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P_2-EQUIVALENT FORM OF THE SP_2 EQUATIONS
Including boundary and interface conditions

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The spherical harmonics (P_N) equations are a moment-based method to solve the Boltzmann transport equation by expanding the angular variable $\hat{\Omega}$ in terms of spherical harmonics functions and then truncating the expansion at some order with a closure. These methods have been shown to work well in problems with moderate amounts of scattering or with appropriate closures [1–4]. The SP_N equations, or simplified P_N equations, were originally derived by Gelbard through taking a spherical harmonics expansion to the 1-D slab geometry transport equation and making some *ad hoc* substitutions to make the equations "look" 3-D. Gelbard was able to show that under many situations, the most general being an infinite medium with a constant cross-section, the SP_N solution for the scalar flux would be the same as the scalar flux solution from the full, and much more complicated, P_N equations. Later variational and asymptotic derivations of the SP_N equations were presented [5–9]. These derivations made it clear that the SP_N equations, in the form they are most commonly solved, do not give the same solution as the P_N equations. Also, there has never been an interpretation of the SP_N unknowns in terms of spherical harmonics moments, except for the scalar flux and current where the intrepretation is trivial. Much of the current knowledge of can be found by the interested reader in a recent special issue of *TTSP* commenorating the 50^{th} anniversary of the SP_N equations [10].

In the 1970's Selengut presented in an inscrutably terse ANS transactions paper a derivation of a P_3-equivalent form of the SP_3 equations with appropriate interface conditions. The trail of this work apparently went cold thereafter, and no numerical solutions or in depth derivations of these equations have surfaced in the literature. The lack of derivation details has made it difficult to extend Selengut's work and verify its correctness, in a similar vein to Fermat's last theorem in that we have the result, but not how it was arrived at*. Of course there would be a large impact of a P_3 -equivalent SP_3 method in computational transport in that SP_3 is a workhorse method for reactor calculations and it has only 3 angular unknowns compared to the 16 unknowns of the P_3 equations in first-order form.

In an ongoing research program we are endeavoring to find P_N -equivalent SP_N methods, and this abstract presents some initial, though theoretically important, results to that end. Specifically, we present a P_2-equivalent form of the SP_2 equations in 2-D Cartesian geometry. We were able to find an interpretation of

*It might be beyond the pale to call this Selengut's last theorem as I believe he did much work after this.

all the SP_2 unknowns and show how it goes to the standard equation for the scalar flux in the case of an infinite medium with constant cross-section.

We will be considering the linear, steady, and one-speed transport equation with isotropic scattering:

$$\left(\Omega \cdot \nabla + \sigma_{\mathrm{t}}\right) \psi = \frac{1}{4\pi} \left(\sigma_{\mathrm{s}} \phi + Q\right), \tag{1}$$

where $\psi(\vec{x}, \Omega, t)$ is the angular flux with scalar flux given by

$$\phi(\vec{x}) = \int_{4\pi} \psi(\vec{x}, \Omega) \, d\Omega. \tag{2}$$

Also, in Eq. (1) σ_{t} is the macroscropic total cross-section, σ_{s} is the macroscopic scattering cross-section, and Q is the isotropic, prescribed source.

The P_2 equations as an approximation to Eq. (1) in 2-D $x - z$ geometry, as derived previously [11, 12], are

$$\sigma_{\mathrm{a}} \psi_0^0 + \frac{1}{\sqrt{3}} \frac{\partial}{\partial z} \psi_1^0 - \sqrt{\frac{2}{3}} \frac{\partial}{\partial x} \psi_1^1 = \frac{Q}{\sqrt{4\pi}}, \tag{3a}$$

$$\sigma_{\mathrm{t}} \psi_1^0 + \frac{\partial}{\partial z} \left(\frac{1}{\sqrt{3}} \psi_0^0 + \frac{2}{\sqrt{15}} \psi_2^0 \right) - \sqrt{\frac{2}{5}} \frac{\partial}{\partial x} \psi_2^1 = 0, \tag{3b}$$

$$\sigma_{\mathrm{t}} \psi_1^1 + \frac{\partial}{\partial x} \left(-\frac{1}{\sqrt{6}} \psi_0^0 + \frac{1}{\sqrt{30}} \psi_2^0 - \frac{1}{\sqrt{5}} \psi_2^2 \right) + \frac{1}{\sqrt{5}} \frac{\partial}{\partial z} \psi_2^1 = 0, \tag{3c}$$

