# Porting RFSP-IST From HP-UX Platform to PC Platform

I. Patrulescu and I. Dumitrache On attachment to AECL from ICN Pitesti, Romania

> W. Shen and D.A. Jenkins Atomic Energy of Canada Limited 2251 Speakman Drive Mississauga, ON L5K 1B2

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#### **ABSTRACT**

RFSP-IST (Reactor Fuelling Simulation Program - Industry Standard Toolset) is a neutron-diffusion code for static and kinetic CANDU® core analysis in three spatial dimensions and two neutron energy groups. The program is a legacy code written in Fortran 77 and executed on UNIX machines. Recently RFSP-IST version 3-00-05 was successfully ported from the HP-UX platform to the PC platform. This paper provides a summary of the work performed in porting RFSP-IST to the PC platform.

## 1. HISTORY OF RFSP

RFSP-IST (Reactor Fuelling Simulation Program - Industry Standard Toolset) is a diffusion code for static and kinetic CANDU core analysis in three spatial dimensions and two neutron energy groups (Reference 1). The program is very extensive, consisting of about 1400 subroutines. The structure of the program is modular: different modules perform different functions.

RFSP-IST is a legacy code with a rich history of development and innovation. In 1974, AECL developed the fuel-management-design program FMDP. This program was created to analyze the neutronics of CANDU reactors. Its intended applications were for both design and core-follow, including expected core behaviour for a variety of different fuelling schemes. FMDP was developed to have considerable flexibility, in order to allow the user to model the reactor in varying degrees of detail and to accommodate design changes as they occurred. Over the years, different separate programs came to be incorporated into FMDP. At the same time, new modules were developed to meet changing requirements. In 1980, a subset of FMDP, specifically designed for use at CANDU generating stations, was developed; it came to be known as RFSP.

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In the 1980s and 90s, frequent computer-platform changes occurred. RFSP was originally written in FORTRAN IV, and ran on NOS/BE CYBER 6600/175 computers at the Chalk River Laboratories (CRL) when portability was not a concern. In 1986, RFSP was converted to run on NOS CYBER 830 computers at Sheridan Park. In 1989, RFSP was converted to run on NOS/VE CYBER 990 computers at CRL, FORTRAN IV was updated to FORTRAN 77, and the fixed central memory was changed to virtual memory management. During all this period, more and more functionalities of FMDP, including those modules related to reactor design, were imported into RFSP at the request of the utilities. In 1990, RFSP was converted to run on the APOLLO UNIX platform. In 1993, RFSP was converted to run on the Hewlett-Packard UNIX (HP-UX) platform, and in 1999, a Y2K-compliant version was developed. In 1999 June, the first IST version, RFSP-IST version 3-00, was created by merging AECL's RFSP version 2-17 and Ontario Power Generation's OHRFSP version R1.06.

#### 2. PLATFORMS

A platform is a combination of operating system (OS) and central processing unit (CPU) that provides a distinct environment in which to write a computer program and to execute it.

Revision control system (RCS) and 'gnu-make' (Reference 2) are currently used to develop and maintain a single platform-independent RFSP source on the HP-UX platform. This source code can be compiled, using 'gnu-make', to run on different operating platforms such as the HP-UX platform (with an HP-UX 10.20 Unix OS) and the IBM-AIX platform (with an AIX 4.3 Unix OS) under a Fortran-77 compiler environment. Recently, and due to the increasing computation speed, growing popularity and capability of PC computers, there has been mounting interest in porting RFSP from the HP-UX platform to the PC platform (with a Windows 2000/NT OS).

### 3. WORK PLAN

A work plan was developed for the porting of the code, as discussed below. This plan ensured that the "trials and errors" made during the porting would not interfere with other on-going work on RFSP. The steps in the work plan are as follows:

- Start with the HP-UX source code
- Attempt compilation on the PC platform
- Examine compiler "error" messages. Many of these were a priori expected to be non-fatal, and to be related to the age of the original source or differences in compiler idiosyncrasy

- Modify the source code to remove all errors, modernizing the source code if necessary
- Recompile (repeating previous step if necessary) and obtain executable on PC platform
- Execute the PC executable on the set of RFSP verification cases. Check that results are the same as on the HP platform (to within possible and expected round-off errors on different platforms)
- Import the source-code modifications back to the HP source code to obtain a platform-independent source code. Verify that the new, modified source code compiles without errors on both platforms and produces the same results.

To date, work on all steps except the last has been completed and the RFSP executable compiled on the PC platform has been created and successfully verified. The work on the last step is currently on-going.

#### 4. PORTING ISSUES

The RFSP version which was ported to the PC is version 3-00-05, released in 2001 March. The compiler used on the PC was DIGITAL Visual Fortran version 6.0.

