The Generalized SP_3 equations: Study of numerical solutions

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The SP_3 unanswered questions

The physical meaning of the SP_3 equations:

- When Gelbard first proposed the theory he formulated it for the convenience of having even scalar fluxes (ϕ_0, ϕ_2).
- The use of SP_3 became popular due to its general improvement of diffusion results and its implementation simplicity.
- However, there is not a real understanding of what these equations mean.
- It is clear that for n=2 ϕ_2 should be a tensor of 5 components and not a scalar.
- Then, *what are the SP_3 equations actually representing*?

The boundary conditions:

- The first derivation of the SP_3 equations was for an infinite homogeneous medium with isotropic distributed sources for which SP_3 and P_3 are equivalent.
- However when applying the SP_3 equations to finite problems users have traditionally applied 1D boundary conditions to the problem subdomains.
- Since the physical meaning of the theory is unknown, *is it appropriate to employ these boundary conditions*?

Dr. Chao's work:

- Dr. Chao carried out a work to answer these questions that resulted in the formulation of the Generalized SP_3 equations.

The physical meaning

- To solve the first question the Davison's P_3 equations formulation is employed.
  - This formulation uses solid harmonics instead of the traditional "surface" harmonics.
  - The P_3 equations have the following form:

$$\Psi_3\;\mathbf{U},r\;=-\frac{5}{7\Sigma_t}\mathbf{U}\cdot\nabla\Psi_2\;\mathbf{U},r\;-\frac{3}{7}U^2\Psi_1\;\mathbf{U},r\;-\frac{1}{7\Sigma_t}U^2\mathbf{U}\cdot\nabla\phi_0$$

$$\left[1-\frac{1}{7\Sigma_t^2}\nabla^2\right]\Psi_2\;\mathbf{U},r\;=-\frac{6}{7\Sigma_t}\mathbf{U}\cdot\nabla\Psi_1\;\mathbf{U},r\;-\frac{1}{7}\left[\frac{3}{5\Sigma_t^2}\;\mathbf{U},r\;^2-\frac{1}{5\Sigma_t^2}U^2\nabla^2+2U^2\right]\phi_0\;r\;+\frac{2}{7\Sigma_t}U^2Q\;r$$

$$\left[1-\frac{3}{7\Sigma_t^2}\nabla^2\right]\Psi_1\;\mathbf{U},r\;=\frac{3}{7\Sigma_t}\mathbf{U}\cdot\nabla\left[\frac{1}{5\Sigma_t^2}\nabla^2-1\right]\phi_0\;r\;+\frac{2}{21\Sigma_t^2}\mathbf{U}\cdot\nabla Q\;r$$

$$\boxed{\left[\frac{9}{\Sigma_t^4}\nabla^4-\frac{90}{\Sigma_t^2}\nabla^2+105\right]\phi_0\;r\;=5\left[21-\frac{11}{\Sigma_t^2}\nabla^2\right]\frac{Q\;r}{\Sigma_t}}$$

- From the SP_3 equations:

$$-\frac{1}{3\Sigma_t}\nabla^2\phi_0-\frac{2}{3\Sigma_t}\nabla^2\phi_2+\Sigma_t\phi_0=Q$$

$$-\frac{2}{15\Sigma_t}\nabla^2\phi_0-\frac{11}{21\Sigma_t}\nabla^2\phi_2+\Sigma_t\phi_2=0 \longrightarrow \phi_2=\frac{1}{14}\left[-\frac{9}{5\Sigma_t^2}\nabla^2\phi_0+11\phi_0-11\frac{Q}{\Sigma_t}\right]$$

- Conclusion:
  - The SP_3 equations are a reformulation of the 0th order P_3 equation.
  - With the solution of ϕ_0 the other flux components (Ψ_1, Ψ_2 and Ψ_3) can be obtained.
  - This "only" a particular solution of the angular flux.

The boundary conditions

- Consequences of the physical meaning for the boundary conditions:
  - Since the solution of the SP_3 equations is the particular angular flux, the condition to be fulfilled at the boundary of the subdomain is precisely the continuity of this particular angular flux.
  - This is the condition even if only the value of ϕ_0 is desired.

