



# Pseudo-Transient Demonstration with PROTEUS-SN

**Nuclear Engineering Division** 

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# Pseudo-Transient Demonstration with PROTEUS-SN

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#### ABSTRACT

In order to demonstrate multi-physics coupling in nuclear reactor simulations, the PROTEUS-SN (SN2ND) neutronics code is in the process of being coupled to the Nek5000 fluid dynamics solver in order to simulate temperature, density, and power feedback. In the proposed coupling demonstration, a series of calculations will be performed to simulate time-dependent behavior. During each time step, Nek calculates densities and temperature and supplies these values to SN2ND, which then modifies the macroscopic material cross sections required for the neutronics solution. The power solution calculated by SN2ND is based upon the updated material cross sections and provided back to Nek to start the next timestep.

The SN2ND-Nek coupling efforts are currently in progress, and the SN2ND code was used in the meantime to simulate a full core "pseudo" transient using a hypothetical inlet temperature perturbation with no connection to Nek. The steady-state SN2ND calculations were carried out on the ALCF's BG/P machine for several "timesteps" over which the inlet temperature distribution changes according to a pre-determined distribution representing a loss of heat sink and corresponding incomplete coolant mixing in the sodium pool. Initial results indicate the correct physical response. The change in eigenvalue from initial to final state is physically consistent with the sodium density reactivity coefficient for the EBR-II reactor. Additionally, the inlet temperature transient produces a power tilt and asymmetric changes in the flux distribution as expected. The decreased sodium density results in reduced moderation and increased leakage which hardens the spectrum. The changes in flux distribution are small but can be seen clearly when plotting the relative change from the initial condition instead of the absolute value. We expect to repeat this calculation in the coming months using the kinetics version of SN2ND as a comparison point. Additionally, these calculations served as a useful diagnostic for defining a suitable "transient" for future SN2ND-Nek coupled calculations.

### **1. INTRODUCTION**

In order to demonstrate multi-physics coupling in nuclear reactor simulations, the PROTEUS-SN (SN2ND) neutronics code [1-2] is in the process of being coupled to the Nek5000 [3] fluid dynamics solver in order to simulate temperature, density, and power feedback. In the proposed coupling demonstration, a series of calculations will be performed to simulate time-dependent behavior. During each time step, Nek calculates densities and temperatures and supplies these values to SN2ND, which then modifies the macroscopic material cross sections required for the neutronics solution. The power solution calculated by SN2ND is based upon the updated material cross sections and sent back to Nek.

Several geometry models have been defined to demonstrate the coupling, including a 3D full core geometry with EBR-II-like assembly layout. In this geometry, the assemblies are modeled homogenously, except for the XX09 assembly which is explicitly modeled. EBR-II was a small, highly enriched, sodium-cooled fast reactor designed by Argonne National Laboratory with a pool-type design whereby the reactor core is submerged in molten sodium.

Figure 1 shows the core geometry model constructed using the frameworks tools Coregen [4] and MeshKit [4]. The explicitly-modeled assembly XX09 is located inside the ring of blue-colored assemblies.



Figure 1. Region number layout in the full core model with explicit XX09.

Since the PROTEUS-Nek coupling capability was not fully functional at the time of this work, we performed a demonstration feedback simulation using only the PROTEUS-SN neutronics code for the geometry model in Figure 1. Representative temperature and density values were inputted into SN2ND in a series of "pseudo" time-dependent calculations.

### 2. DETERMINATION OF A SUITABLE PSEUDO-TRANSIENT

A transient was originally proposed to change the inlet temperature in the XX09 assembly and determine the effect on core neutronics. In the PROTEUS model, the active core region was divided into 5 axial zones, each of which experiences a rise in temperature over the time period, starting with the region closest to the inlet. A series of steady state SN2ND simulations were performed to simulate time dependence, where the material cross sections were interpolated linearly between the initial state and final state temperatures according to the specified temperature distribution. The sodium density was also modified as a function of temperature for more realistic feedback.

At the initial condition, the inlet sodium is uniform at 600 K and the outlet sodium is uniform at 800 K. A sodium temperature rise of 400 K at each axial region was enforced on the XX09 assembly over a number of timesteps. This temperature rise is quite drastic and corresponds to sodium nearly reaching its boiling point at the outlet of XX09. Figure 2 shows an example power distribution of the EBR-II-XX09 model calculated by PROTEUS at the initial condition. The figure has been graphically clipped such that the radial and axial gradient in the XX09 pin power result can be easily seen.



Figure 2. Initial power distribution (clipped to show explicit XX09 assembly).

In an infinite lattice of assemblies, temperature feedback has a significant impact on the reactivity. However, the full core model for this reactor (with vacuum boundaries) has a significant amount of neutron leakage, and each assembly has only a small reactivity worth. Perturbing the coolant temperature in a single assembly such as XX09 therefore introduces only a small change in the global eigenvalue. Furthermore, the Doppler feedback in EBR-II is known to be small due to the high-enrichment and corresponding lack of U-238 (the main isotope

contributing to Doppler feedback) in nuclear fuel. The Doppler reactivity coefficient for the actual EBR-II reactor was calculated [5] as -30 pcm for an assumed doubling of fuel temperature everywhere in the core and upper plenum. The sodium density reactivity coefficient was calculated as -636 pcm for an assumed 10% decrease everywhere in the core and plenum. These coefficients are nearly negligible when considering a temperature or density change in a single fuel assembly.

