# nTRACER/ESCOT Initial Coupling and Assessment

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# 1. Introduction

The simulation of the entire core of light water reactors is now possible thanks to the Direct Whole Core Calculation (DWCC) [1] and the enhancements of computing power. To calculate both the thermal feedbacks and the coolant conditions is necessary an integrated simulation of the neutronics and the thermalhydraulics.

The Seoul National University Reactor Physics Laboratory (SNURPL) developed nTRACER [2], a deterministic transport code which employs 2D/1D scheme with planar Methods of Characteristics (MOC) and axial Simplified P<sub>N</sub> implemented within the 3D CMFD framework. The nTRACER code is highly parallelized with a hybrid approach assigning [2] employing axial domain decomposition. Recently, the SNURPL has developed ESCOT, a pin-level nuclear reactor core thermal-hydraulics code [3]. The ESCOT code adopts a four-equation drift-flux model, SIMPLEC algorithm, and fuel conduction model which uses the FRAPCON code empirical models for the solid equations of state [4]. This code is highly parallelized with MPI, employing both axial and radial domain decomposition, and provides an accurate yet fast core T/H solution. Fig. 1 provides the two flowcharts of the nTRACER and the ESCOT codes.



Fig. 1: flowcharts of the nTRACER (*left*) and the ESCOT (*right*) codes.

This paper is to assess the initial sequential coupling between nTRACER and ESCOT. The neutronics-T/H platform will be described inside the first section while the accuracy and performances will be provided in the third section.

#### 2. Development of the nTRACER/ESCOT Coupled Platform

To maximize nTRACER and ESCOT parallel performances, the implementation of a wrapping system was in order since the two codes adopt a different parallelization scheme. The wrapper code (parent process) uses the MPI capability of spawning two children processes and manages the exchange of information between the two codes. Fig. 2 depicts the scheme of this platform.

The optimum number of required MPI processes has to be set equal to the number of axial planes for nTRACER, plus the number of fuel assemblies for ESCOT, plus one more process where the Wrapper code runs. The calculation is started by the Wrapper code which initializes both codes, after that the neutronics calculations is started. After the axial sweep nTRACER sends directly to ESCOT power and burnup. Then ESCOT calculates the T/H variables. The Wrapper receives the  $ho_{cool}, T_{cool}, T_{fuel}$  distributions, adjusts the T/H information according to the neutronics ordering scheme and sends it back to nTRACER. The choice of passing the T/H data to the Wrapper code and not directly to nTRACER is related to future applications of different coupling schemes or acceleration techniques which can be partly found in the Lee J. dissertation [5] and will not treated in this paper.



Fig. 2: nTRACER/ESCOT entire coupled platform.

# 3. Assessment of nTRACER/ESCOT

The and assessment capability of the nTRACER/ESCOT coupled code have been performed by comparing the solutions obtained by nTRACER standalone and the coupled platform nTRACER/ESCOT. The nTRACER code has its own simple internal T/H solver which is for closed channels and involves no pressure drops.

Four reactors have been used for this analysis, a fictitious core obtained by combining assemblies of the YeongGwang Unit 3 core (see Fig. 3), the YeongGwang Unit 3, the APR-1400 and the BEAVRS one. BEAVRS core has been simulated at 75% and 100% of the nominal power. TABLE I provides the main information of the simulated reactors.

This analysis has been carried out using the SNURPL cluster (Soochiro3) which has the following characteristics:

- # of nodes: 27,
- CPU per node: 2 X Intel Xeon E5-2640 v3 (16 cores, 2.8 GHz), and
- Interconnection: Intel Omni-path Infiniband EDR (58Gbps).



Fig. 3: scheme of the fictitious 5x5 core used for the initial assessment of nTRACER/ESCOT.

TABLE I: summary of the four simulated cores.

	Yeong Gwang Unit 3	APR-1400	BEAVRS Cycle 1	Fictitious Core
Abbrev.	YG3	SKN3	BEAVRS	FC
Number of FA	177	241	193	40
Power [MW <sub>th</sub> ]	2,815	3,983	3,410	636
Gd <sub>2</sub> O <sub>3</sub> wt. [%]	4.0	8.0	-	4.0

#### 3.1 Analysis of the Results

The calculations have been carried out targeting the critical boron concentration (CBC), using a quarter core symmetry and applying the Xenon equilibrium model. The conditions for the neutronics calculation options have been set to the default one:

- Ray: 0.05 8 4, and
- pseudo convergence for the fission source:  $1.0 \cdot 10^{-5}$ .

The fictitious core has been simulated also applying 500 ppm and seeking the correspondent eigenvalue for this input condition.

The results of this quarter core analysis is shown inside TABLE II. The maximum eigenvalue difference was encountered when simulating the fictitious core and the boron concentration was applied (27 pcms). For the other cases, the critical k-eff never exceeded 2 pcm and the correspondent CBC has never been bigger than 2.5 ppm. The 2D axially integrated power root mean square difference (RMS) had values below 0.20% while the maximum (MAX) was found to be equal to 0.74%.

