Final Report – Improvements in Neutronics/Thermal-Hydraulics Coupling in Two-Phase Flow Systems Using Stochastic-Mixture Transport Models

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Project Summary

In this NEER project, researchers from Oregon State University have investigated the limitations of the treatment of two-phase coolants as a *homogeneous* mixture in neutron transport calculations. Improved methods of calculating the neutron distribution in binary stochastic mixtures have been developed over the past 10-15 years and are readily available in the transport literature. These methods are computationally more expensive than the homogeneous (or atomic mix) models, but can give much more accurate estimates of ensemble average fluxes and reaction rates provided statistical descriptions of the distributions of the two materials are known. A thorough review of the two-phase flow literature has been completed and the relevant mixture distributions have been identified. Using these distributions, we have performed Monte Carlo criticality calculations of fuel assemblies to assess the accuracy of the atomic mix approximation when compared to a resolved treatment of the two-phase coolant. [Appendix A contains a summary of this work accepted for publication to the PHYSOR 2002 conference in Seoul, South Korea.] To understand the benefit of more advanced binary stochastic mixture models, we have also compared Levermore-Pomraning BSM transport calculations to atomic mix and benchmark calculations in mixtures of a material in a near void. These comparisons yield valuable information about both the ensemble average scalar flux and the variance in the scalar flux.

Phase 1 Summary of Objectives and Accomplishments

Phase 1 of the project, performed in the first project year, addressed two objectives: determine the relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes, and compare benchmark and atomic mix simulation results to evaluate the importance of coolant heterogeneity in the neutronic behavior of fuel assemblies. The primary goal of the first year of the project was to develop an understanding of the limitations of atomic mix applied to two-phase steam/water mixtures. The specific tasks and accomplishments associated with each objective are outlined below.

Objective 1: Determine the relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes.

Accomplishments: The thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes have been determined for bubbly, slug, and annular flow regimes.
In the bubbly flow regime, bubbles are in spherical, elliptical or small cap shapes. For simplicity, a spherical bubble shape is a rational approximation that can greatly simplify the mathematical derivations. Since bubbles are highly dispersed in turbulent liquid, bubble size and space distribution are assumed to be independent of each other (experimental data of Wu et al. confirm this claim [1]). A typical distribution function is the upper-limit log-normal distribution function. However, the true distribution function depends on phase change rate, bubble nucleation mechanism, and bubble coalescence/breakage, which rely on the full solution of the two-fluid

thermal-hydraulics model with the addition of interfacial area transport equation. Unfortunately, such a model capability is not available yet. In this study, we shall take two approximate approaches. The first approach is to define an upper-limit log-normal distribution function throughout the bubbly flow regime. Subsequently, the void fraction increase due to vaporization can only boost the total bubble population. This artificial distribution function is effective in validating the proposed higher order Stochastic Mixture Transport Model, without involving the complexity of solving the fully coupled thermal-hydraulics equations. The second approach is to employ a uniform bubble size distribution that allows the mean bubble size to change in the flow direction. In this case, a one-dimensional thermal-hydraulics model can be applied along with the one-group interfacial area transport equation developed by Wu et al. [1]. The spatial variation of the distribution function is independent of the bubble size, but depends on the heating arrangement. For near saturation boiling on nuclear fuel clad surface, bubbles intend to accumulate in the center core region, resulting in a center-peaking void distribution, except in the bubble incipient region where wall-peaking void distribution presents. It can be modeled by $(1-(r/R)^n)$ without loss its generality. In the slug flow regime, bubbles are assumed to be of a lateral size close to the flow channel size. Small bubbles in the wake region are neglected. Therefore, the slug frequency plays a vital role in the analysis. Depending on the overall void fraction $(0.3 < a < 0.8)$, the slug frequency can be readily assigned in the proposed higher order Stochastic Mixture Transport Model. In the annular flow regime, a thin liquid film attaches to the pipe wall and a small amount of liquid is dispersed in the vapor core in the form of droplets. As a approximation, only the liquid film is considered and the film thickness is obtained from void fraction. A more detailed description of the results of this work in this Task is included in our NEER Year 1 Progress Report. [3]

Objective 2: Compare benchmark and atomic mix simulation results evaluate the importance of coolant heterogeneity in the neutronic behavior of fuel assemblies.