- But what is the form of these conditions:
  - Employing the Davison's formulation to obtain the new boundary conditions is cumbersome.
  - As an alternative Chao proposes the use of the variational derivation of the SP_3 equations to define the new set of conditions.

- The new boundary conditions:
  - The derivation is somehow lengthy therefore we will skip it here.
  - The final form of the conditions are:

$$\left.\begin{aligned}
\Phi_0(r) &= \frac{1}{4}\phi_0 + \frac{5}{16}\left[\phi_2 - G_\phi \frac{3}{2}\frac{\partial^2}{\partial y^2}\left(\frac{2}{15\Sigma_t^2}\phi_0 + \frac{11}{21\Sigma_t^2}\phi_2\right)\right] \\
\Phi_2(r) &= \frac{1}{16}\phi_0 + \frac{5}{16}\left[\phi_2 - G_\phi \frac{3}{2}\frac{\partial^2}{\partial y^2}\left(\frac{2}{15\Sigma_t^2}\phi_0 + \frac{11}{21\Sigma_t^2}\phi_2\right)\right] \\
J_0(r) &= -\frac{1}{3\Sigma_t}\frac{\partial}{\partial x}\phi_0 - \frac{2}{3\Sigma_t}\frac{\partial}{\partial x}\phi_2 \\
J_2(r) &= -\frac{2}{15\Sigma_t}\frac{\partial}{\partial x}\phi_0 - \frac{4}{15\Sigma_t}\frac{\partial}{\partial x}\phi_2 - \frac{9}{35\Sigma_t}\left[\frac{\partial}{\partial x}\phi_2 - G_J \frac{5}{2}\frac{\partial}{\partial x}\frac{\partial^2}{\partial y^2}\left(\frac{2}{15\Sigma_t^2}\phi_0 + \frac{11}{21\Sigma_t^2}\phi_2\right)\right]
\end{aligned}\right]$$

- If G_ϕ and G_J are set 0 the equations are equivalent to the traditional BC.
- If they are 'switch on', then ϕ_2 is not continuous anymore.
- In this case the 'corrected' ϕ_2 is the continuous one.

A 2D numerical solution

- To prove the validity and potential of the new boundary conditions a 2D nodal solution is proposed.
  - More specifically, the 2D Source Expansion Nodal Method is employed.
  - To begin with the SP_3 equations need to be decoupled (i.e. similarity transformation) resulting in two non-homogeneous Helmholtz equations.

$$\nabla^2\tilde{\phi} - k^2\tilde{\phi} = \tilde{Q}$$

  - The flux solution consists of a homogeneous and a particular component.

$$\tilde{\phi}\ \ x,y\ \ = \tilde{\phi}_h\ \ x,y\ \ + \tilde{\phi}_p\ \ x,y$$

  - The particular part is expanded in Legendre Polynomials whose coefficients are obtained from the right hand side (the source here) which is also expanded in Legendre Polynomials.

$$\tilde{\phi}_p\ \ x,y\ \ = \sum_{\substack{i=0\\ i+j}}^{2}\sum_{\substack{j=0\\ \leq 2}}^{2} p_{i,j} P_i\left(\frac{2x}{h_x}\right) P_j\left(\frac{2y}{h_y}\right) \longleftrightarrow \tilde{Q}\ \ x,\mathrm{y}\ \ = \sum_{\substack{i=0\\ i+j}}^{2}\sum_{\substack{j=0\\ \leq 2}}^{2} q_{i,j} P_i\left(\frac{2x}{h_x}\right) P_j\left(\frac{2y}{h_y}\right)$$

  - The homogeneous solution is expanded as a sum of hyperbolic functions.
  - In order to incorporate the transverse terms of the boundary conditions the following 8 coefficients form with cross terms is selected:

$$\begin{aligned}\tilde{\phi}_h &= a_1\sinh(kx) + a_2\cosh(kx) + a_3\sinh(k\,\mathrm{y}) + a_4\cosh(k\,\mathrm{y})\\ &\quad + a_5\,\mathrm{y}\sinh(kx) + a_6\,\mathrm{y}\cosh(kx) + a_7\,\mathrm{x}\sinh(k\,\mathrm{y}) + a_8\,\mathrm{x}\cosh(k\,\mathrm{y})\end{aligned}$$

