A Direct Coupling between RFSP and CATHENA Using PVM

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Abstract

An increasing number of safety analyses are being performed with coupled neutronic and thermalhydraulic calculations. Neutronic and thermalhydraulic computer codes, namely RFSP and CATHENA, are currently coupled using scripts. These scripts are used to read and write input files and restart files for both codes, resulting in long computation times.

This work presents modifications implemented in RFSP for both the *CERBERUS and *CERBRRS modules, to allow direct coupling with CATHENA using PVM, thus reducing the simulation time. Results obtained with the direct PVM-based coupling are compared to the results produced with scripts for verification purposes. The results are found identical and the simulation time is considerably reduced.

1. Introduction

Coupled neutronic and thermalhydraulics calculations are often used for safety analyses. For fast transient as large-break Loss-of-Coolant Accident (LOCAs) analysis, the computer codes RFSP [2] and CATHENA [3] are executed in tandem. The *CERBERUS module of RFSP is specifically used to solve the time-dependent two-energy-group neutron diffusion equation [4]. The *CERBERUS module requires input from CATHENA for each simulation step, namely, coolant density, coolant temperature and fuel temperature at each thermalhydraulic calculation node within the core. After the *CERBERUS calculation is complete, a set of normalized powers corresponding to the nodes in the thermalhydraulics model is made available to CATHENA. This interchange of data forms the basis of the coupling of the two codes. Safety analyses of slower transients such as loss-of-flow accidents or small LOCA can also be performed using coupling between RFSP and CATHENA. For these types of slower events, the *CERBRRS module of RFSP, which simulates the response of the CANDU® 6 regulating system, is used to solve the time-dependent neutron diffusion equations. These calculations are performed coupled with CATHENA as well.

The current coupling methodology uses scripts to process and pass information between the two codes. It is often time consuming and although scripts can be modified to suit many different plant models, such changes require re-qualification of the scripts. This work intends to develop a more direct coupling between CATHENA and RFSP to reduce computational time and increase the applicability of the coupling strategy. The coupling is implemented using PVM [1] since CATHENA already contains a REMOTE PROCESS implementation [7] in PVM. The two coupling methodologies are introduced in this section.

1.1 Coupling Methodology Using Scripts

In the past [6], CATHENA and RFSP have been coupled using scripts such as RFSPCB [5] and, more recently, RCCTS.

The calculation scheme of these PERL-based scripts is presented in

Figure 1. The tasks performed by the scripts consist of input file preparation, simulation initialization, code execution, and output and restart file preparation. Once the thermalhydraulic code execution is completed, these steps are applied to the physics code. This sequence is repeated every coupling interval. Coupling in this manner often results in long computational times as both computer codes need to load their restart files at each time step of the coupling instead of only once at the beginning of the transient.

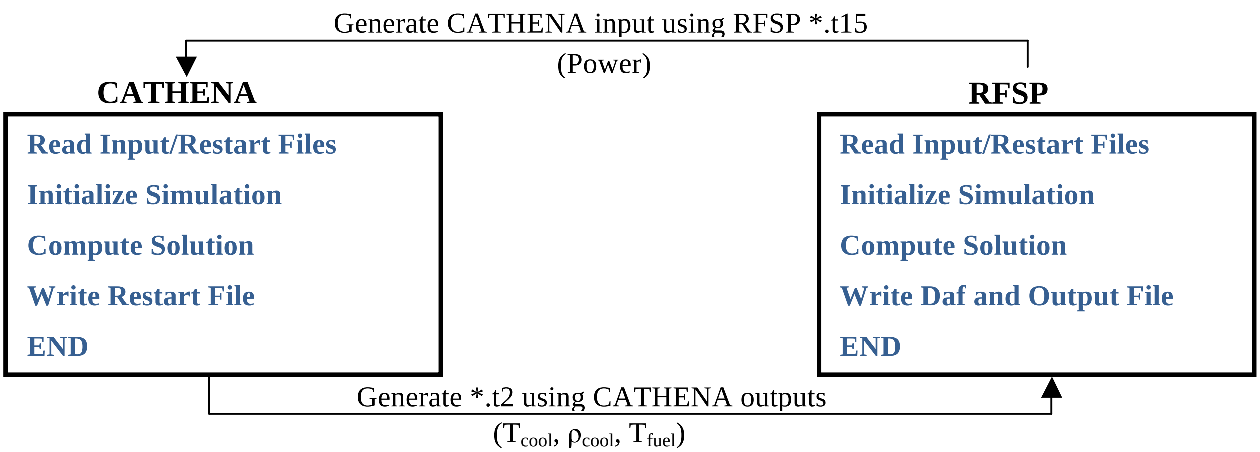

Figure 1 Script-based Coupling Calculation Scheme.