Scoping calculations with SN2ND confirmed that the XX09 assembly perturbation yielded essentially no impact on the core eigenvalue (11 pcm change). These results indicate that the original proposed coupling problem is not meaningful, as no significant reactivity or power distribution changes will result from the proposed transient.

The simulation goal was therefore modified to consider a whole core change in the temperature and sodium density (unprotected loss of heat sink). In this case, the core eigenvalue was affected considerably, with most of the effect resulting from the sodium density change. However, changing the inlet temperature everywhere uniformly does not yield a "compelling" picture in neutronics. It was decided that a transient consisting of a stratified and lagged temperature change in the inlet temperature across the core would occur. This type of transient could arise from some lack of complete mixing in the inlet plenum due to multiple inlet paths. As shown in the following results, this transient produces both radial and axial perturbations in the calculation.

#### **3. PSEUDO-TRANSIENT RESULTS**

#### **3.1 Description of the "Pseudo"-Transient**

In order to demonstrate a visible effect, the following pseudo-transient problem was simulated. The reactor's initial condition is a uniform inlet temperature of 600 K. A loss of heat sink is assumed to occur in the sodium pool, which causes a "stratified" temperature increase in the inlet sodium temperature. The red "amoeba" region, depicted in Figure 3, experiences the first rise in inlet temperature. Each time step corresponds to a +5 K increase in inlet temperature, and the axial temperatures also increase by +5 K in a staggered way to simulate flow of sodium up through the active core. The orange region maintains its initial inlet temperature until the red region has risen by +50 K (e.g. 50 K stratification). The yellow and green amoebas are subsequently delayed similarly. The 50 K stratification is somewhat aggressive (unrealistic) but was necessary in order to see a noticeable radial tilt in the core neutronics over time. The maximum temperature reached in any given region is 300 K above the initial condition. Thus, at the end of the calculation, every region is 300 K higher in temperature than the initial condition. These temperatures were passed into SN2ND without using the Nek5000 coupling (i.e. they are contrived rather than computed).



# Figure 3. Core map showing assemblies subject to different inlet temperature conditions ("amoeba" regions).

Because Doppler broadening is negligible in this model, the temperature change in the fuel was ignored. Similarly, temperature effects on sodium microscopic cross sections can be ignored. However, sodium density is strongly dependent on temperature due to its liquid form and thus a density change is important to model. The sodium density in each axial region of each assembly was adjusted to be consistent with the assigned temperature. The +300 K increase in sodium temperature corresponds to an approximately 8% decrease in sodium density. Several scripts were written to automate the generation of SN2ND input files as well as the submission of these jobs on BG/P.

It is very important to note that this is not the EBR-II reactor model, but a vast simplification of it used for initial testing only. The number of fuel assembly types and compositions is significantly reduced from the actual experiment and thus the results (eigenvalues) appearing in the following sections are not representative of EBR-II.

#### 3.1 Angular Convergence Study

A convergence study was performed for the initial condition in order to determine angular cubature requirements. Various combinations of Legendre-Tchebychev cubature were used as this cubature conveniently allows for the number of "x-y" angles and "axial" angles to be varied independently. Table 1 lists the angular cubatures which were tested as well as the resulting eigenvalue. All calculations used the same 33 energy group structure.

	# Angles in 3D	
Cubature	SN2ND	Eigenvalue
L3T5	24	0.93088
L5T7	48	0.93132
L7T7	64	0.93140
L7T11	96	0.93136
L7T15	128	0.93140

#### Table 1. Eigenvalue at initial condition computed using different angular cubatures.

The eigenvalue converges in both Legendre and Tchebychev orders at L7T7, which is 64 angles in the SN2ND 3D formulation. The L7T7 cubature was therefore used for subsequent calculations.

#### **3.2 Transient Effect on Eigenvalue**

The eigenvalue behavior was plotted as a function of the pseudo time step in Figure 4. The eigenvalue drops off throughout the transient as expected from the negative sodium density reactivity coefficient of this problem. There is a total change of -697 pcm in the eigenvalue. This is physically expected given that the EBR-II sodium density coefficient is -636 pcm for 10% decrease in sodium everywhere in the core. This problem undergoes a slightly smaller sodium density change (8% decrease in sodium everywhere in the core) but is not exactly identical to the EBR-II compositions.



Figure 4. Eigenvalue throughout the transient.

Note that the reactor would shut down in this transient due to the negative reactivity insertion. However, one major purpose of this work is to visualize the change in power and flux <u>distributions</u> resulting from the transient. We therefore held the power constant at each time step.

#### **3.3 Transient Effect on Power Distribution**

The pseudo-transient produces a small yet visible tilt in the core power. Figure 5 shows the power distribution in a slice taken 7 cm above the bottom of the active core. The pins in the explicitly-modeled XX09 assembly are clearly visible.