A 2D numerical solution

- To obtain the homogeneous flux coefficients the four surface averaged incoming currents are imposed.
- Additionally, four surface averaged projected incoming currents are used.
- Where the surface averaged projected fluxes and currents are defined as:

$$\hat{\phi}_{x^+} = \frac{1}{h_y} \int_{-\frac{h_y}{2}}^{\frac{h_y}{2}} w(y) \phi(\frac{h_x}{2}, y) dy \qquad \hat{J}_{x^+} = -\frac{D_0}{h_y} \int_{-\frac{h_y}{2}}^{\frac{h_y}{2}} w(y) \frac{\partial}{\partial x} \phi(\frac{h_x}{2}, y) dy$$

- And the projection function is the following step function:

$$w(y) = \begin{cases} -1 & \text{for y < 0} \\ 1 & \text{for y} \geq 0 \end{cases}$$

- To obtain the homogeneous part of the incoming currents the particular part needs to be subtracted from the total current:

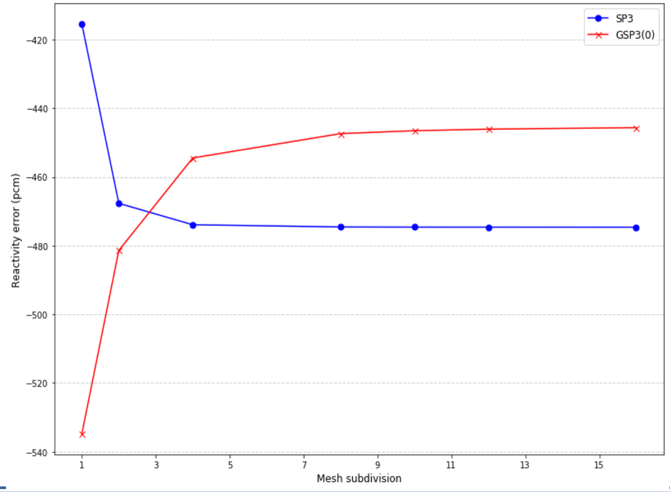
$$J_h^- = J^- - J_p^- \qquad \hat{J}_h^- = \hat{J}^- - \hat{J}_p^-$$

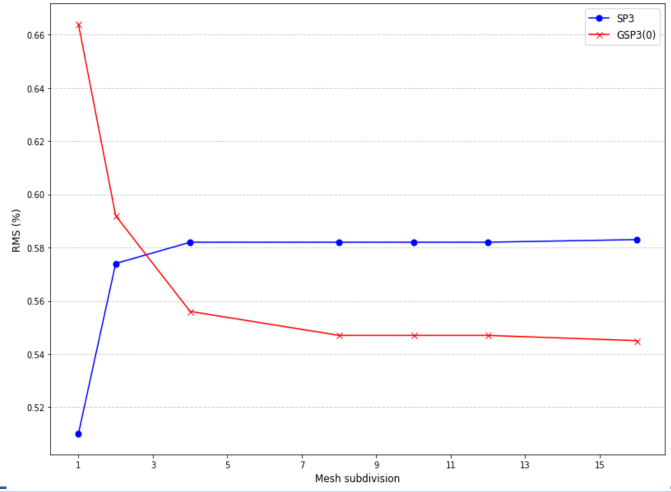
- To update the source coefficients the total flux must be expressed in the same shape as the source:

$$c_{i,j} = \frac{\int_{-1}^{1}\int_{-1}^{1} (\tilde{\phi}_h + \tilde{\phi}_p) P_i\left(\frac{2x}{h_x}\right) P_j\left(\frac{2y}{h_y}\right) dxdy}{\int_{-1}^{1}\int_{-1}^{1} P_i^2\left(\frac{2x}{h_x}\right) P_j^2\left(\frac{2y}{h_y}\right) dxdy} \longrightarrow \tilde{\phi}\ x, y = \sum_{\substack{i=0 \\ i+j}}^{2} \sum_{\substack{j=0 \\ \leq 2}}^{2} c_{i,j} P_i\left(\frac{2x}{h_x}\right) P_j\left(\frac{2y}{h_y}\right)$$