1.2 Direct Coupling Methodology with CATHENA

The REMOTE PROCESS implemented in CATHENA provides the ability to couple the code with other programs. The REMOTE PROCESS uses library routines from the Parallel Virtual Machine (PVM) [1] to launch and exchange data with a child process or code.

PVM is a software package that enables a collection of heterogeneous computers to be used as a single computational resource. PVM consists of essentially two parts: a background process that runs on each computer in the virtual machine (commonly known as a daemon process) and a library of C or FORTRAN routines to which the computer code links. A code will communicate with another code by first sending a message to its local PVM Daemon process (PVMD). This PVMD will then send the message to the PVMD on the appropriate remote computer and pass the message onto the second code.

The REMOTE PROCESS is already used in GOLFER [7], a version of the fuel code ELOCA linked with CATHENA. The approach used here to couple CATHENA with RFSP is therefore to implement similar PVM routines in RFSP to those in ELOCA. RFSP is then launched during the execution of

CATHENA and PVM is used to transfer data between the codes. The calculation scheme is then simplified as shown in Figure 3.

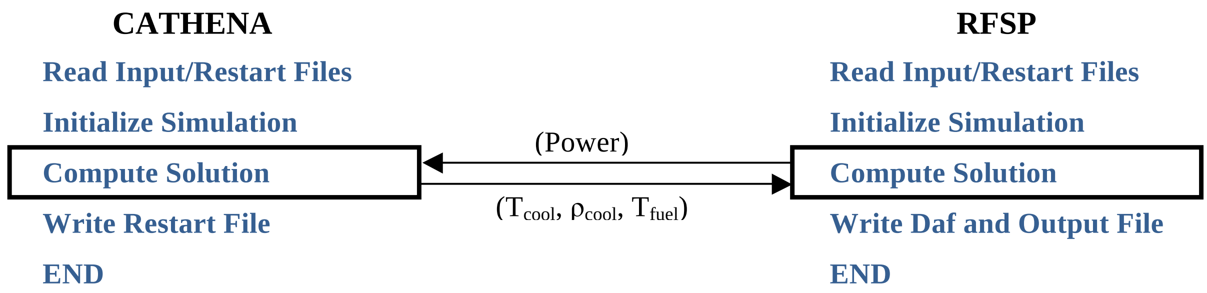

Figure 3 Direct Coupling Calculation Scheme.

2. Implementation of the Direct Coupling between CATHENA and RFSP

RFSP has been slightly modified to allow internal coupling with CATHENA. Code modifications were implemented in both the *CERBERUS and *CERBRRS modules. As such direct coupling with CATHENA is available with and without the reactor regulating system**.** The resulting calculation scheme for PVM-based coupling is shown in Figure 4. The coupling is initiated by launching CATHENA. Then, the code reads the input file and initializes the simulation. PVM will be launched if an adequate REMOTE PROCESS is defined in the CATHENA input file. Next, PVM launches RFSP and communication is established between the two codes using data defined in a coupling input file.