Accomplishments: In our proposal we indicated that we would investigate the impact of homogenized vs. spatially resolved two-phase coolant mixtures on neutron energy spectra and multiplication factor (k) in one and two dimensions. We instead approached the problem by modeling computing the multiplication factor in an infinite array of BWR coolant channels using the Monte Carlo neutron transport code MCNP4B. We perform two sets of calculations: "atomic mix", in which cross-sections for the coolant in the flow channel are calculated using an average number density (using the void fraction of the steam/water mixture, independent of the flow regime), and "benchmark", in which the steam/water interface is resolved and the cross sections of each phase are calculated using the density of that phase. In general, many realizations of the statistical distribution of the two-phase mixture must be generated in the benchmark case, and the results averaged over these realizations to compare properly with atomic mix. Figure 1 shows a two-dimensional slice of the geometry of the MCNP simulations, and describes one trend in our calculations: for a given number of vapor bubbles, realizations with bubbles in the narrowest part of the channel have a larger k than realizations containing bubble clusters in the central part of the channel. Figure 2 shows a slice of the MCNP geometry in which each plane of the problem contains eight bubbles, and the bubble size is varied to yield different void fractions. Because we are simulating an infinite lattice of BWR fuel pins, we reduced the enrichment of the fuel to 1% to cause the multiplication factor to be nearer to unity.
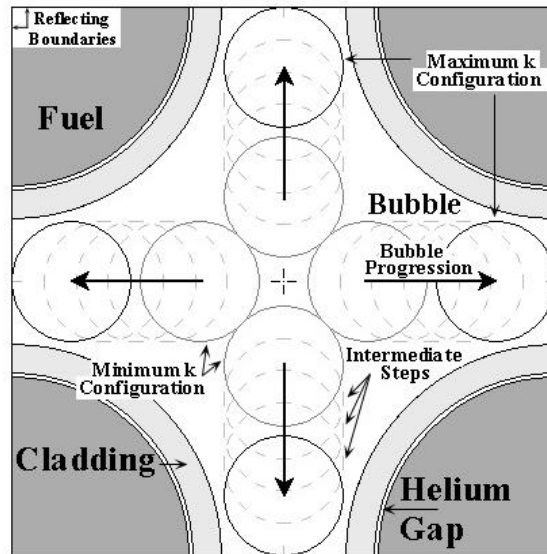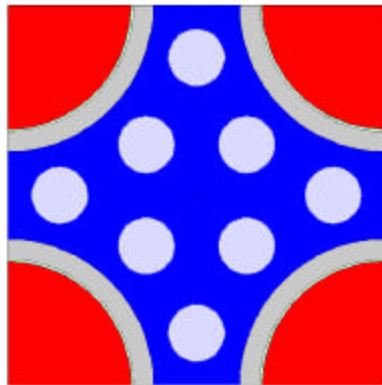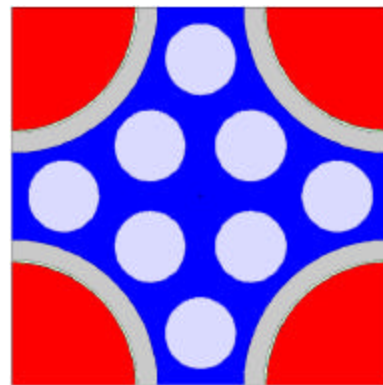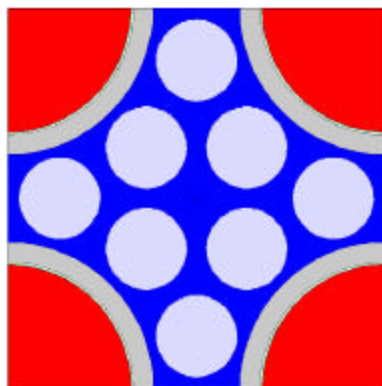
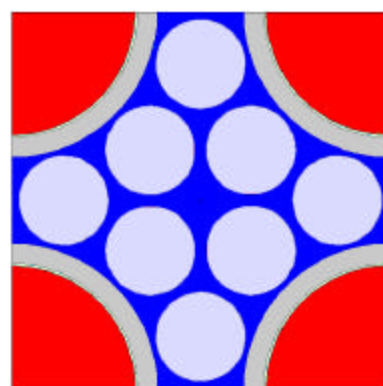Figure 1: MCNP4B model of BWR lattice channel