Isolation of the transport error

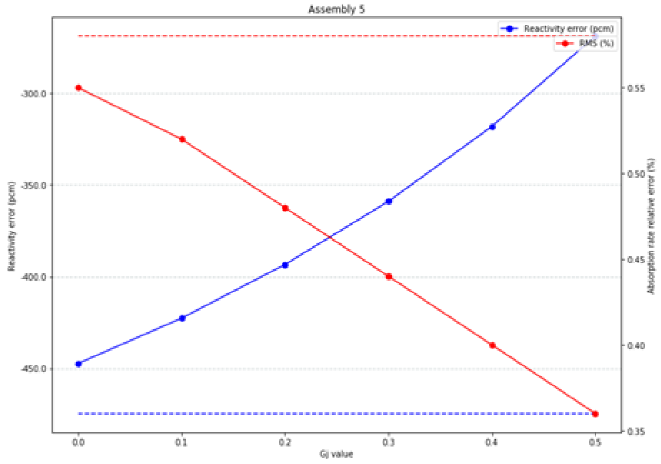
- With the introduction of the new boundary conditions a reduction of the transport error is expected.:
  - The evaluation of the transport error requires the elimination of the other sources of error.
  - The energy collapse and the geometry homogenization errors are removed by employing the same set of group constants for the comparison.
  - For the elimination of the discretization error a sensitivity analysis is carried out to set the minimum mesh per pin that eliminates this error.
  - The reference is set with an MOC calculation with pin homogenized 8 groups group constants obtained with NTRACER with a 32x32 mesh per pin.
- The transverse term in the boundary condition J_2 causes divergence in the calculation.
  - The cause of this instability probably arises from the linearity of the cross terms in the homogeneous flux expansion ($ycosh(kx)$).
  - For now we will set G_J equal to 0.
  - The discretization error will be assessed employing here the assembly 5 of the VERA benchmark (enrichment 2.6 % and 24 burnable absorbers)



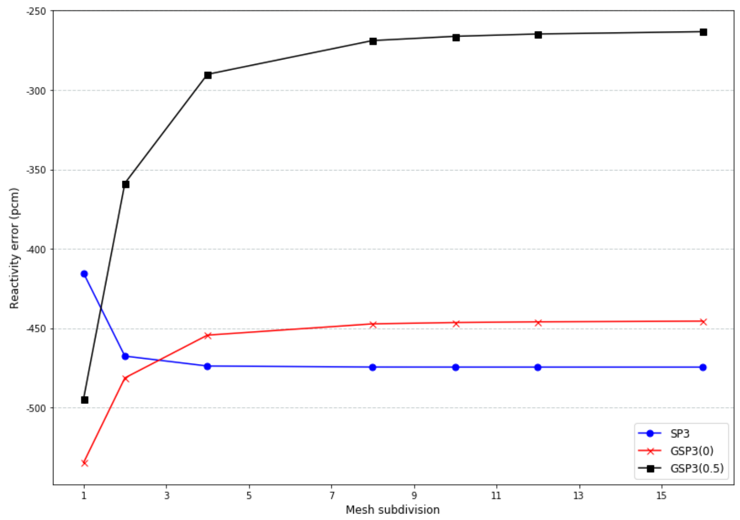


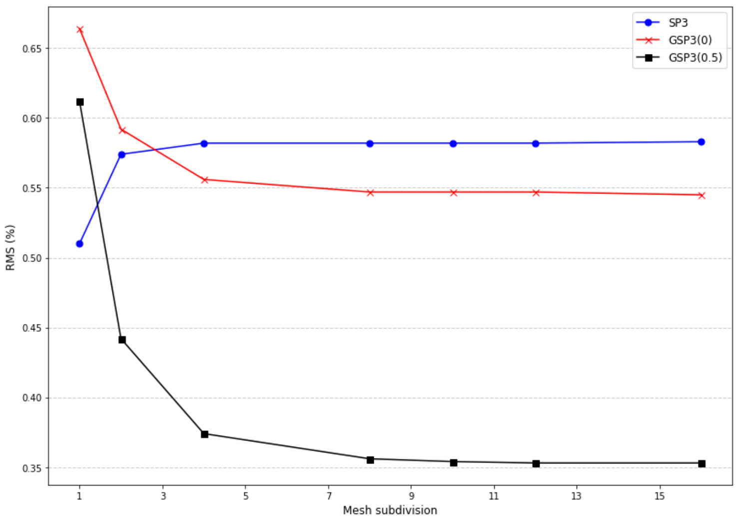
Analysis of the G_J term

- The isolation of the transport error is achieved with a mesh size of at least 4x4 subdivision per pin.
  - However, although the new boundary conditions ($GSP_3(0)$) reduce the error, this reduction is very modest.
  - Therefore, we decided to explore the impact of the G_J term.