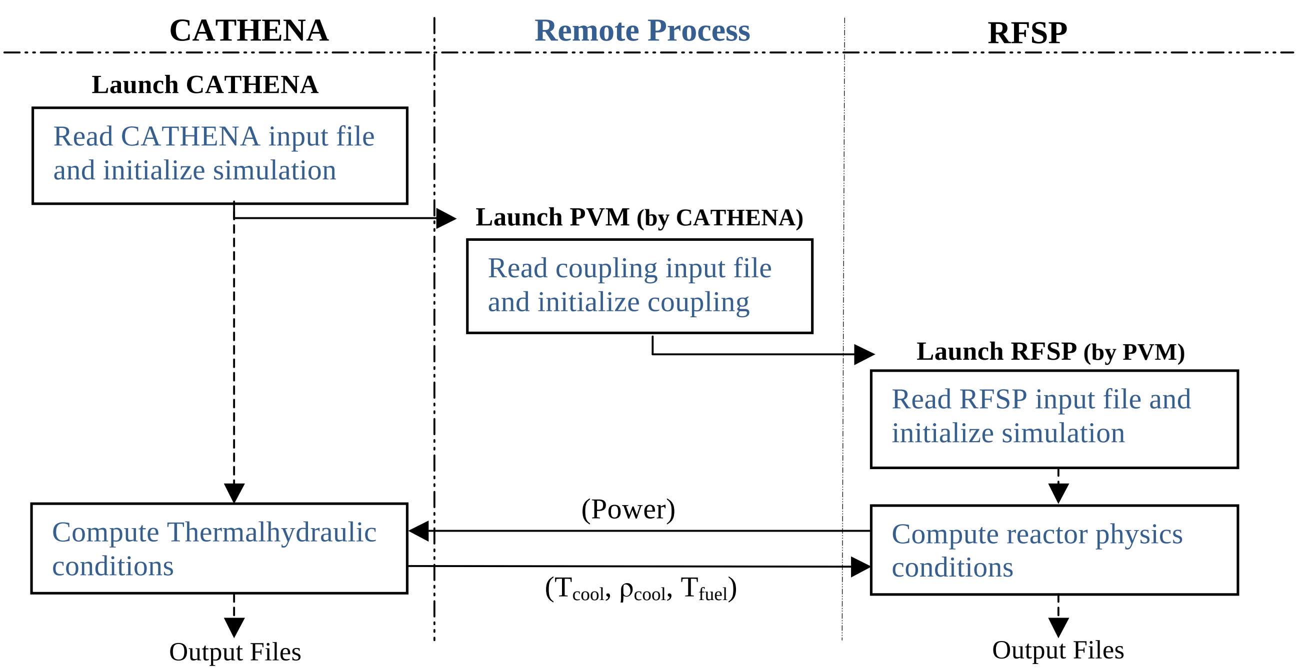

Figure 4 General PVM-based Coupling Calculation Scheme.

When coupled, RFSP is executed normally until thermalhydraulic data is needed (i.e. the coolant temperature and density and the fuel temperature) in *CERBERUS or in *CERBRRS. The execution of RFSP is then paused until the code receives this data from CATHENA. RFSP then computes the power distribution in the core, which is then sent back to CATHENA. Simultaneously, CATHENA runs normally until it needs the power distribution, which will be sent by RFSP. The execution of the two codes continues until the total number of RFSP cases (KCERB) defined in the RFSP input file is reached or until the execution of CATHENA is ended. The data exchanged through the REMOTE PROCESS at every coupling interval is presented in Table 2 and Table 3.

For coupled simulations, the user must prepare an additional coupling input file. This file contains the path of the RFSP working directory, the number of thermalhydraulic channels in the CATHENA and RFSP models and the number of axial nodes in the two models. No modification is required to the RFSP input file. The current modifications made to RFSP only allow for PVM-based coupling to be performed on the transient cases (RFSP/CATHENA Case 3 on). The steady state RFSP case (Case 1) must be converged with the corresponding CATHENA steady state model; and the RFSP adjoint case must exist in the RFSP direct access file before the PVM-based coupling can begin.. The CATHENA input file must include the appropriate REMOTE PROCESS that will launch RFSP and exchange appropriate data. Special attention should be paid to the time interval between data transfers in the REMOTE PROCESS, which should be set to a synchronization time (‘TIM_SYNC’) that forces CATHENA to evaluate its time step at a fixed interval.

3. Verification Results

A series of testing exercises have been identified for verification purpose. Verification is independent of the model selected. As such, the CATHENA and RFSP models used for the testing are not models used for safety analysis, but rather consist of typical CANDU® 6 models. Results presented in this section are not to be taken as safety analysis results but only as comparison tests verifying the direct coupling.

Here, the CATHENA PHTS model uses 5 average channels per core pass. The convergence between the two models in steady-state is achieved prior to the testing by performing a succession of steady state calculations, each model using the result from the other. The RCCTS scripts were used to perform this calculation. Moreover, the transient initialization (cases 1 to 3) of both CERBERUS and CERBRRS are carried out coupled to CATHENA using the same RCCTS scripts.

