

P₂-Equivalent form of the SP₂ Equations

Including boundary and interface conditions Ryan G. McClarren Texas A&M University



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SP_n Equations



Not news to anyone here but...

- The SP_n equations are a simplified form of the full spherical harmonics (P_n) equations for the linear transport equation.
 - > The SP_n equations have n+1 angular unknowns in first-order form
 - > The P_n equations have $(n+1)^2$ unknowns
- This large reduction of unknowns comes with a price
 - ➤ The SP_n solution does not necessarily converge to the transport solution as n goes to ∞
 - > As a result there is a order n that gives the optimal solution
 - Another way of saying that: the error between the SP_n solution and the transport solution is lowest for some finite n.

A colloquial rule of thumb: "Where diffusion is ok, SP_n is better. Where diffusion is bad, SP_n is worse."



The SP_n equations were originally derived by Gelbard in 1960 by

- \succ Taking the 1-D P_n equations
- Replacing 1-D spatial derivatives
 - With a gradient in the odd order equations
 - With a divergence in the even order equations
- Interpreting odd order unknowns as vectors and even order unknowns as scalars

Despite this ad hoc "derivation" the SP_n equations have the property that

- > For an infinite medium, the SP_n solution is equivalent to the P_n solution provided that the total cross-section is constant and sources are isotropic
- > This fact has been used to solve some problems to high accuracy.
 - Gelbard used it to compute the leakage from a cylinder by surrounding the cylinder with a pure absorber.

Example: Uniform medium with local sources





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Example: Uniform medium with local sources



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The SP_n equations aren't just some ad hoc equations that happen to be correct in some limits.

The SP_n equations can also be derived via an asymptotic expansion

- One approach does a similar expansion to that used to derive the diffusion limit (Larsen, Morel, and Miller)
 - That is, scattering is large and absorption and sources are small.
 - This explains the rule of thumb expressed earlier
- The other approach expands the dependence of the solution in 2 of 3 spatial directions (Pomraning)
 - This derivation shows that if the transport solution is "locally 1-D" the SPn solution will be accurate.
- Variational derivations also exist for the
 - SP2 equations (Larsen and Tomasevic)
 - > SP3 equations (Larsen and Brantley)



- We know that in a uniform, infinite medium the P_n and SP_n equations give the same scalar flux.
- Therefore, if we think of a heterogeneous materials in a finite problem as a patchwork of uniform media
 - > The only difference between the P_n and SP_n solutions comes down
 - Material interface conditions
 - Boundary conditions

 If we can express the P_n conditions at boundaries and interfaces using SP_n unknowns

- We can derive an SP_n system that is equivalent to the P_n system in the scalar flux solution.
- Of course, this might not be possible.
- At low order, one might have hope because the SP_n and P_n unknowns are the same through first-order
 - > The scalar flux and the current unknowns are the same in both systems.



In a terse ANS transactions paper in 1970, Selengut claimed to have derived a form of the P₃ approximation

- That could be expressed entirely in terms of the SP₃ unknowns in second-order form
- > This approximation included interface conditions.
- > No boundary conditions though.
- The brevity of the derivation makes reproducing the result difficult.
- No numerical results were presented
 - I'm not aware of any attempts to solve these equations.
- Some more recent analysis suggests that the solution used to construct these SP₃ equations might not be the most general solution.

Selengut, D. S. (1970). A new form of the P3 approximation. Trans. Am. Nucl. Soc. 13:625.



This is the entirety of the technical content in Selengut's ANS transactions.