DIGITAL Fortran provides a superset of the Fortran 90 standard, along with a number of extensions that are compatible with Fortran 77. One major issue in the porting is the compatibility of DIGITAL Visual Fortran-90 compiler with HP-UX Fortran-77 compiler supplied by different vendors for different platforms. Fortunately, DIGITAL Fortran 90 provides all the original features of Fortran 77, and adds modern extensions and flexibility. Some features of the older standard have been declared obsolete. While Visual Fortran still recognizes the obsolete features, it encourages new coding to use the new structures provided.

As with other legacy codes, RFSP has passed through different dialects of Fortran, picking up features from each, even after those features have become outmoded. Porting such a program may sometimes be as simple as identifying and removing the non-portable features. However, this was not the case in porting RFSP to the PC – it was necessary in this exercise to find ways around incompatibilities between the HP-UX Fortran 77 compiler and the DIGITAL Visual Fortran 90 compiler.

The total number of routines modified during the porting was about 90. Of these, only a few routines were modified due to compiler errors. Most modifications were due to a mismatch between parameter type in a subroutine call and the corresponding parameter type as declared in the subroutine; this mismatch had not previously been identified, but had apparently not caused any errors. This fixing of linker errors was the most time-consuming part of the work. Run-time errors were also present, and several routines were modified to fix these errors. In addition, all compiler warnings were analyzed. As

expected, most of these were evaluated as being irrelevant, and only a few routines were changed to eliminate warnings that indicated possible run-time errors.

## 5. VERIFICATION

After creating the RFSP executable on the PC, 32 verification test cases were run on the PC platform and results were compared with the reference results obtained on the HP-UX platform. The PC runs were made under Windows NT on Intel Pentium hardware with 400 MHz speed and 320 MB memory. The HP-UX runs were made on a HP9000 series Model 889, with the operating system HP-UX 10.20 and the CPU version 2.0PA 8000.

Table 1 contains the values compared for most of the test cases. The comparison was made on the basis of number of iterations required, final value of  $k_{\rm eff}$  after convergence, the maximum channel power and the maximum bundle power. In addition, in the test runs for the \*CERBERUS module, the values of the flux amplitude and reactivity were compared as shown in Table 2.

Overall, the values obtained on the two platforms for  $k_{eff}$ , maximum channel power and maximum bundle power were very close. The largest differences for the maximum channel power are ~0.04% for all cases. The largest differences for the maximum bundle power are around  $\pm 0.06\%$  for all cases, except that the difference is ~0.14% for the "SimpleCell" case, a complex calculation invoking the Simple-Cell Method (SCM) lattice calculation for each bundle, which may result in greater truncation error.

Figure 1 shows the changes (in %) induced by the PC calculation, relative to the reference HP-UX calculation, in the channel-power distributions for the "SimpleCell" case. Taking into account the truncation errors, the differences are acceptable, with the maximum difference again less than  $\pm 0.05\%$ .

In summary, the comparison showed very small differences between the results on the PC and those on the HP-UX. Most of these small differences are related to differences in numerical truncation; this is consistent with the known fact that, in general, results provided by distinct compilers and computers are not exactly identical. No unacceptable differences in the results were identified.

The CPU time required for a typical RFSP run (with no optimization option during the compilation on both the PC and HP-UX platforms) was about three times shorter on the PC than on the HP-UX platform. The computational speed on the PC is further increased by up to 50% without any effect on the calculation accuracy when the optimization option is used during compilation. Therefore the optimized PC version of RFSP is about 6 times faster than the non-optimized HP-UX version of RFSP. Note however that only one RFSP case can be run at a time and that the performance of other tasks will be decreased significantly while this RFSP case is running.

#### 6. CONCLUSION

RFSP-IST version 3-00-05 has been successfully ported from the HP-UX platform to the PC platform. The use of RFSP will no longer be strictly dependent on the availability of (more expensive) UNIX machines. Even when PCs and UNIX machines are both available, the existence of an RFSP executable on the PC may offer several advantages for code users. Very often, UNIX servers have many end users and may be very heavily loaded. In such instances, and even though the UNIX network may have several servers available, computationally intensive tasks requiring many RFSP simulations may be performed in much shorter real time using PC nodes.

#### **ACKNOWLEDGEMENTS**

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#### **REFERENCES**

- 1. B. Rouben, "RFSP-IST, The Industry Standard Tool Computer Program for CANDU Reactor Core Design and Analysis", in Proceedings of the 13<sup>th</sup> Pacific Basin Nuclear Conference, Shenzhen, China, 2002 October 21-25.
- 2. D. Bolinger and T. Bronson, "Applying RCS and SCCS", O'Reilly &Associates, Inc., 1995.