$$\sigma_{\mathrm{t}} \psi_2^0 + \frac{2}{\sqrt{15}} \frac{\partial}{\partial z} \psi_1^0 + \sqrt{\frac{2}{15}} \frac{\partial}{\partial x} \psi_1^1 = 0, \tag{3d}$$

$$\sigma_{\mathrm{t}} \psi_2^1 + \frac{1}{\sqrt{5}} \frac{\partial}{\partial z} \psi_1^1 - \frac{1}{\sqrt{10}} \frac{\partial}{\partial x} \psi_1^0 = 0, \tag{3e}$$

$$\sigma_{\mathrm{t}} \psi_2^2 - \frac{1}{\sqrt{5}} \frac{\partial}{\partial x} \psi_1^1 = 0, \tag{3f}$$

where

$$\psi_l^m(\vec{x}) = \int_{4\pi} \bar{Y}_l^m(\hat{\Omega}) \psi(\vec{x}, \hat{\Omega}) \, d\hat{\Omega},$$

with

$$Y_l^m(\mu, \varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^{|m|}(\mu) e^{im\varphi}. \tag{4}$$

Now we will define a re-normalized moment by undoing the normalization constant used in the above definition of the moments and removing the Condon-Shortley phase term:

$$\psi_{lm} = (-1)^m \psi_l^m \sqrt{\frac{4\pi (l+m)!}{(2l+1)(l-m)!}}, \tag{5}$$

making

$$\psi_{00} = \sqrt{4\pi}\psi_0^0, \quad \psi_{10} = \frac{4\pi}{\sqrt{3}}\psi_1^0, \quad \psi_{11} = -\sqrt{\frac{8\pi}{3}}\psi_1^1, \quad \psi_{20} = \sqrt{\frac{4\pi}{5}}\psi_2^0, \quad \psi_{21} = -\sqrt{\frac{24\pi}{5}}\psi_2^1, \quad \psi_{22} = \sqrt{\frac{96\pi}{5}}\psi_2^2.$$

Under this normalization $\psi_{00} = \phi$ and $\vec{J} = (\psi_{11}, 0, \psi_{10})^{\mathrm{t}}$. These definitions make the P_2 equations

$$\sigma_{\mathrm{a}}\psi_{00} + \frac{\partial}{\partial z}\psi_{10} + \frac{\partial}{\partial x}\psi_{11} = Q, \tag{6a}$$

$$\sigma_{\mathrm{t}}\psi_{10} + \frac{\partial}{\partial z}\left(\frac{1}{3}\psi_{00} + \frac{2}{3}\psi_{20}\right) + \frac{1}{3}\frac{\partial}{\partial x}\psi_{21} = 0, \tag{6b}$$

$$\sigma_{\mathrm{t}}\psi_{11} + \frac{\partial}{\partial x}\left(\frac{1}{3}\psi_{00} - \frac{1}{3}\psi_{20} + \frac{1}{6}\psi_{22}\right) + \frac{1}{3}\frac{\partial}{\partial z}\psi_{21} = 0, \tag{6c}$$

$$\sigma_{\mathrm{t}}\psi_{20} + \frac{2}{5}\frac{\partial}{\partial z}\psi_{10} - \frac{1}{5}\frac{\partial}{\partial x}\psi_{11} = 0, \tag{6d}$$

$$\sigma_{\mathrm{t}}\psi_{21} + \frac{3}{5}\frac{\partial}{\partial z}\psi_{11} + \frac{3}{5}\frac{\partial}{\partial x}\psi_{10} = 0, \tag{6e}$$

$$\sigma_{\mathrm{t}}\psi_{22} + \frac{6}{5}\frac{\partial}{\partial x}\psi_{11} = 0. \tag{6f}$$

These equations are starting to look like the SP_2 equations, but there are still some algebraic hoops to jump through.

