme is compatible with void.

4. CONCLUSION

In conclusion, we have derived boundary conditions for LS which are consistent to the SAAF weak formulation with void treatment [1], independently of the angular discretization. With such boundary conditions, LS and SAAF are then equivalent if the cross-section σ_t is constant over the spatial domain

Table I: Value for k_{eff} for different methods.

Refinement	N	LS-P$_N$	Quad order	LS-S$_N$	SAAF-S$_N$
0	1	1.911364	2	1.441561	1.354652
0	3	1.591152	4	1.455436	1.350099
0	9	1.454500	10	1.454254	1.347603
0	19	1.441763	20	1.453473	1.347430
1	3	1.549035	2	1.383950	1.354182
1	9	1.401521	4	1.384094	1.349362
1	19	1.383698	10	1.382194	1.346884
1	29	1.379677	20	1.382080	1.346677
2	9	1.387192	2	1.365296	1.354136
2	19	1.365902	4	1.362090	1.349267
2	29	1.360969	10	1.359796	1.346791
2	39	1.359555	20	1.357283	1.346566
3	9	1.383306	2	1.359100	1.354129
3	19	1.360183	4	1.354512	1.349267
3	29	1.354673	10	1.352033	1.346779
3	39	1.353057	20	1.350871	1.346549

and if the mesh is uniform. Our method gave the expected convergence behaviors in space and angle. In particular, solving only for the even-parity component of the angular flux, when possible, decreases the spatial order of convergence by one. However, being globally non-conservative, LS differs noticeably on heterogeneous problems from the SAAF results before convergence is achieved.

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