$P_2$-Equivalent form of the $SP_2$ Equations

Including boundary and interface conditions

Ryan G. McClarren
Texas A&M University
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Ryan G. McClarren
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Unindicted co-conspirators
Marvin Adams, Jim Morel, Cory Hauck
SP\textsubscript{n} Equations

◆ Not news to anyone here but…

◆ The SP\textsubscript{n} equations are a simplified form of the full spherical harmonics (P\textsubscript{n}) equations for the linear transport equation.
  ➢ The SP\textsubscript{n} equations have \( n+1 \) angular unknowns in first-order form
  ➢ The P\textsubscript{n} equations have \((n+1)^2\) unknowns

◆ This large reduction of unknowns comes with a price
  ➢ The SP\textsubscript{n} solution does not necessarily converge to the transport solution as \( n \) goes to \( \infty \)
  ➢ As a result there is a order \( n \) that gives the optimal solution
    • Another way of saying that: the error between the SP\textsubscript{n} solution and the transport solution is lowest for some finite \( n \).

◆ A colloquial rule of thumb: “Where diffusion is ok, SP\textsubscript{n} is better. Where diffusion is bad, SP\textsubscript{n} is worse.”
What do the SP\textsubscript{n} equations represent?

◆ The SP\textsubscript{n} equations were originally derived by Gelbard in 1960 by
  ➢ *Taking the 1-D P\textsubscript{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\textsubscript{n} equations have the property that
  ➢ *For an infinite medium, the SP\textsubscript{n} solution is equivalent to the P\textsubscript{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

- (a) $P_1$
- (b) $SP_1$
- (c) $P_5$
- (d) $SP_5$
Example: Uniform medium with local sources

![Graph showing scalar flux along the diagonal of the test problem](image)

For most of the lines the \( P_1 \) solution is obscured by the \( P_7 \) solution. We have found that the maximum pointwise relative difference between the \( P_1 \) and \( P_7 \) solution is about 1%. This is remarkable agreement considering the different numerical methods used and the large differences between the solutions at different \( N \) levels. We did not solve the problem with \( P_7 \) or higher approximations. The principal reason for this is that the problem size becomes intractable for serial computing. For the linear discontinuous Galerkin method with \( N \times \times l \), the \( P_7 \) solution requires \( l \times 10^6 \) unknowns. On the other hand, \( P_7 \) calculations with this many computational cells can be easily accomplished on a laptop computer.

**Conclusions**

We have shown the equivalence of \( P_1 \) and \( P_7 \) in a homogeneous medium. In some sense this is a remarkable fact because \( P_7 \) has so many fewer unknowns than \( P_1 \). Also, given that in a homogeneous medium these two systems give the same scalar flux PDE, the correct boundary and initial conditions should make the \( P_7 \) solution the same as the \( P_1 \) solution for a multimaterial problem.

**References**


[m] Ryan G. McClarren, Thomas M. Evans, Robert B. Lowrie, and Jeremy D. Densmore, Semigimplicit time integration for \( P_1 \) thermal radiative transfer, *J. Comput. Phys.*
What do the $\text{SP}_n$ equations represent?

◆ The $\text{SP}_n$ equations aren’t just some ad hoc equations that happen to be correct in some limits.

◆ The $\text{SP}_n$ 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)
Why look for $P_n$ Equivalvent Forms of $SP_n$

◆ 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 $P_3$ approximation

- *That could be expressed entirely in terms of the $SP_3$ 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 $SP_3$ equations might not be the most general solution.

This is the entirety of the technical content in Selengut’s ANS transactions.
The linear transport equation and SP\textsubscript{2} equations

We’ll begin the derivation of a P\textsubscript{2}-equivalent form of the SP\textsubscript{2} equations with a steady, one-speed transport equation with isotropic scattering

\[
(\Omega \cdot \nabla + \sigma_t) \psi = \frac{1}{4\pi} (\sigma_s \phi + Q)
\]

In this situation the SP\textsubscript{2} equations are

\[
\begin{align*}
\sigma_a \phi_0 + \nabla \cdot \vec{\phi}_1 &= Q, \\
\sigma_t \vec{\phi}_1 + \frac{1}{3} \nabla \phi_0 + \frac{2}{3} \nabla \phi_2 &= 0, \\
\sigma_t \phi_2 + \frac{2}{5} \nabla \cdot \vec{\phi}_1 &= 0,
\end{align*}
\]
The \( P_2 \) Equations in 2-D Cartesian geometry