(a) 10%

(b) 20%

(a) 30%

(b) 40%

Figure 2: Channel geometry with 8 bubbles and various void fractions

The detailed procedure for generating the realizations, and the complete results of these calculations can be found in our Year 1 Progress Report [3]. Our findings are that for void fractions less than 20%, 10^6 neutrons per generation, 25 skipped generations and 100 active generations, the difference in k between the atomic mix and benchmark calculations is less than or equal to the standard error in the MCNP calculation of the atomic mix k – meaning that the atomic mix approximation accurately reproduces the benchmark calculation. In the 45%-35% void range the multiplication factor calculated with resolved fluid-vapor interfaces is markedly different than that calculated by the atomic mix model; the average difference in k for any number of bubbles was $0.74, $0.57, and $0.36 for 45%, 40%, and 35% void fraction, respectively. In the 30%-20% void range the difference between the two models decreases, dropping from an average of $0.25 at 30% to $0.12 at 25%, and then down to an average of only $0.05 at 20% which is lost within the error range of the calculations ($0.085).

The 30% void calculations, augmented by the calculations at other void fractions, show that the moderation properties of a coolant channel with resolved vapor-liquid interfaces are substantially different than that of an atomically mixed channel. The average difference in the calculated multiplication factor was $0.25, which was three times higher than the standard deviation of the calculations. A summary of these results was submitted to the PHYSOR 2002 International Meeting on Reactor Physics in Seoul, South Korea [4]. Although the summary was accepted, the first author declined to submit a full paper to the conference for personal reasons.

Phase 2 Summary of Objectives and Accomplishments

Phase 2 of the project, performed in the second project year, addressed three objectives: develop two deterministic transport codes to perform benchmark (B), atomic mix (AM) and Levermore-Pomraning (LP) transport calculations, compare estimates of ensemble average neutron fluxes from the three approaches, and compare Levermore-Pomraning estimates of the variance in scalar flux to benchmark variances. The primary goal of the second year of the project is to determine if an advanced model for binary stochastic mixture transport is a significant improvement over atomic mix for two-phase coolant mixtures. In these calculations we have focused on neutron transport in the coolant mixture, and we treat it as water mixed with void. Given the density ratio of steam and water, this is a good approximation.

Objective 1: Develop two deterministic transport codes to perform benchmark, atomic mix and Levermore-Pomraning transport calculations.

Accomplishments: Our slab geometry, monoenergetic, fixed source transport codes both utilize the diamond-difference spatial discretization and the discrete ordinates approximation in angle. In our benchmark calculations, we have treated the water and void materials as Markovian (meaning the mean chord lengths in two materials have an exponential distribution) and homogeneous (meaning the distribution of material "chunk" sizes is independent of space). A Markovian distribution has recently been shown to accurately represent the distribution of chord lengths in a background material randomly populated with a second material in the form of fixed-radii disks in 2D or spheres in 3D [5]. The distribution of chords in the disks and spheres are not Markovian, but we use this approximation as a first step. Benchmark (B) calculations are performed by generating realizations of the statistical mixture given mean chord lengths (and corresponding void fractions), solving the transport equation, and then averaging the results over the realizations to compute both the ensemble average scalar flux and the variance in the scalar flux. Atomic mix (AM) calculations are performed by solving the transport equation in a single, homogenized coolant region, where the cross sections are calculated using the void fraction to