3.1.1 Data Transferred between RFSP and CATHENA

The REMOTE PROCESS data transfer is first verified independently from any code calculation. The data exchanged between CATHENA and RFSP is presented in Table 2 and Table 3. The appropriate transfer of these data is verified by comparing the outputs of the two codes. For example, the coolant density in the first average group in core pass 1 for bundles 1, 5 and 9 is presented in Figure 5 from RFSP and CATHENA output files and the power transferred between the two codes is presented for core pass 4, average group 4 for bundles 4, 8 and 12 in Figure 6 . All data transferred between CATHENA and RFSP was found identical.

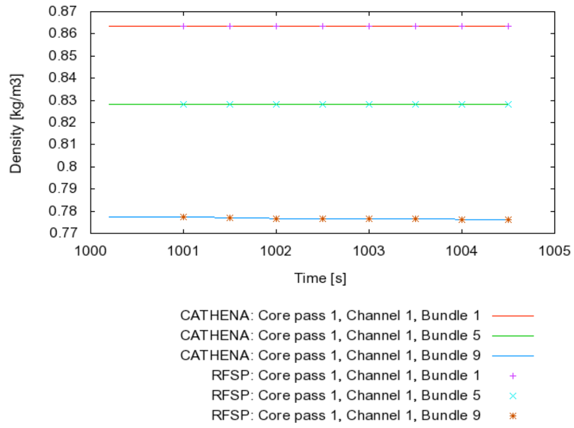

Figure 5 Testing Data Exchange: Coolant Densities in CATHENA and RFSP

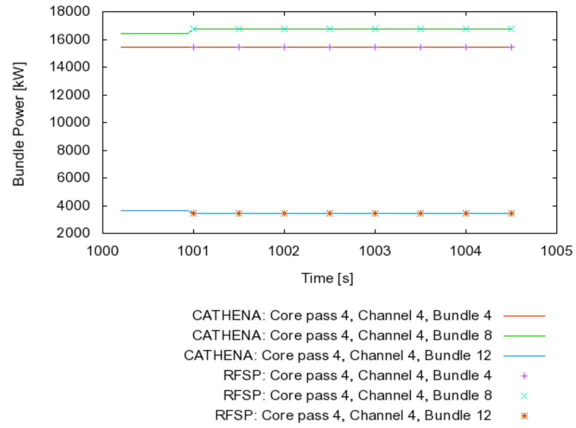

Figure 6 Testing Data Exchange: Bundle Powers in CATHENA and RFSP

3.1.2 Steady-state Convergence

The convergence of steady-states generated by both *CERBRRS and *CERBERUS modules has been verified. A steady-state transient is a do-nothing transient where no perturbation is initiated. Convergence confirms the coupling capability with PVM. A time step of 0.5s is used in the *CERBRRS calculations with a synchronization time of 0.5 s in CATHENA. A time step and synchronization time of 0.1 s are chosen for *CERBRRS.

A steady state calculation with the *CERBERUS module is not expected to converge in the long term, since no reactor regulation is simulated in the module or in CATHENA. Therefore, only the first second of the simulation can be examined to determine that no unexpected divergence is observed.

For the two modules, CATHENA and RFSP are run for 396 transient cases (from KCERB = 4 to KCERB = 400). The simulation results confirm convergence of the CATHENA and RFSP models. As an example, the total reactor power for CATHENA coupled to *CERBRRS and the reactor inlet header mass flow for CATHENA coupled to *CERBERUS are presented in Figure 7 and in Figure 8.

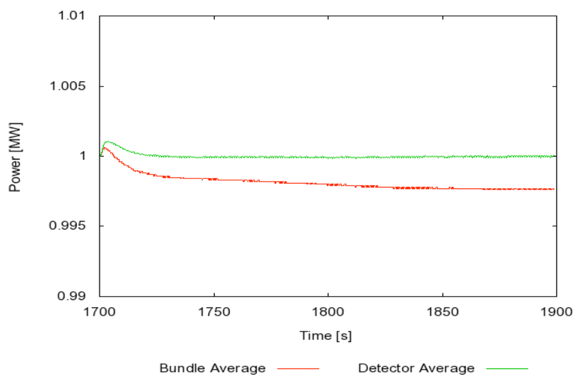

Figure 7 Steady-state: Total Reactor Power, CATHENA coupled to *CERBRRS.