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Transport The

The neutron angular distribution can be written

 $\psi(\mathbf{r}, \Omega) = \left(1 - \frac{1}{\Sigma} \ \Omega \cdot \nabla\right) \psi_0(\mathbf{r}, \Omega) \quad , \qquad (1)$ where the even part satisfies the second-order Boltzmann equation^{2,4}

$$-\Omega \cdot \nabla \frac{1}{\Sigma} \Omega \cdot \nabla \psi_e + \Sigma \psi_e = \frac{1}{4\pi} \Sigma_B \int d\Omega \psi_e + \frac{1}{4\pi} S$$
. (2)

 $\Psi_{e}(\mathbf{r}, \Omega) \simeq \frac{1}{4\pi} \phi(\mathbf{r}) + \frac{15}{8\pi} \sum_{ij} \rho_{ij}(\mathbf{r}) \Omega_{i} \Omega_{j},$ (3)

where ρ_{1j} is a traceless second-rank Cartesian tensor related to the second moment of ψ , and Ω_i is the l'th component of a unit vector along the neutron velocity.

Requiring conservation of the zero'th and second moments of Eq. (2) yields the tensor P3 equations

$$\rho_{ij} = \frac{15}{8\pi} \sum_{klmn} \omega_{ijklmn} D_{kl} \rho_{mn}$$

 $+\frac{1}{4\pi}\sum_{kl}\omega_{ijkl}D_{kl}\phi + \frac{1}{3\Sigma}\delta_{ij}(S - \Sigma_R\phi)$, (4)

where ω_{1jk} , $= \int d\Omega \Omega_1 \Omega_1 \Omega_j \Omega_k$... is a family of isotropic tensors which can be evaluated explicitly and $D_{1j} = (\Sigma)^{-1} \partial_1(\omega_1) (\Sigma)^{-1} \partial_1(\omega_2)$. Contracting Eq. (4) with the operator D_{1j} , and using the trace of Eq. (4), one obtains

 $\frac{3}{35\Sigma^{3}} \nabla^{4} \phi + \frac{11}{21\Sigma} \nabla^{2} (S - \Sigma_{R} \phi) - \frac{1}{3\Sigma} \nabla^{2} \phi = S - \Sigma_{R} \phi , \quad (5)$

the known 4'th-order differential equation for the flux, which holds for both the complete and simplified forms of P₃ theory.

Applying Gauss' theorem to Eq. (2) implies that n. $\Omega(\Sigma)^{-1} \nabla \cdot \Omega \psi_{0}$ must be continuous at interfaces between modif, where n is the unit normal to the surface. This leads to the continuity of

$$\begin{array}{c} \phi \ , \ \sum_{\substack{ij \\ e \in S}} n_i \rho_i j_n \ , \ \ \frac{1}{3\Sigma} \mathbf{n} \cdot \nabla \phi + \sum_{\substack{ij \\ e \in S}} \frac{1}{2} n_i \nabla_j \rho_{ij} \ , \ \\ \frac{1}{3\Sigma} \frac{2}{15\Sigma} \mathbf{n} \cdot \nabla \phi + \frac{1}{2} n_i \nabla_j \rho_{ij} \ , \ \\ \frac{1}{2} \sum_{\substack{i \in S}} \frac{2}{15\Sigma} \mathbf{n} \cdot \nabla \phi + \frac{1}{2} (\mathbf{n} \cdot \nabla) \sum_{\substack{ij \\ e \in S}} n_i \rho_{ijn} \ , \ \\ \end{array}$$

To evaluate these interface conditions in terms of the flux, we can write the solution to Eq. (4) as

$$\rho_{1j} = \delta_{1j} \left[\frac{11}{42\Sigma} \left(S - \Sigma_{R} \phi \right) + \frac{3}{70\Sigma^{2}} \nabla^{2} \phi \right]$$

$$+ D_{11} \left[\frac{2}{4} + \frac{121}{42\Sigma} \left(S - \Sigma_{R} \phi \right) + \frac{33}{70\Sigma^{2}} \nabla^{2} \phi \right]$$

+ $D_{ij}\left[\frac{a}{15}\phi - \frac{aa}{294\Sigma}(S - \Sigma_R\phi) - \frac{aa}{490\Sigma^2}\nabla^2\phi\right]$. (7)

The flux Eq. (5) can now be solved using a coupled diffusion-theory code, after which the angular distribution is given explicitly by Eqs. (1), (3), and (7).