Table 1: Summary of the RFSP Verification Results Calculated on the PC and HP-UX Platforms (Differences between HP and PC power results are reported as % differences in last 2 columns)

Docation of input	dle		
PC   100   1.00069   6.899 (0.03%)   797.516 (0.028)     After 10 FPD   HP-UX   71   0.998329   6.937   809.185     PC   100   0.998326   6.936 (-0.01%)   809.099 (-0.028)     PC   100   1.00813   7.390   762.904     PC   100   1.00813   7.389 (-0.01%)   762.731 (-0.028)     PC   100   1.00813   7.392   763.127     Coarse mesh model   HP-UX   100   1.00813   7.391 (-0.01%)   762.949 (-0.028)     Monic_1.5g   HP-UX   156   0.982358         PC   159   0.982358         PowderPufs   HP-UX   156   0.982358         PC   159   0.982358         PC   140   0.998371   6.778   759.521     PC   140   0.998371   6.739 (0.01%)   744.394 (-0.028)     PC   140   0.998371   6.739 (0.01%)   744.394 (-0.028)     PC   140   0.998371   6.739 (0.01%)   744.394 (-0.028)     PC   22   1.00246   6.749 (0%)   750.320 (0.028)     Simulate_20FPD   C6_FPD0_new.input   HP-UX   100   1.00070   6.897   797.208     E=0 (FRESH CORE)   PC   100   1.00069   6.899 (0.03%)   797.516 (0.028)     PC   100   1.00069   6.899 (0.03%)   797.516 (0.028)     PC   100   1.00069   6.899 (0.03%)   797.516 (0.028)			
After 10 FPD			
PC   100   0.998326   6.936 (-0.01%)   809.099 (-0.01%)			
Collapse			
PC	)1%)		
PC   100   1.00813   7.389 (-0.01%)   762.731 (-0.01%)   762.731 (-0.01%)   763.127			
Coarse mesh model   HP-UX   100   1.00813   7.392   763.127			
PC   90   1.00813   7.391 (-0.01%)   762.949 (-0.			
Monic_1.5g			
PC   159   0.982358			
PowderPufs	-		
SimpleCell         Fresh Core         HP-UX         75         1.00778         6.778         759.521           PC         132         1.00777         6.779 (0.01%)         760.560 (0.30)           10 EFPD         HP-UX         109         0.998383         6.738         744.816           PC         14         0.998371         6.739 (0.01%)         744.394 (-0.00)           20 EFPD w. refuelling         HP-UX         100         1.00248         6.749         750.320 (0.00)           simulate_20FPD         c6_FPDO_new.input         HP-UX         100         1.00070         6.897         797.208           E=0 (FRESH CORE)         PC         100         1.00069         6.899 (0.03%)         797.516 (0.00)			
SimpleCell         Fresh Core         HP-UX         75         1.00778         6.778         759.521           PC         132         1.00777         6.779 (0.01%)         760.560 (0.20%)           10 EFPD         HP-UX         109         0.998383         6.738         744.816           PC         14         0.998371         6.739 (0.01%)         744.394 (-0.00%)         750.249           20 EFPD w. refuelling         HP-UX         100         1.00248         6.749         750.320 (0.00%)           simulate_20FPD         c6_FPDO_new.input         HP-UX         100         1.00070         6.897         797.208           E=0 (FRESH CORE)         PC         100         1.00069         6.899 (0.03%)         797.516 (0.00%)	ing —		
PC 132 1.00777 6.779 (0.01%) 760.560 (0.132) 10 EFPD HP-UX 109 0.998383 6.738 744.816 PC 14 0.998371 6.739 (0.01%) 744.394 (-0.0132) 1.00248 6.749 750.249 PC 14 0.998371 6.749 (0.01%) 750.320 (0.0132) 1.00248 6.749 (0.0132) 750.320 (0.0132) 1.00248 6.749 (0.0132) 1.00248 6.749 (0.0132) 1.00248 6.749 (0.0132) 1.00249			
10 EFPD     HP-UX     109     0.998383     6.738     744.816       PC     14     0.998371     6.739 (0.01%)     744.394 (-0.01%)       20 EFPD w. refuelling     HP-UX     100     1.00248     6.749     750.249       PC     22     1.00246     6.749 (0%)     750.320 (0.01%)       simulate_20FPD     c6_FPD0_new.input     HP-UX     100     1.00070     6.897     797.208       E=0 (FRESH CORE)     PC     100     1.00069     6.899 (0.03%)     797.516 (0.01%)			
PC         14         0.998371         6.739 (0.01%)         744.394 (-0.01%)           20 EFPD w. refuelling         HP-UX         100         1.00248         6.749         750.249           PC         22         1.00246         6.749 (0%)         750.320 (0.01%)           simulate_20FPD         c6_FPD0_new.input         HP-UX         100         1.00070         6.897         797.208           E=0 (FRESH CORE)         PC         100         1.00069         6.899 (0.03%)         797.516 (0.01%)	4%)		
20 EFPD w. refuelling     HP-UX     100     1.00248     6.749     750.249       simulate_20FPD     PC     22     1.00246     6.749 (0%)     750.320 (0.0000)       simulate_20FPD     c6_FPD0_new.input     HP-UX     100     1.00070     6.897     797.208       E=0 (FRESH CORE)     PC     100     1.00069     6.899 (0.03%)     797.516 (0.0000)	,		
refuelling	06%)		
simulate_20FPD         c6_FPD0_new.input         HP-UX         100         1.00070         6.897         797.208           E=0 (FRESH CORE)         PC         100         1.00069         6.899 (0.03%)         797.516 (0.00)	-		
E=0 (FRESH CORE) PC 100 1.00069 6.899 (0.03%) 797.516 (0.0	1%)		
100 1100000 0.00000 1771.010 (0.0			
C6_FPD10_new.input HP-UX 71 0.998329 6.937 809.189	4%)		
E=494736 PC 100 0.998326 6.936 (-0.01%) 809.099 (-0.	)1%)		
C6_FPD20_new.input HP-UX 85 1.00420 7.055 836.063			
E=989472 PC 92 1.00420 7.052 (-0.04%) 835.644 (-0.	)5%)		
simulate_2Group E=0 (FRESH CORE) HP-UX 174 1.01296 6.897 819.15			
PC 134 1.01296 6.897 (0%) 819.15 (0°	%)		
10 EFPD with Xenon HP-UX 104 0.999419 6.960 833.02			
PC 104 0.999419 6.960 (0%) 833.02 (0°	%)		
20 EFPD HP-UX 117 1.00367 7.081 860.13	860.13		