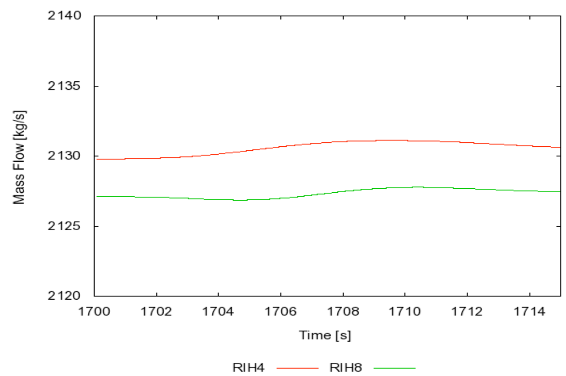

Figure 8 Steady-state: Reactor Inlet Header Mass Flow, CATHENA coupled to *CERBERUS.

3.1.3 Transient calculations

Coupled simulation results produced using PVM-based coupling and using RCCTS are compared to complete verification of the implementation of PVM-based coupling. The transient corresponds to a simultaneous loss of the 4 PHTS pumps. No reactor trip is assumed. As specified previously, these results are not to be taken as safety analysis results but are only used to compare the results produced by the two coupling methodologies.

For the *CERBRRS module, a synchronization time of 0.5 s is used in CATHENA in conjunction with a time step of 0.5 s in RFSP. Similarly, a synchronization time of 0.1 s in CATHENA and a time step of 0.1 s in RFSP are used with the *CERBERUS module.

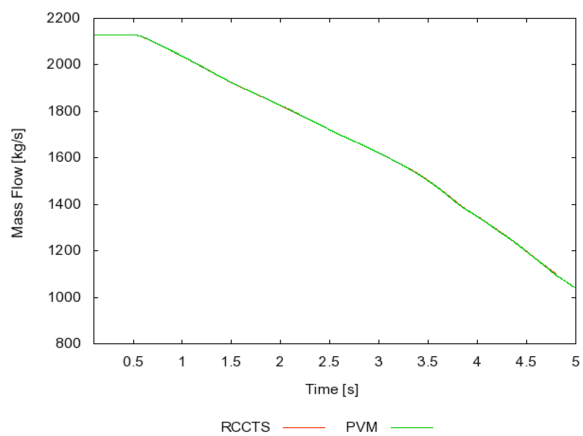

Figure 9 Total Mass Flow in a Core Pass, CATHENA coupled to *CERBRRS.

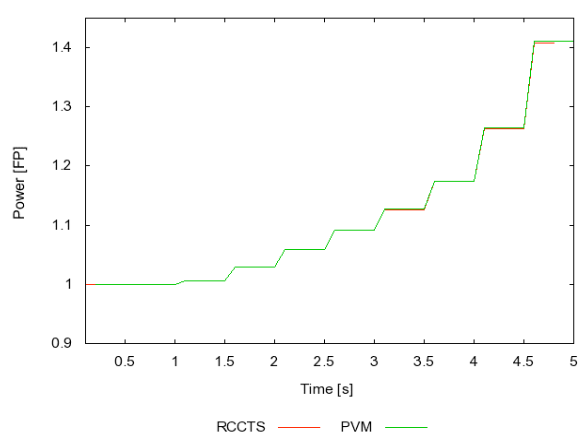

Figure 10 Bulk Reactor Power, CATHENA coupled to *CERBRRS.

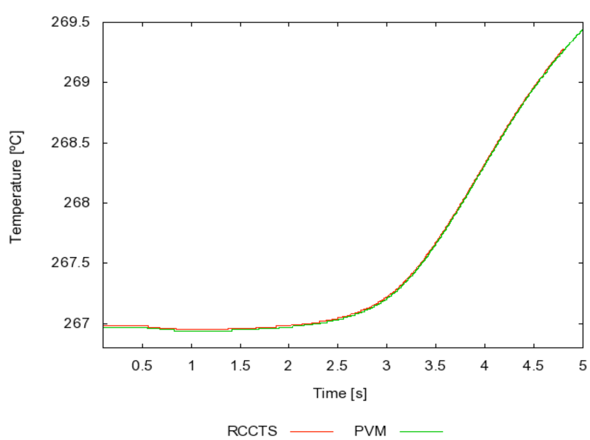

Figure 11 Reactor Inlet Header Temperature, CATHENA coupled to *CERBERUS.