A convenient way to carry this out is to introduce the ''pseudoflux'' θ to obtain

$$-\frac{9}{55\Sigma}\nabla^2\phi-\frac{7}{11}\Sigma\theta+\Sigma_{\bf a}\phi={\bf S}$$

(8)

 $+\frac{9}{28\Sigma}\,\nabla^2\theta-\frac{5}{4}\,\Sigma\theta+\Sigma_R\phi=S$ subject to the continuity at interfaces of

$$\phi$$
, $\frac{1}{\Sigma} \mathbf{n} \cdot \nabla(\phi + \theta)$, $\theta - \frac{1}{\Sigma^2} (\mathbf{n} \mathbf{x} \nabla)^2 \left(\frac{28}{55} \phi + \theta\right)$,
and

$$\frac{1}{\Sigma} \mathbf{n} \cdot \nabla \theta + \frac{1}{\Sigma^2} (\mathbf{n} \mathbf{x} \nabla)^2 \frac{1}{\Sigma} \mathbf{n} \cdot \nabla \left(\frac{2}{3} \phi + \frac{55}{42} \theta \right) . \quad (5)$$

The cross-product terms are missing in the simplified \mathbf{P}_3 approximation; for the case of spherical or cylindrical

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The linear transport equation and SP₂ equations



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

In this situation the SP₂ equations are

$$\begin{aligned} \sigma_{\mathrm{a}}\phi_{0} + \nabla\cdot\vec{\phi}_{1} &= Q, \\ \sigma_{\mathrm{t}}\vec{\phi}_{1} + \frac{1}{3}\nabla\phi_{0} + \frac{2}{3}\nabla\phi_{2} &= 0, \\ \sigma_{\mathrm{t}}\phi_{2} + \frac{2}{5}\nabla\cdot\vec{\phi}_{1} &= 0, \end{aligned}$$



• If we restrict our system to 2-D x-z geometry, the full P2 equations are $\sigma_a \psi_{00} + \frac{\partial}{\partial} \psi_{10} + \frac{\partial}{\partial} \psi_{11} = Q$,

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

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

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

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

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

• The moments are defined as $\psi_{lm} = \int_{4\pi} Y_{lm}(\Omega) \psi(\Omega) \, d\Omega$

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The first step to writing the P2 equations in SP2 form defines

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

Then we add the ψ_{20} equation to one-half times the ψ_{22} equation to get $2 \ \partial \qquad 2 \ \partial$

$$\sigma_{t}\phi_{2} + \frac{2}{5}\frac{\partial}{\partial z}\psi_{10} + \frac{2}{5}\frac{\partial}{\partial x}\psi_{11} = 0,$$

 \clubsuit Upon defining the current to be $\Vec{J}=(\psi_{11},0,\psi_{10})^t$, this equation becomes

$$\sigma_{\rm t}\phi_2 + \nabla \cdot \vec{J} = 0,$$

 \bullet This is exactly the last equation in the SP₂ system.

From the original equations we can add equations to make simplifications

$$\begin{aligned} \sigma_{a}\psi_{00} + \frac{\partial}{\partial z}\psi_{10} + \frac{\partial}{\partial x}\psi_{11} &= Q, \\ \sigma_{t}\psi_{10} + \frac{\partial}{\partial z}\left(\frac{1}{3}\psi_{00} + \frac{2}{3}\psi_{20}\right) + \frac{1}{3}\frac{\partial}{\partial x}\psi_{21} &= 0, \\ \sigma_{t}\psi_{11} + \frac{\partial}{\partial x}\left(\frac{1}{3}\psi_{00} - \frac{1}{3}\psi_{20} + \frac{1}{6}\psi_{22}\right) + \frac{1}{3}\frac{\partial}{\partial z}\psi_{21} &= 0, \\ \sigma_{t}\psi_{20} + \frac{2}{5}\frac{\partial}{\partial z}\psi_{10} - \frac{1}{5}\frac{\partial}{\partial x}\psi_{11} &= 0, \\ \sigma_{t}\psi_{21} + \frac{3}{5}\frac{\partial}{\partial z}\psi_{11} + \frac{3}{5}\frac{\partial}{\partial x}\psi_{10} &= 0, \\ \sigma_{t}\psi_{22} + \frac{6}{5}\frac{\partial}{\partial x}\psi_{11} &= 0. \end{aligned}$$