calculate the average atom density of the coolant. No information about the variance in the scalar flux is available from AM calculations. Both the benchmark and atomic mix calculations employ diffusion synthetic acceleration to efficiently iterate the transport equation to convergence. The Levermore-Pomraning (LP) binary stochastic mixture model involves two coupled transport equations for the angular flux in each of the two materials. The two equations have the form of a standard transport equation, with the added complexity of terms accounting for the transfer of particles across the interface between the two materials. Our LP code also utilizes an acceleration technique to obtain efficient solutions to these coupled equations, even for problems whose materials have drastically different neutronic properties [6]. To date, we have investigated only physical systems with no interior source, driven on one boundary by an isotropic incident angular flux, but our codes are general enough to handle a variety of boundary conditions and source configurations. In fact, these codes can be leveraged to investigate a variety of interesting binary stochastic mixture transport problems in which the background material is a void – solar radiation in cloudy atmospheres, pebble bed reactors, etc.

Objective 2: Compare estimates of ensemble average neutron fluxes from the B, AM and LP transport calculations.

Accomplishments: We have simulated a wide variety of problems to understand the range of applicability of the AM approximation, and to investigate the potential improvement in accuracy of the LP equations. We present here the results of two representative problems that show the scalar fluxes from all three methods. Figure 3 shows the scalar flux distribution in a 5 cm coolant mixture with a void fraction $[l_2/(l_1 + l_2)]$ of 25% . The scattering ratio in the simulated water is 0.99, and the total cross section is 1.0 cm^{-1}. Both the AM and LP approximate transport methods predict the benchmark results very accurately. This figure also shows the variance in the benchmark calculation of the scalar flux due to the statistical nature of the mixing.
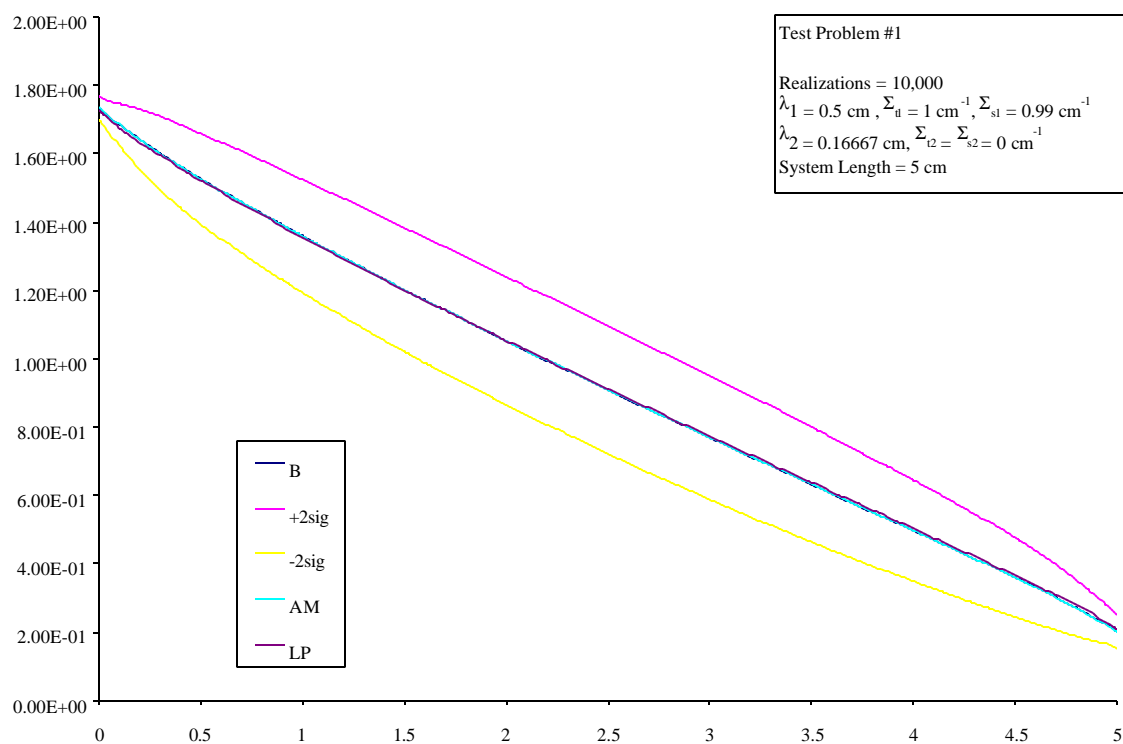
Figure 3: Scalar flux comparison for Test Problem #1