The next step is to define a linear combination of ψ_{20} and ψ_{22} as a new unknown. If we take Eq. (6d) and add it with one-half times Eq. (6f) we get that

$$\sigma_{\mathrm{t}}\phi_2 + \frac{2}{5}\frac{\partial}{\partial z}\psi_{10} + \frac{2}{5}\frac{\partial}{\partial x}\psi_{11} = 0, \tag{7}$$

where

$$\phi_2 = \psi_{20} + \frac{\psi_{22}}{2}.$$

From Eqs. (6d) and (6f) we also get that

$$\frac{3}{2}\psi_{20} + \frac{1}{4}\psi_{22} = -\frac{3}{5\sigma_{\mathrm{t}}}\frac{\partial}{\partial z}\psi_{10}. \tag{8}$$

Next, we will eliminate ψ_{20} and ψ_{22} in favor of ϕ_2 in Eqs. (6b) and (6c). We note that

$$\frac{2}{3}\left(\phi_2 + \frac{3}{5\sigma_{\mathrm{t}}}\frac{\partial}{\partial z}\psi_{10}\right) = \frac{2}{3}\left(\psi_{20} + \frac{1}{2}\psi_{22} - \frac{3}{2}\psi_{20} - \frac{1}{4}\psi_{22}\right) = -\frac{1}{3}\psi_{20} + \frac{1}{6}\psi_{22}, \tag{9}$$

which is exactly what we need to write the x-derivative term in Eq. (6c) in terms of ϕ_2. Using this result and solving Eq. (6e) for ψ_{21} makes Eq. (6c):

$$\sigma_{\mathrm{t}}\psi_{11} + \frac{\partial}{\partial x}\left(\frac{1}{3}\psi_{00} + \frac{2}{3}\phi_2\right) = \frac{\partial}{\partial z}\frac{1}{5\sigma_{\mathrm{t}}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial z}\frac{1}{5\sigma_{\mathrm{t}}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial x}\frac{2}{5\sigma_{\mathrm{t}}}\frac{\partial}{\partial z}\psi_{10}. \tag{10}$$

To we will deal with Eq. (6b) we need to write ψ_{20} in terms of ϕ_2 and ψ_{11}. We do this by writing

$$\frac{2}{3}\psi_{20} = \frac{2}{3}\phi_2 - \frac{1}{3}\psi_{22} = \frac{2}{3}\phi_2 + \frac{2}{5\sigma_{\mathrm{t}}}\frac{\partial}{\partial x}\psi_{11},$$

where we have used Eq. (6f) to write ψ_{22} in terms of ψ_{11}. This makes Eq. (6b)

$$\sigma_\mathrm{t}\psi_{10} + \frac{\partial}{\partial z}\left(\frac{1}{3}\psi_{00} + \frac{2}{3}\phi_2\right) = \frac{\partial}{\partial x}\frac{1}{5\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\frac{1}{5\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial z}\frac{2}{5\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{11}, \tag{11}$$

The P_2 equations can now be written in terms of 4 variables that can be interpreted as the SP_2 unknowns:

$$\sigma_\mathrm{a}\phi_0 + \nabla\cdot\vec{\phi}_1 = Q, \tag{12a}$$

$$\sigma_\mathrm{t}\vec{\phi}_1 + \frac{1}{3}\nabla\phi_0 + \frac{2}{3}\nabla\phi_2 = \begin{pmatrix} \frac{\partial}{\partial z}\frac{1}{5\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial z}\frac{1}{5\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial x}\frac{2}{5\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{10} \\ 0 \\ \frac{\partial}{\partial x}\frac{1}{5\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\frac{1}{5\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial z}\frac{2}{5\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{11} \end{pmatrix}, \tag{12b}$$

$$\sigma_\mathrm{t}\phi_2 + \frac{2}{5}\nabla\cdot\vec{\phi}_1 = 0, \tag{12c}$$

where $\phi_0 = \psi_{00}$ and $\vec{\phi}_1 = (\psi_{11}, 0, \psi_{10})^\mathrm{t}$, and $\frac{\partial}{\partial y}\psi_{lm} = 0$. These equations are the SP_2 equations for $x - z$ geometry with extra terms on the right-hand side of the ϕ_1 equations. We can simplify these terms using vector calculus operators. Here we will see the curl operator, an operator not commonly seen in transport theory. Parsing the righthand side of Eq. (12b) yields

$$\frac{1}{5}\begin{pmatrix} \frac{\partial}{\partial z}\frac{1}{\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial z}\frac{1}{\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial x}\frac{2}{\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{10} \\ 0 \\ \frac{\partial}{\partial x}\frac{1}{\sigma_\mathrm{t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\frac{1}{\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial z}\frac{2}{\sigma_\mathrm{t}}\frac{\partial}{\partial x}\psi_{11} \end{pmatrix} = \frac{1}{5\sigma_\mathrm{t}}\begin{pmatrix} \frac{\partial^2}{\partial z^2}\psi_{11} - \frac{\partial^2}{\partial x\partial z}\psi_{10} \\ 0 \\ \frac{\partial^2}{\partial x^2}\psi_{10} - \frac{\partial^2}{\partial x\partial z}\psi_{11} \end{pmatrix}$$
$$- \frac{2}{5}\begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} \end{pmatrix} + \frac{1}{5}\begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\psi_{10}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{10} + \frac{\partial}{\partial z}\psi_{11}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1}. \end{pmatrix} \tag{13}$$