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•We make the substitutions

$$-\frac{1}{3}\psi_{20} + \frac{1}{6}\psi_{22} = \frac{2}{3}\left(\phi_2 + \frac{3}{5\sigma_t}\frac{\partial}{\partial z}\psi_{10}\right)$$
$$\frac{2}{3}\psi_{20} = \frac{2}{3}\phi_2 - \frac{1}{3}\psi_{22} = \frac{2}{3}\phi_2 + \frac{2}{5\sigma_t}\frac{\partial}{\partial x}\psi_{11},$$

This leads to the equations

$$\begin{aligned} \sigma_{\rm t}\psi_{10} + \frac{\partial}{\partial z}\left(\frac{1}{3}\psi_{00} + \frac{2}{3}\phi_2\right) &= \frac{\partial}{\partial x}\frac{1}{5\sigma_{\rm t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\frac{1}{5\sigma_{\rm t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial z}\frac{2}{5\sigma_{\rm t}}\frac{\partial}{\partial x}\psi_{11},\\ \sigma_{\rm t}\psi_{11} + \frac{\partial}{\partial x}\left(\frac{1}{3}\psi_{00} + \frac{2}{3}\phi_2\right) &= \frac{\partial}{\partial z}\frac{1}{5\sigma_{\rm t}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial z}\frac{1}{5\sigma_{\rm t}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial x}\frac{2}{5\sigma_{\rm t}}\frac{\partial}{\partial z}\psi_{10}. \end{aligned}$$

At this point we have the standard SP2 equations with a strange right-hand side

$$\sigma_{\mathbf{a}}\phi_{0} + \nabla \cdot \vec{\phi_{1}} = Q,$$

$$\sigma_{\mathbf{t}}\vec{\phi_{1}} + \frac{1}{3}\nabla\phi_{0} + \frac{2}{3}\nabla\phi_{2} = \begin{pmatrix} \frac{\partial}{\partial z}\frac{1}{5\sigma_{\mathbf{t}}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial z}\frac{1}{5\sigma_{\mathbf{t}}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial x}\frac{2}{5\sigma_{\mathbf{t}}}\frac{\partial}{\partial z}\psi_{10} \\ 0 \\ \frac{\partial}{\partial x}\frac{1}{5\sigma_{\mathbf{t}}}\frac{\partial}{\partial z}\psi_{11} + \frac{\partial}{\partial x}\frac{1}{5\sigma_{\mathbf{t}}}\frac{\partial}{\partial x}\psi_{10} - \frac{\partial}{\partial z}\frac{2}{5\sigma_{\mathbf{t}}}\frac{\partial}{\partial x}\psi_{11} \end{pmatrix}$$

$$\sigma_{\mathbf{t}}\phi_{2} + \frac{2}{5}\nabla \cdot \vec{\phi_{1}} = 0,$$

with $\phi_0 = \psi_{00}$ and $\vec{J} = (\psi_{11}, 0, \psi_{10})^t$.

The RHS can be rewritten in terms of common vector calculus operators.



• First, we separate the RHS into a piece where σ_t is constant and a piece where σ_t is spatially varying using the product rule

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

• We note that

$$\begin{pmatrix} \frac{\partial^2}{\partial z^2} \psi_{11} - \frac{\partial^2}{\partial x \partial z} \psi_{10} \\ 0 \\ \frac{\partial^2}{\partial x^2} \psi_{10} - \frac{\partial^2}{\partial x \partial z} \psi_{11} \end{pmatrix} = -\nabla \times \nabla \times \vec{\phi_1}.$$