If we restrict our system to 2-D x-z geometry, the full \( P_2 \) equations are

\[
\sigma_a \psi_{00} + \frac{\partial}{\partial z} \psi_{10} + \frac{\partial}{\partial x} \psi_{11} = Q,
\]

\[
\sigma_t \psi_{10} + \frac{\partial}{\partial z} \left( \frac{1}{3} \psi_{00} + \frac{2}{3} \psi_{20} \right) + \frac{1}{3} \frac{\partial}{\partial x} \psi_{21} = 0,
\]

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

\[
\sigma_t \psi_{20} + \frac{2}{5} \frac{\partial}{\partial z} \psi_{10} - \frac{1}{5} \frac{\partial}{\partial x} \psi_{11} = 0,
\]

\[
\sigma_t \psi_{21} + \frac{3}{5} \frac{\partial}{\partial z} \psi_{11} + \frac{3}{5} \frac{\partial}{\partial x} \psi_{10} = 0,
\]

\[
\sigma_t \psi_{22} + \frac{6}{5} \frac{\partial}{\partial x} \psi_{11} = 0.
\]

The moments are defined as

\[
\psi_{lm} = \int_{4\pi} Y_{lm}(\Omega) \psi(\Omega) \, d\Omega
\]
Simplifying these equations

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

\[ \phi_2 = \psi_{20} + \frac{\psi_{22}}{2} \]

◆ Then we add the \( \psi_{20} \) equation to one-half times the \( \psi_{22} \) equation to get

\[ \sigma_t \phi_2 + \frac{2}{5} \frac{\partial}{\partial z} \psi_{10} + \frac{2}{5} \frac{\partial}{\partial x} \psi_{11} = 0, \]

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

\[ \sigma_t \phi_2 + \nabla \cdot \vec{J} = 0, \]

◆ This is exactly the last equation in the SP\(_2\) system.
The $\psi_{1m}$ equations are not so easily simplified.

From the original equations we can add equations to make simplifications

$$\sigma_a \psi_{00} + \frac{\partial}{\partial z} \psi_{10} + \frac{\partial}{\partial x} \psi_{11} = Q,$$

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

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

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

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

$$\sigma_t \psi_{22} + \frac{6}{5} \frac{\partial}{\partial x} \psi_{11} = 0.$$
The $\psi_{1m}$ equations are not so easily simplified.

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

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

$$\sigma_t \psi_{11} + \frac{\partial}{\partial x} \left( \frac{1}{3} \psi_{00} + \frac{2}{3} \phi_2 \right) = \frac{\partial}{\partial z} \frac{1}{5\sigma_t} \frac{\partial}{\partial z} \psi_{11} + \frac{\partial}{\partial z} \frac{1}{5\sigma_t} \frac{\partial}{\partial x} \psi_{10} - \frac{\partial}{\partial x} \frac{2}{5\sigma_t} \frac{\partial}{\partial z} \psi_{10}.$$
Putting this together leads to the SP2 equations, almost

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

\[
\sigma_t \vec{\phi}_1 + \frac{1}{3} \nabla \phi_0 + \frac{2}{3} \nabla \phi_2 = \begin{aligned}
\sigma_a \phi_0 + \nabla \cdot \vec{\phi}_1 &= Q, \\
\left(\begin{array}{c}
\frac{\partial}{\partial z} \frac{1}{5\sigma_t} \frac{\partial}{\partial z} \psi_{11} + \frac{\partial}{\partial z} \frac{1}{5\sigma_t} \frac{\partial}{\partial x} \psi_{10} - \frac{\partial}{\partial x} \frac{2}{5\sigma_t} \frac{\partial}{\partial z} \psi_{10} \\
\frac{\partial}{\partial x} \frac{1}{5\sigma_t} \frac{\partial}{\partial z} \psi_{11} + \frac{\partial}{\partial x} \frac{1}{5\sigma_t} \frac{\partial}{\partial x} \psi_{10} - \frac{\partial}{\partial z} \frac{2}{5\sigma_t} \frac{\partial}{\partial x} \psi_{11}
\end{array}\right) &= 0,
\end{aligned}
\]