Using the definition of the curl operator we get

$$\begin{pmatrix} \frac{\partial^2}{\partial z^2}\psi_{11} - \frac{\partial^2}{\partial x\partial z}\psi_{10} \\ 0 \\ \frac{\partial^2}{\partial x^2}\psi_{10} - \frac{\partial^2}{\partial x\partial z}\psi_{11} \end{pmatrix} = -\nabla\times\nabla\times\vec{\phi}_1. \tag{14}$$

We can also make the simplification:

$$-2\begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} \end{pmatrix} + \begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\psi_{10}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{10} + \frac{\partial}{\partial z}\psi_{11}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1}. \end{pmatrix} = -(\nabla\times\vec{\phi}_1)\times\nabla\sigma_\mathrm{t}^{-1} + 2\begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} - \left(\frac{\partial}{\partial z}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1} - \left(\frac{\partial}{\partial x}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} \end{pmatrix} \tag{15}$$

Putting this all together gives the P_2 equivalent SP_2 equations:

$$\sigma_\mathrm{a}\phi_0 + \nabla\cdot\vec{\phi}_1 = Q, \tag{16a}$$

$$\sigma_\mathrm{t}\vec{\phi}_1 + \frac{1}{3}\nabla\phi_0 + \frac{2}{3}\nabla\phi_2 = -\frac{1}{5\sigma_\mathrm{t}}\nabla\times\nabla\times\vec{\phi}_1 - \frac{1}{5}\left(\nabla\times\vec{\phi}_1\right)\times\nabla\sigma_\mathrm{t}^{-1} + \frac{2}{5}\begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} - \left(\frac{\partial}{\partial z}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_\mathrm{t}^{-1} - \left(\frac{\partial}{\partial x}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_\mathrm{t}^{-1} \end{pmatrix}, \tag{16b}$$

$$\sigma_\mathrm{t}\phi_2 + \frac{2}{5}\nabla\cdot\vec{\phi}_1 = 0. \tag{16c}$$

It is entirely possible that the last term in Eq. (16b) can be simplified using some other operators, but this simplification has to date escaped this author.

Properties of the P_2 Equivalent SP$_2$ equations

When σ_t is constant the $\vec{\phi}_1$ equation becomes

$$\sigma_\mathrm{t}\vec{\phi}_1 + \frac{1}{3}\nabla\phi_0 + \frac{2}{3}\nabla\phi_2 = -\frac{1}{5\sigma_\mathrm{t}}\nabla\times\nabla\times\vec{\phi}_1, \tag{17}$$

which when we apply the divergence operator $(\nabla\cdot)$ becomes

$$\nabla\cdot\vec{\phi}_1 = -\frac{1}{3\sigma_\mathrm{t}}\nabla^2\phi_0 - \frac{2}{3\sigma_\mathrm{t}}\nabla^2\phi_2, \tag{18}$$

because $\nabla\cdot(\nabla\times\vec{F}) = 0$ for any vector field $\vec{F}$. Substituting Eq. (18) into the equations for ϕ_0 and ϕ_2 gives

$$-\frac{1}{3\sigma_\mathrm{t}}\nabla^2\phi_0 - \frac{2}{3\sigma_\mathrm{t}}\nabla^2\phi_2 + \sigma_\mathrm{a}\phi_0 = Q, \tag{19a}$$

$$-\frac{1}{15\sigma_\mathrm{t}}\nabla^2\phi_0 - \frac{2}{15\sigma_\mathrm{t}}\nabla^2\phi_2 + \sigma_\mathrm{t}\phi_2 = 0. \tag{19b}$$

These are precisely the SP$_2$ equations when σ_t is uniform.

The procedure to derive boundary and interface conditions that we are currently pursuing will take standard P$_2$ conditions and repeat the derivation above to get the proper conditions in terms of ϕ, $\vec{\phi}_1$, and ϕ_2.

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