- G_J effectively reduces way further the transport error.
  - This being said, the nodal solution proposed only allows a G_J value of 0.5.
  - It seems clear that the introduction of the complete boundary conditions should be achieved if a notable improvement of the results is desired.





Single Assembly calculations

- To generalize this conclusion the rest of the assemblies of the benchmark are calculated.
  - The value of G_J is et to 0.5 for all the calculations.
  - The mesh size is set to 4x4.
  - The new boundary conditions are more effective as the heterogeneity of the problem increases.

Assembly	Enrichment (%)	#Burnable absorbers
1	2.1	0
2	2.6	0
3	2.6	16
4	2.6	20
5	2.6	24
6	3.1	0
7	3.1	8
8	3.1	16
9	3.1	20
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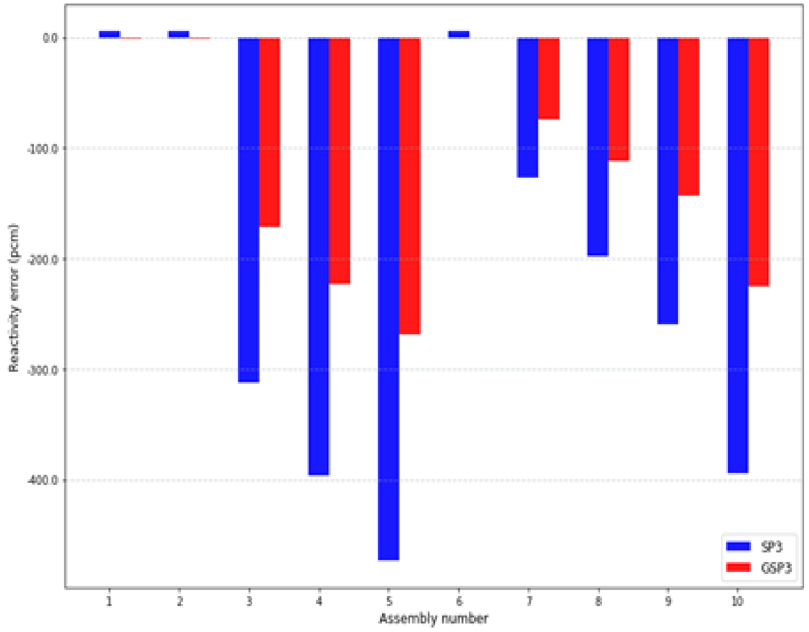
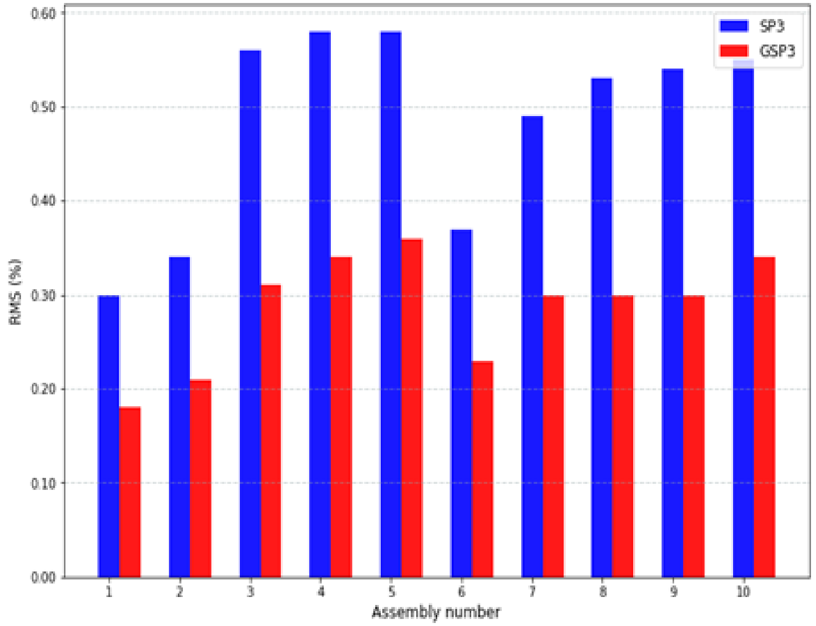
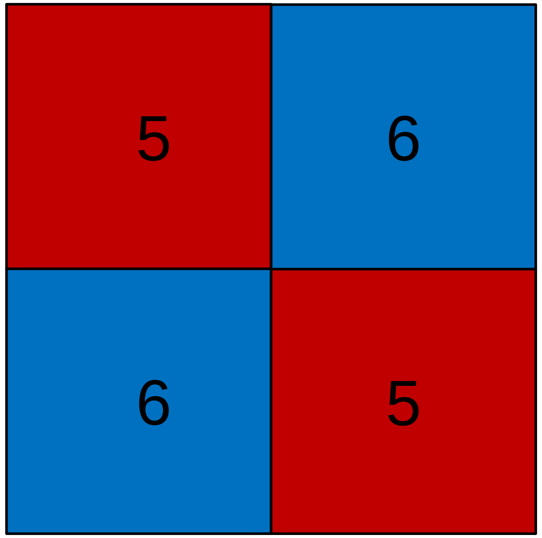