TABLE II: summary of the quarter core analysis
performed for the assessment of the coupled platform
nTRACER/ESCOT.

	k-eff diff ( <i>pcm</i> )		CBC (ppm)		2D power Difference [%]	
	Simple	ESCOT	Simple	ESCOT	RMS	MAX
FC (500 ppm)	1.00046	1.00073 (27)	500*	500*	0.14	0.46
FC	1.00002	1.00003 (1)	503.28	505.29 (2.1)	0.14	0.45
YG3	1.00000	0.99999 (1)	751.25	753.6 (2.35)	0.19	0.52
SKN3	1.00000	1.00000 (0)	819.86	822.13 (2.27)	0.20	0.74
BEAVRS 75%	1.00001	1.00000 (-1)	671.11	672.35 (1.24)	0.08	0.30
BEAVRS 100%	1.00002	1.00000 (-2)	630.92	632.61 (1.69)	0.12	0.44

The 2D axially integrated power obtained by nTRACER/ESCOT is shown inside Fig. 4 (*top*) together with the difference against the power calculated with nTRACER standalone (*bottom*). The maximum differences are located at the boundary of each assembly; in those positions ESCOT provides a better approximation of cross flow and mixing which increase the power difference against the standalone solution. Similar results have been obtained with the YG3 core calculations as Fig. 5 depicts.



Fig. 4: SKN3 2D axially integrated power obtained by nTRACER/ESCOT (top) and difference against the one obtained with nTRACER standalone (bottom).



Fig. 5: YG3 2D axially integrated power obtained by nTRACER/ESCOT (top) and difference against the one obtained with nTRACER standalone (bottom).

# 3.2 Analysis of the Performances

Each simulated calculation has been performed using both codes at their maximum parallel performances: nTRACER has assigned one plane per MPI process while ESCOT used one MPI process per assembly. For example, for the APR-1400 case the 20 nodes of the cluster were distributed as follows:

- nTRACER used 30 MPI processes, each of them used 8 OpenMP threads, while
- ESCOT used 69 MPI processes for its calculation.

The summary of the performance analysis is given TABLE III. The maximum difference inside encountered was of about 6 minutes for the calculation at 75% of the BEAVRS cycle 1 core. It is important to notice that nTRACER/ESCOT number of neutronics-T/H iterations have always been smaller or equal than the one of nTRACER standalone. For example, the fictitious core calculations in boron search mode has a similar calculation times for the two simulations, the reason why those two values are similar can be explained by the fact that nTRACER standalone performed two fix point iterations (FPI) more.

Fig. 6 shows the average time per FPI. Adding a higher fidelity T/H solver cost per iteration about a minute.



	Wall Ti Tot	me (min) / TH	Number of Fix Point Iterations		
	Simple	ESCOT	Simple	ESCOT	
FC (500 ppm)	17/<0.1	21 / 5	9	8	
FC	19/<0.1	20 / 5	10	8	
YG3	60 / 0.3	63 / 9	9	8	
SKN3	50 / 0.3	53 / 3	6	6	
BEAVRS 75%	53 / 0.2	59 / 7	7	7	
BEAVRS	69 / 0.3	70 / 10	9	8	

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Average Time per Fix Point Iteration



Fig. 6: average time to perform a complete neutronics-T/H iterations for each simulated case.

# 4. Summary and Conclusions

nTRACER and ESCOT, the two whole core high fidelity codes developed by the SNURPL, have been successfully coupled for steady-state neutronics-T/H analyses.

The two codes adopt different parallelization schemes. Therefore, the implementation of a wrapper system which allowed the two codes of running at their higher performances have been in order. The wrapper system uses the MPI capability of spawning two children processes and manages the exchange of information between the two codes.

The scope of this work can be found in the fact that ESCOT provides a more accurate prediction of cross-flow, mixing effects, spacer-grid effects, fuel temperature and possible presence of local void fraction is necessary when simulating a full core of nuclear reactor ensuring a higher fidelity in contrast to the simple internal T/H solver which was initially implemented inside nTRACER.

The new platform has then been assessed using reactor core calculations: one fictitious core designed using some of the YG3 fuel assemblies, the YG3, the APR-1400 and the BEAVRS cycle 1 (simulated both at 75% and 100% of the nominal power).

The maximum encountered eigenvalue difference was 27 pcms while the critical boron concentration differences never exceeded 2.5 ppm. Moreover, the 2D axially integrated power RMS difference had values below 0.20% while the MAX was found to be equal to 0.74%.

It turned out that the maximum differences are located at the edges of each assembly; in those positions in fact, ESCOT gives a better approximation of cross flow and mixing which increase the power difference against the standalone solution.

The coupled platform has also good performances; a coupled calculation nTRACER/ESCOT has usually comparable solution time with the standalone one.

# 5. Future Plans

The use of a sequential coupling and a wrapper code implies that one of the two codes has to be in stand-by while the other code is completing its own calculation. To avoid this stand-by phase, the SNURPL is now investigating the benefits of using a simultaneous (tandem) solution of coupled problems. In this case the two codes run separately and exchange the necessary information online. This topic will be part of a future publication.

Moreover, nTRACER/ESCOT per single fix point iteration costs on average one minute more than nTRACER standalone as it was suggested at the end of the performance analysis section. Therefore, if the number of Picard iterations could be reduced down the time-gap between nTRACER standalone and nTRACER/ESCOT could be furthermore decreased. Currently, the application of the Anderson Acceleration [6] for this kind of steady-state neutronics-T/H problems is under deep study. This method approximates the solution of the  $(k+1)^{th}$  iteration as a linear combination of the solution history g. The coefficients, which determine the  $x^{(k+1)}$ , are calculated by minimizing the square norm of the residual vectors f. An initial assessment of the benefits obtainable from the application of this technique can be found here [7], for the coupling platform nTER/ESCOT.

Finally, the SNURPL is converting and adapting its codes to the GPU architecture [8], [9]. Therefore, the steady-state coupling for GPU architecture is in order.

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