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.
Simplifying the RHS (Yes, that is the curl operator)

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

\[
\frac{1}{5} \left( \frac{\partial}{\partial z} \frac{1}{\sigma_t} \frac{\partial}{\partial z} \psi_{11} + \frac{\partial}{\partial z} \frac{1}{\sigma_t} \frac{\partial}{\partial x} \psi_{10} - \frac{\partial}{\partial x} \frac{2}{\sigma_t} \frac{\partial}{\partial z} \psi_{10} \right) = \frac{1}{5\sigma_t} \left( \frac{\partial^2}{\partial z^2} \psi_{11} - \frac{\partial^2}{\partial x \partial z} \psi_{10} \right)
\]

\[
- \frac{2}{5} \left( \left( \frac{\partial}{\partial z} \psi_{10} \right) \frac{\partial}{\partial x} \sigma_t^{-1} \right) + \frac{1}{5} \left( \left( \frac{\partial}{\partial x} \psi_{11} + \frac{\partial}{\partial x} \psi_{10} \right) \frac{\partial}{\partial z} \sigma_t^{-1} \right)
\]

• We note that

\[
\left( \begin{array}{c}
\frac{\partial^2}{\partial z^2} \psi_{11} - \frac{\partial^2}{\partial x \partial z} \psi_{10} \\
0 \\
\frac{\partial^2}{\partial x^2} \psi_{10} - \frac{\partial^2}{\partial x \partial z} \psi_{11}
\end{array} \right) = -\nabla \times \nabla \times \vec{\phi}_1.
\]
The final SP2 equations are then

\[ \sigma_a \phi_0 + \nabla \cdot \phi_1 = Q, \]

\[ \sigma_t \phi_1 + \frac{1}{3} \nabla \phi_0 + \frac{2}{3} \nabla \phi_2 = -\frac{1}{5\sigma_t} \nabla \times \nabla \times \phi_1 - \frac{1}{5} \left( \nabla \times \phi_1 \right) \times \nabla \sigma_t^{-1} \]

\[ + \frac{2}{5} \left( \begin{array}{c} \left( \frac{\partial}{\partial z} \psi_{11} \right) \frac{\partial}{\partial z} \sigma_t^{-1} - \left( \frac{\partial}{\partial z} \psi_{10} \right) \frac{\partial}{\partial x} \sigma_t^{-1} \\ 0 \\ \left( \frac{\partial}{\partial x} \psi_{10} \right) \frac{\partial}{\partial x} \sigma_t^{-1} - \left( \frac{\partial}{\partial x} \psi_{11} \right) \frac{\partial}{\partial z} \sigma_t^{-1} \end{array} \right), \]

\[ \sigma_t \phi_2 + \frac{2}{5} \nabla \cdot \phi_1 = 0. \]
The SP2 equations with constant cross-section

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

\[
\sigma_t \vec{\phi}_1 + \frac{1}{3} \nabla \phi_0 + \frac{2}{3} \nabla \phi_2 = -\frac{1}{5\sigma_t} \nabla \times \nabla \times \vec{\phi}_1,
\]

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 Differences between the SP2 equations and the P2 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
Deriving material interface conditions

- To get interface conditions we write the P2 equations as a hyperbolic system
  \[
  \left( A_x \frac{\partial}{\partial x} + A_z \frac{\partial}{\partial z} + \sigma_t \right) \vec{\psi} = \delta_{l0} \delta_{m0} (\sigma_s \phi_0 + \mathcal{Q})
  \]

- 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 Mark-type boundary conditions
The eigenvalues for both the Jacobians are

\[
\left( -\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, -\frac{1}{\sqrt{5}}, \frac{1}{\sqrt{5}}, 0, 0 \right)
\]

- The zero eigenvalues mean 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 \( P_n \) expansions are generally avoided

From the eigenvectors we get that across an interface in the \( z \) direction, the following are continuous

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

In the \( x \) direction, these are continuous

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

It’s not clear how to enforce these conditions using just \( \phi \) and \( \phi_2 \).
Summary

◆ 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