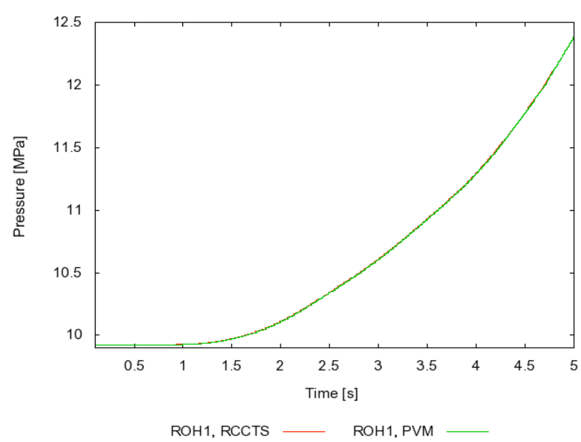

Figure 12 Reactor Outlet Header Pressure, CATHENA coupled to *CERBERUS.

The total mass flow in a core pass of the reactor is shown for the two coupling methodologies in Figure 9.The total reactor power computed by the reactor regulation system in *CERBRRS is shown in

Figure 10 respectively for PVM-based coupling and RCCTS coupling. The staircase step representation is due to the 0.5 s interval calculation of the reactor power evaluation in the Reactor Regulating System rules.

For the *CERBERUS simulations, a synchronization time of 0.1 s is used in CATHENA with a 0.1 s time interval in RFSP. Figure 11 and Figure 12 show the inlet header temperature and the outlet header pressure respectively for the *CERBERUS simulations for the two coupling strategy.

Comparison of the results shows that all the parameters are identical for the two coupling strategies, both direct coupling and RCCTS coupling.

3.1.4 Simulation Time

The direct coupling methodology between CATHENA and RFSP was implemented to reduce the simulation time compared to when scripts are used for coupling. The transient simulations presented above for 400 coupling intervals have been simulated on two different computers and the simulation computer times are shown in Table 1 for the two coupling methodologies. In all cases, the PVM-based coupled simulations took almost half the time of the same simulation coupled using the RCCTS scripts. Note that the speed of the computer used also has a significant impact.

Table 1 Computation Time for the Transient Coupled Simulations

	*CERBERUS/CATHENA		*CERBRRS/CATHENA	
	PVM	scripts	PVM	scripts
Simulation Time on Computer 1 (min)	36	85	62	110
Simulation Time on Computer 2 (min)	16	29	19	35

4. Conclusion

Direct coupling between CATHENA and RFSP has been implemented based on PVM, through the REMOTE PROCESS. The required modifications have been included in both the *CERBERUS and *CERBRRS modules of RFSP.

Steady-state (do-nothing) transients as well as perturbation transients (instantaneous pressurized heat transport system 4-pump trip) on standard CANDU-6 CATHENA and RFSP models have been used to verify the implementation of PVM-based coupling. Results produced with the PVM-based coupling scheme have been compared to results obtained with RCCTS scripts. Results were found to be identical. Furthermore, the simulation time is considerably reduced when using the PVM-based coupling rather than scripts.

PVM-based direct coupling between CATHENA and RFSP has been shown to produce the same results as current, qualified coupling scripts. In the context of the safety analyses improvement initiative, where coupled analyses are being performed, PVM-based coupling shows a great benefit by reducing simulation times.

5. Acronyms and Nomenclature

CANDU®	CANadian Deuterium Uranium
CATHENA	Canadian Algorithm for THErmalhydraulic Network Analysis
CERBERUS	Kinetics module for reactor physics code RFSP
GENHTP	GENeralized Heat Transfer Package for the CATHENA code
GOLFER	Communication Interface for ELOCA: Gain Open Link to Fuel Element Response
PHTS	Primary Heat Transport System
PVM	Parallel Virtual Machine
RCCTS	Coupling script for running CATHENA-RFSP coupled cases
RFSP	Reactor Fuelling Simulation Program
RIH	Reactor Inlet Header
ROH	Reactor Outlet Header