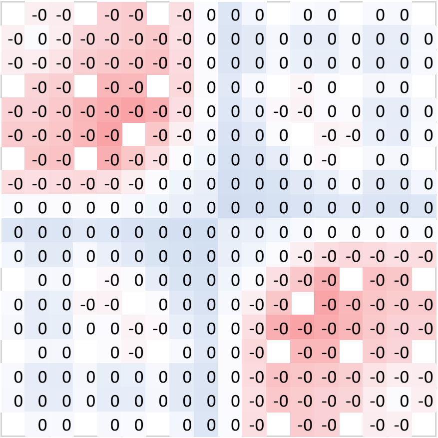


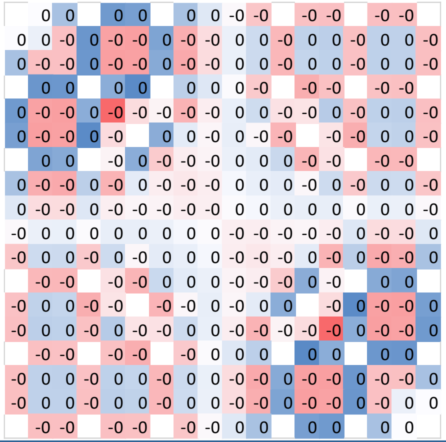
Checkerboard calculation

- To test the equations with a more challenging problem a checkerboard problem is calculated.
  - The assemblies 5 and 6 are selected to introduce a big inter-assembly gradient.
  - The mesh size is set to 4x4.
  - In this case although the reactivity error is again reduced the pin power error worsens.



Core		VERA
Discretization		4x4
Assemblies		5-6
SP3	drho	-182.57
	max	0.10%
	min	-0.23%
	RMS	0.08%
GSP3	drho	-110.31
	max	0.35%
	min	-0.39%
	RMS	0.16%





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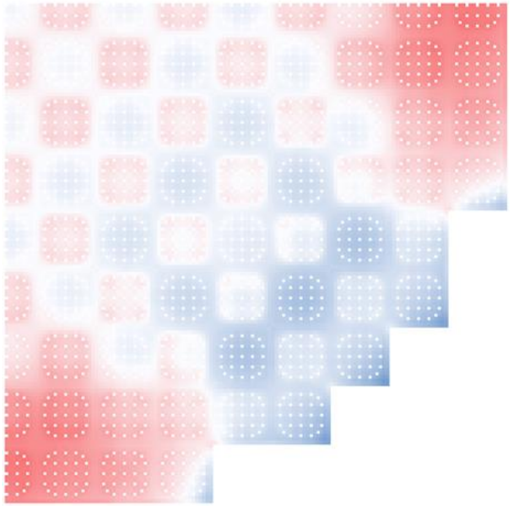
Core calculations

- The analysis is now extended to whole core calculations.
  - The core problems employed are the VERA benchmark problems.
  - The first corresponds to an ARO problem.
  - The second one has the CR bank D inserted (P5).
  - The mesh refinement is 2x2 per pin.