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

$$\begin{aligned} \sigma_{t}\vec{\phi}_{1} + \frac{1}{3}\nabla\phi_{0} + \frac{2}{3}\nabla\phi_{2} &= -\frac{1}{5\sigma_{t}}\nabla\times\nabla\times\vec{\phi}_{1} - \frac{1}{5}\left(\nabla\times\vec{\phi}_{1}\right)\times\nabla\sigma_{t}^{-1} \\ &+ \frac{2}{5}\begin{pmatrix} \left(\frac{\partial}{\partial z}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_{t}^{-1} - \left(\frac{\partial}{\partial z}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_{t}^{-1} \\ 0 \\ \left(\frac{\partial}{\partial x}\psi_{10}\right)\frac{\partial}{\partial x}\sigma_{t}^{-1} - \left(\frac{\partial}{\partial x}\psi_{11}\right)\frac{\partial}{\partial z}\sigma_{t}^{-1} \end{pmatrix}, \\ \sigma_{t}\phi_{2} + \frac{2}{5}\nabla\cdot\vec{\phi}_{1} = 0. \end{aligned}$$



In the case when the total cross-section is constant, the right hand of the current equation simplifies, but does not go to zero:

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

However, these terms do not influence the scalar flux

Because the divergence of J does not contain them

$$\nabla \cdot \vec{\phi}_1 = -\frac{1}{3\sigma_t} \nabla^2 \phi_0 - \frac{2}{3\sigma_t} \nabla^2 \phi_2,$$

Therefore there are modes in the solution that are in the P2 equations but not the SP2 equations.



The extra terms in the reduced P2 equations, do not influence the scalar flux

- Because the divergence of a curl is zero.
- Equivalently, the null space of the P2 equations is not the same as that of the SP2 equations
- The scalar flux in the SP2 equations is the same as the P2 equations
- The current is not necessarily the same in the two systems.
- Of course, unless boundary/interface conditions introduce these modes
 - > These modes won't be created.
- Yet, if we solve the SP2 equations, w/o the extra terms but with the correct interface/boundary conditions

We would get the same scalar flux as the P2 equations



To get interface conditions we write the P2 equations as a hyperbolic system

$$\left(\mathbf{A}_{x}\frac{\partial}{\partial x} + \mathbf{A}_{z}\frac{\partial}{\partial z} + \sigma_{t}\right)\vec{\psi} = \delta_{l0}\delta_{m0}\left(\sigma_{s}\phi_{0} + Q\right)$$

We can derive interface conditions by hypothesizing an interface in either the x or z directions

- > And then diagonalizing the appropriate Jacobian
- > To find the waves that move in each direction

These interface conditions can then be expressed in terms of the SP2 unknowns.

This approach to obtaining boundary conditions will yield Marktype boundary conditions



The eigenvalues for both the Jacobians are

$$-\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, -\frac{1}{\sqrt{5}}, \frac{1}{\sqrt{5}}, 0, 0$$

- The zero eigenvalues means that there are two waves that do not move for each direction
- These zero-eigenvalues can cause problems in numerical calculations
- These are also a reason why even-over Pn expansions are generally avoided
- From the eigenvectors we get that across an interface in the z direction, the following are continuous $\int_{\Delta} d$

$$\left(\phi + \frac{4}{5}\psi_{20}, \psi_{10}, \psi_{11}, \psi_{21}\right)$$

In the x direction, these are continuous

$$\left(\phi - \frac{1}{5}\psi_{20} + \frac{6}{5}\psi_{22}, \psi_{10}, \psi_{11}, \psi_{21}\right)$$

igoplus It's not clear how to enforce these conditions using just $\,\phi\,$ and $\,\,\,\phi_2$



Using some simple manipulations the P2 equations in 2-D geometry can be written as an SP2 system

With some extra terms that don't influence the scalar flux

- Except through boundary and interface conditions
- These equations demonstrate that even though the scalar flux between the two equations is consistent in a uniform media

> The solution for the current is, in general, different.

What about 3-D?

- I've not had any luck getting a similar manipulation to work in 3-D for the P2 equations
- P3 or higher order?
 - Same story; partially due to the fact that in 2-D P3 has 4 more unknowns than P2