6. Acknowledgements

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7. References

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8. Tables

Table 2 RFSP to CATHENA Message Buffer

No.	Data Description	Data Type	Units	CATHENA Variable	GOLFER / ELOCA Variable	Usage
Messages exchanged at the initial handshake between the parent and child program						
I	PVM ID number of child program	Integer	-	IDTASK(2)	IDTASK(2)	
ii	Integer translation of this child program name i.e., "MSWIN: GOLFER 0.1 (ELOCA 2.1c)"	Integer	-	IPRONM	IPRONM	
iii	Connection status flag (0 child program working directory found, else error)	Integer	-	ISTAT(3)	ISTAT(3)	
Messages exchanged at each CORE call form CATHENA						
1	Current time $T + \Delta T$	Real	S	`TSIMNET`	`Pvm%Time`	Start time
2	Time step ΔT	Real	S	`DTNET`	`Pvm%DT`	Simulation time (length)
3	Stop flag	Logical		`NETSTOP`	`Pvm%Stop`	Control (always set to .FALSE.)
4	Redo time step flag	Logical		`NETREDO`	`Pvm%Redo`	Control (always set to .FALSE.)
5	Write restart flag	Logical		`NETWRST`	`Pvm%Write`	Control (always set to .FALSE.)
6	Total reactor power	Real	W			Total reactor Power
7 to (7+`ngr*nbun`)	Power	Real	W		`PWR()`	To be applied the to the GENTHP power generation model.

Table 3 CATHENA to RFSP Message Buffer

No.	Data Description	Data Type	Units	CATHENA Variable	RFSP Variable	Usage
Messages exchanged at the initial handshake between the parent and child program						
I	PVM ID number of parent program	Integer	-	IDTASK(1)	IDTASK(1)	
ii	Integer translation of parent program name i.e., “CATHENA MOD-3.5d Rev 2”	Integer	-	IPRONM	IPRONM	
iii	Integer translation of working directory for child program	Integer	-	IWDIR	IWDIR	
iv	Integer translation of input file name for child program	Integer	-	IINFL	IINFL	
Messages exchanged at each CORE call form CATHENA						
1	Current time T	Real	S	TSIM	Pvm%Time	Start time
2	Time step ΔT	Real	S	DT	Pvm%DT	Simulation time (length)
3	Stop flag (indicating that CATHENA simulation is to be terminated after completion of this time step).	Logical		STOPRN	Pvm%Stop	Control
4	Redo time step flag (indicating that step starting with current time to be recalculated with a smaller time step).	Logical		REDO	Pvm%Redo	Control
5	Write restart flag (indicating that restart record should be written after completion of the current time step calculation).	Logical		WRST	Pvm%Write	Control
6 to (6+ngr*nbun)[1]	Local coolant density	Real	kg/m^3 [2]	ROMIX (ex:'ROMIX:CHAN1-1(1)')	FBTIMpvm(1,ngr,nbun)[1]	Local coolant density
(6+ngr*nbun) to (6+2*ngr*nbun)	Local liquid temperature	Real	ºC	TEMPF (ex: 'TEMPF:CHAN1-1(1)')	FBTIMpvm(2,ngr,nbun)[3]	Local liquid temperature (eventually quality averaged)
(6+2*ngr*nbun) to (6+3*ngr*nbun)	Local gas temperature	Real	ºC	TEMPG (ex: 'TEMPG:CHAN1-1(1)')	FBTIMpvm(2,ngr,nbun)[3]	Local liquid temperature (eventually quality averaged)
(6+3*ngr*nbun) to (6+4*ngr*nbun)	Local mass quality	Real		QUALITY (ex: 'QUALITY:CHAN1-1(1)')	FBTIMpvm(2,ngr,nbun)[3]	Local temperature averaging
(6+4*ngr*nbun) to (6+5*ngr*nbun)	Local fuel average temperature	Real	ºC	TWALL/AVG (ex.'TWALL/AVG:P1C1B01(1-1,1-5,1-99,1-99)')	FBTIMpvm(3,ngr,nbun)	Local fuel average temperature

[1] Ngr is the number of thermalhydraulic groups implemented in the CATHENA model and as defined in the CORE inputfile. nbunis the number of axial thermalhydraulic nodes (i.e. bundles, typically 12) and as defined in the CORE inputfile.
[2] Converted in g/m^3 once received by RFSP.
[3] Once quality averaged