Test Problem #1

Realizations = 10,000
$\lambda_1 = 0.5$ cm , $\Sigma_{t1} = 1$ cm^{-1}, $\Sigma_{s1} = 0.99$ cm^{-1}
$\lambda_2 = 0.16667$ cm, $\Sigma_{t2} = \Sigma_{s2} = 0$ cm^{-1}
System Length = 5 cm
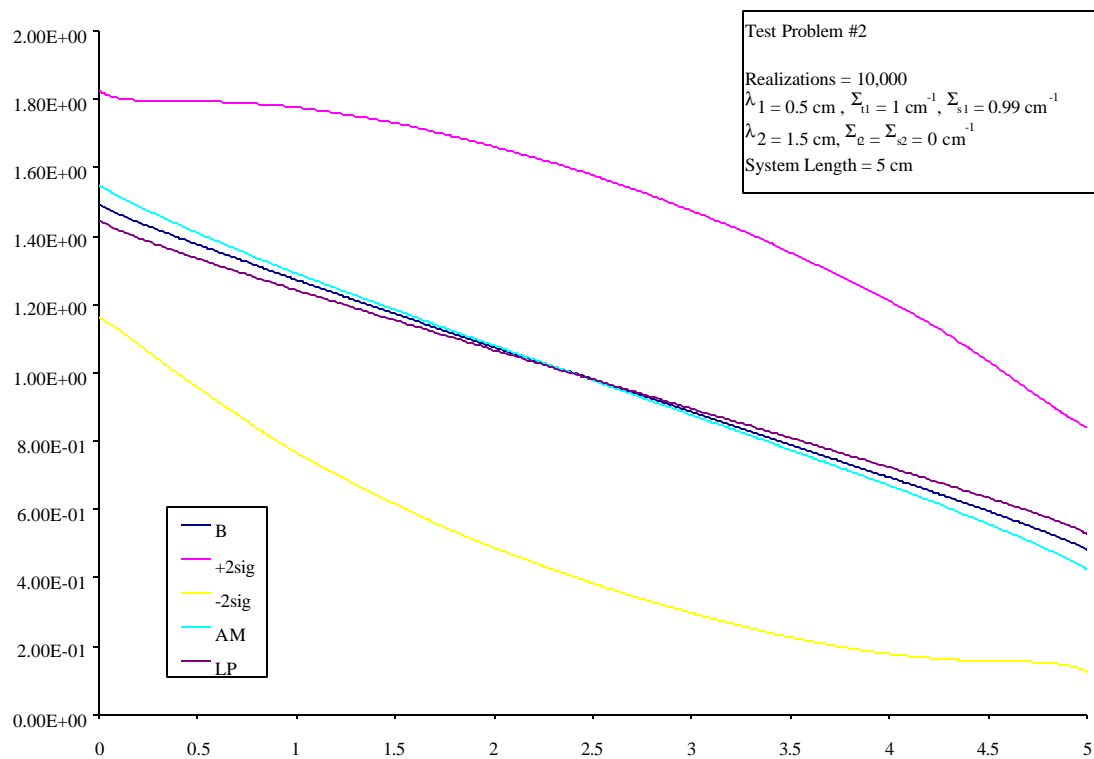
Figure 4: Scalar flux comparison for Test Problem #2

Test Problem #2

Realizations = 10,000
$\lambda_1 = 0.5$ cm , $\Sigma_{t1} = 1$ cm^{-1}, $\Sigma_{s1} = 0.99$ cm^{-1}
$\lambda_2 = 1.5$ cm, $\Sigma_{t2} = \Sigma_{s2} = 0$ cm^{-1}
System Length = 5 cm

Figure 4 shows the scalar flux distribution in a 5 cm coolant mixture where the void fraction is 0.75. Both the AM and LP results differ from the benchmark results on both ends of the slab 3%, though their differences are in opposite directions. Calculations of other problems follow these trends: 1) AM predictions of the scalar flux are most inaccurate when the scattering ratio of the non-void material is in the intermediate range (0.3-0.7); 2) LP predictions of scalar flux more closely match the benchmark solutions unless the non-void material scattering ratios are very near one; 3) in general, discrepancies between the approximate methods and the benchmark calculations are more pronounced as the size of the problem (in mean free paths) increases.