Figure 5. Power distribution at z=7 cm for initial condition.

The induced power change is small ( $\sim \pm 1\%$ ) compared to the range of power in the entire core, so plots of the power at different time steps are not very informative. Instead, the percent change in power is plotted in Figure 6, where the radial power tilt can easily be seen.



Figure 6. Percent change in power at t=50 (left) and final condition (right) at z=7 cm.

The left side of Figure 6 clearly shows the decreased power in the vicinity of the red and orange amoebas, as expected due to the negative reactivity associated with increased sodium temperature in these regions. Physically, the reduction in sodium density reduces down-scattering, and allows fast neutrons to stream out of the core. The power near the transient region (lower right quadrant) at t=50 is clearly reduced due to the increased neutron leakage in this region. The power on the opposite side of the core is forced to increase as an artifact of power normalization (total power in the core was kept constant for each timestep). The symmetric

power distribution is recovered at the final condition (t=104), where all regions are uniformly +300 K from the initial condition.

We also examine the power shift in the heterogeneously modeled XX09 assembly in Figure 7. This figures illustrates the relative power change from the initial condition in various slices of the XX09 assembly, at timesteps 50 and 104 (final condition). We observe that a power shift in the individual XX09 assembly does occur but is very small (at most 0.3% increase).



#### Figure 7. Percent change in power in XX09 at t=50 (left) and final condition (right).

The whole core power distribution returns to a symmetrical radial distribution at the final condition as in Figure 6, but the individual XX09 assembly which is located near the periphery of the active core experiences a permanent power shift due to the transient. This occurs due to the increased leakage from the core which is most prominent in assemblies near the reflector. The power is suppressed in the part of XX09 closest to the core external boundary (lower right pins in the figure). The axial slices in Figure 7 also illustrate the effect of the "staggered" temperature rise in the axial direction as the hot sodium moves up the channels.

#### **3.3 Transient Effect on Group Flux Distributions**

Several short movies were created to show the time evolution behavior of the flux in selected groups. Numerous images were also created but are not as informative as the time-lapse movies. We note again that the power was renormalized to 1.0 at each time step in order to see the change in flux shape over time.

The 33-group flux spectrum for this EBR-II model is shown in Figure 8. The peak of the flux occurs in group 8 (approximately 300-500 keV).



### Figure 8. EBR-II flux spectrum for 33-group structure.

Figure 9 shows the percent change in the group 8 flux (peak flux group in the 33 group structure) at t=20, alongside another image of the power profile in order to show the geometry orientation. The image shows contour lines of percent change in the group flux.



Figure 9. Power profile at initial condition shown to illustrate geometry (left) and contour surfaces showing constant percent change in group 8 flux at t=20.

At time step 20, the sodium temperature in the red amoeba (from Figure 3) has increased by approximately +100 K. The red amoeba is physically located in the front right quadrant of the geometry. The circular ball in the center of Figure 9 (left) is the active core region. The tilting contour lines above and below the active core lie in the upper and lower plenums. Figure 9 demonstrates the radial (and axial) asymmetry introduced in the group 8 flux due to the stratified temperature increase. Again we note that the group 8 flux shows a small increase (about 1-2 percent for this time step) in the red amoeba region due to hardening of the spectrum.

Multiple images were generated to illustrate the flux changes such as that in Figure 9, but we omit these figures for brevity. In general, those figures show the asymmetrical changes physically expected with the introduction of the specified transient. Brief movies showing the time-evolution of the flux are available upon request.

#### **3.4 Computational Requirements**

The simulations in this work were performed on Intrepid (a Blue Gene/P machine) at the Argonne Leadership Computing Facility. As aforementioned, the "pseudo"-transient was simulated via a series of steady-state simulations. Each steady state calculation required approximately 30 minutes of wall-clock time on 4096 nodes (16,384 cores in VN mode). Since 105 timesteps were performed including the initial and final conditions, roughly 885,000 corehours were consumed on BG/P for the entire simulation. Computer time was provided via an ALCC allocation.

#### **4. CONCLUSIONS**

The PROTEUS-SN code was used to simulate a full core "pseudo" transient using a hypothetical inlet temperature perturbation. The steady-state PROTEUS-SN calculations were carried out on the ALCF's BG/P machine for several "timesteps" over which the inlet temperature distribution changes according to a pre-determined distribution. Initial results indicate the correct physical response. The change in eigenvalue from initial to final state is physically consistent with the sodium density reactivity coefficient for the EBR-II reactor. Additionally, the inlet temperature transient produces a power tilt and asymmetric changes in the flux distribution as expected. The decreased sodium density in the high temperature areas results in reduced moderation and increased leakage which hardens the spectrum. The changes in flux distribution are small but can be seen clearly when plotting the relative change from initial condition instead of the absolute value. We expect to repeat this calculation in the coming months using the kinetics version of PROTEUS-SN as a comparison point. Additionally, these calculations served as a useful diagnostic for defining a suitable "transient" for SN2ND-Nek coupled calculations.

#### **5. ACKNOWLEDGMENTS**

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