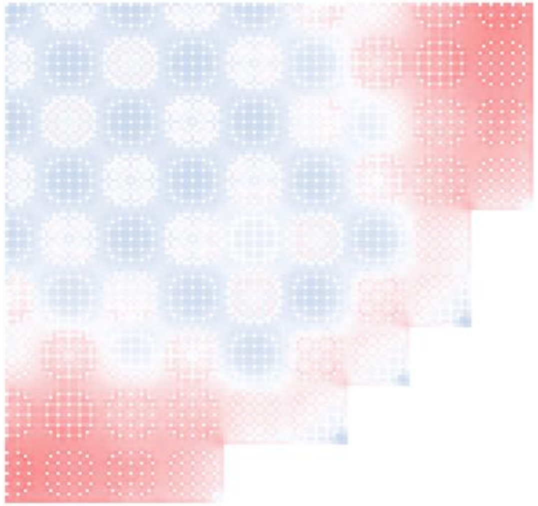
Discretization		2x2	
Control rods		ARO	P5
SP3	$\Delta\rho$ (pcm)	-170.27	-198.24
	Max. (%)	1.26	3.69
	Min (%)	-1.41	-3.96
	RMS (%)	0.48	0.93
GSP3	$\Delta\rho$ (pcm)	-134.03	-158.15
	Max. (%)	0.52	0.95
	Min (%)	-1.27	-2.96
	RMS (%)	0.40	0.42

ARO

SP3



GSP3



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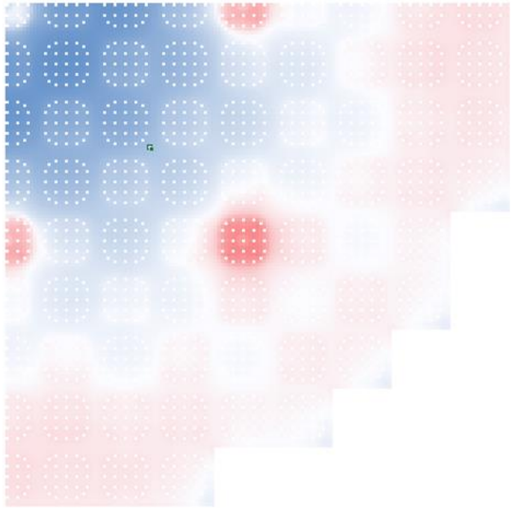
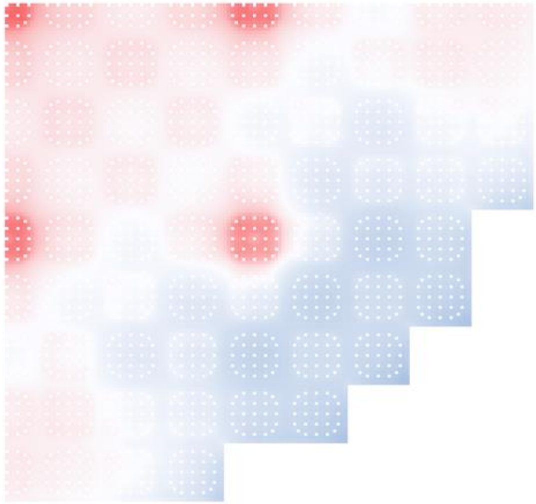
P5

SP3



GSP3



Conclusions

- A first numerical solution is achieved with the application of 2D SENM.
  - However this solution is "incomplete".
  - The rigorous boundary condition for the second moment current is only satisfied for a maximum G_J=0.5.

- The Generalized SP_3 equations reduce effectively the transport error.
  - This reduction, nonetheless, is only notable if G_J is set equal 0.5.
  - Consequently we can conclude that a complete solution of the GSP_3 should be obtained.

- In this regard, other numerical solutions have been attempted.
  - For example 2D SENM with 45º homogenous flux expansion with current continuity or FDM discretization.
  - This being said, the search for better solutions is still ongoing.