Objective 3: Compare Levermore-Pomraning estimates of the variance in scalar flux to benchmark variances.

Accomplishments:

Larsen [7] has recently developed a coupled set of transport equations that can be used to estimate the variance in the scalar flux in a binary stochastic mixture. The approximation is exact if the true angular flux solution is separable in angle and space. The scalar flux variance is a very important quantity in our evaluation of the LP transport model as a possible improvement over atomic mix. A large variance in the scalar flux signifies that the inherent stochasticity of the problem is so significant that the system being analyzed may not be predictable and/or engineerable. Figures 5 and 6 compare the LP approximation of the variance to that calculated by the benchmark for two test problems presented in the previous section – the first has a void fraction of 0.048 and the second a void fraction of 0.66. In both figures, we see that the benchmark estimate of the relative variance is small (very near zero for small void fraction), whereas the LP estimate starts at zero on the left edge of the problem and increases significantly toward the right edge of the slab. This indicates a serious inaccuracy in the LP approximation for the variance in these water/void problems. In fact, the LP estimate of the variance is substantially incorrect for many problems of practical interest, and will be the subject of future research.
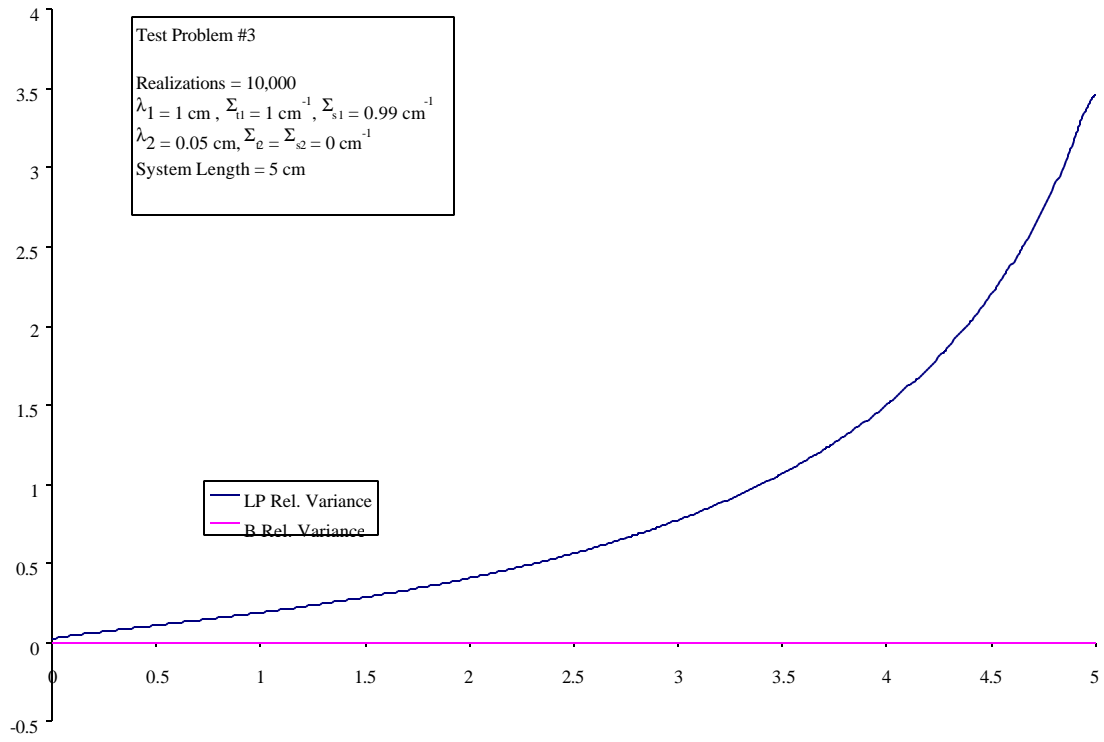
Test Problem #3

Realizations = 10,000
$\lambda_1 = 1$ cm , $\Sigma_{t1} = 1$ cm^{-1}, $\Sigma_{s1} = 0.99$ cm^{-1}
$\lambda_2 = 0.05$ cm, $\Sigma_{t2} = \Sigma_{s2} = 0$ cm^{-1}
System Length = 5 cm

LP Rel. Variance
B Rel. Variance

Figure 5: Relative variance in scalar flux for Test Problem #1

Test Problem #4

Realizations = 10,000
$\lambda_1 = 1$ cm , $\Sigma_{t1} = 1$ cm^{-1}, $\Sigma_{s1} = 0.99$ cm^{-1}
$\lambda_2 = 2$ cm, $\Sigma_{t2} = \Sigma_{s2} = 0$ cm^{-1}
System Length = 5 cm
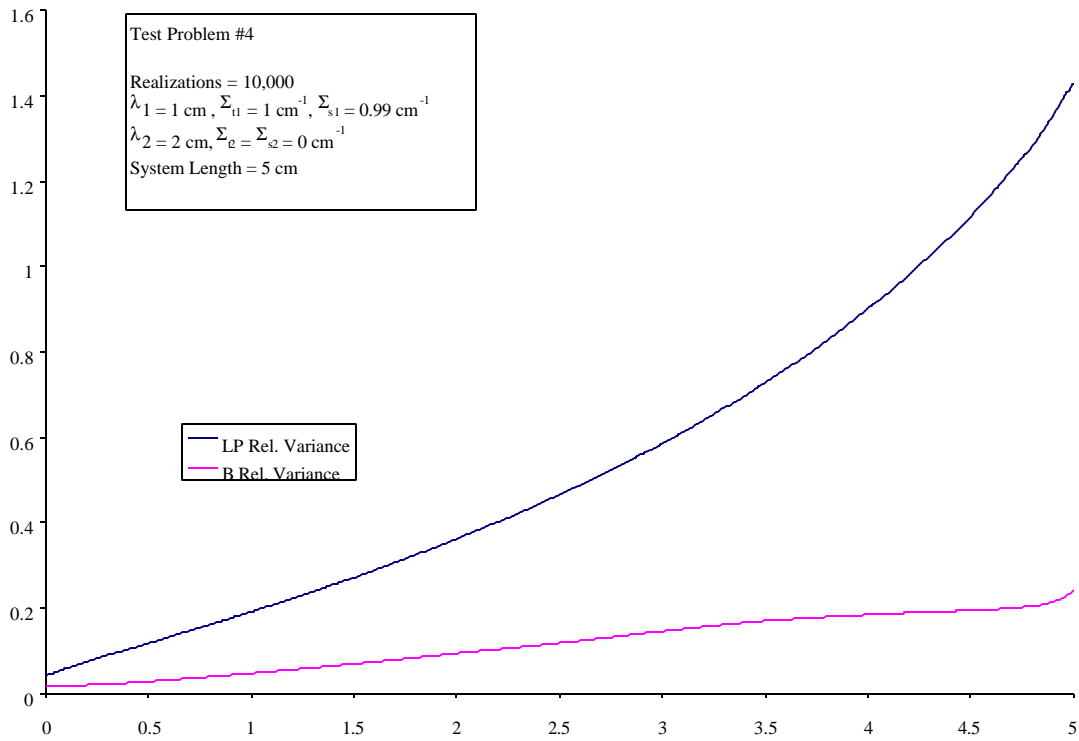
LP Rel. Variance
B Rel. Variance

Figure 6: Relative variance in scalar flux for Test Problem #4

A full conference paper is in preparation containing a complete description of these findings [8] and it will be submitted to PHYSOR 2004 in Chicago, IL.

References

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8. Davis, I., and Palmer, T.S., "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void", in preparation for PHYSOR 2004, Chicago IL.

Presentations

1. Davis, I., and Palmer, T.S., "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void", Presented to CCS-4 at Los Alamos National Laboratory, August 7, 2003.
2. Davis, I., and Palmer, T.S., "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void", Presented to Bettis Laboratory, September 9, 2003.