		PC	85	1.00367	7.082 (0.01%)	860.19 (0.01%)
tave_equiv.2g	TIME-AVER	HP-UX	20	1.01692	6.79875	764.91
		PC	42	1.01693	6.79992 (0.02%)	765.02 (0.01%)
	TAVEQUIV	HP-UX	85	1.00601	6.790	766.363
		PC	87	1.00601	6.791 (0.01%)	766.483 (0.02%)
tavequiv_1.5g	TIME-AVER	HP-UX	40	0.999787	6.77163	826.77
1 _ 0		PC	42	0.999787	6.77147 (0%)	826.76 (0%)
	TAVEQUIV	HP-UX	41	1.00031	6.775	828.564
		PC	40	1.00031	6.774 (-0.01%)	828.509 (-0.01%)
Unfold	xleft_symmetry.input	HP-UX	80	1.00758	7.41438	772.53
		PC	80	1.00757	7.41462 (0%)	772.53 (0%)
	xright.input	HP-UX	100	1.00755	7.431	775.258
		PC	100	1.00755	7.432 (0.01%)	775.531 (0.04%)
	yfloor.input	HP-UX	100	1.00755	7.431	775.258
	•	PC	100	1.00755	7.432 (0.01%)	775.531 (0.04%)
	ytop.input	HP-UX	100	1.00755	7.431	775.258
		PC	100	1.00755	7.432 (0.01%)	775.531 (0.04%)
	zback.input	HP-UX	100	1.00755	7.431	775.258
	•	PC	100	1.00755	7.432 (0.01%)	775.531 (0.04%)
	zfront.input	HP-UX	100	1.00755	7.431	775.258
	•	PC	100	1.00755	7.432 (0.01%)	775.531 (0.04%)

Table 2: Summary of the RFSP \*CERBERUS Results Calculated on the PC and HP-UX Platforms

Directory location of input	Case	System	Iterations	k <sub>eff</sub>	Max. Channel Power, MW	Max. Bundle Power, kW	Amplitude	Reactivity
Cerberus	cerb_case1.input	HP-UX	83	0.999400	6.83	751.18		
		PC	80	0.999398	6.83 (0%)	751.80 (0.08%)		
	cerb_case2.input	HP-UX	226	0.999400				
		PC	224	0.999400				
	cerb_case3.input	HP-UX	21	0.999386			1.0037	9.2926E-05
		PC	21	0.999382			1.0038 (0.01%)	9.5618E-05 (2.90%)
	cerb_case4.input	HP-UX	25	0.999392			1.0250	4.9777E-04
		PC	25	0.999393			1.0252 (0.02%)	5.00050E-04 (0.46%)
Cerberus_2G	cerb_scmcase1.input	HP-UX	400	0.998041	6.79	743.91		
		PC	204	0.998041	6.79 (0%)	743.92 (0%)		
	cerb_scmcase2.input	HP-UX	400	0.998032				
		PC	240	0.998041				
	cerb_scmcase3.input	HP-UX	400	0.998042			1.0047	1.1312E-04
		PC	240	0.998041			1.0047 (0%)	1.1326E-04 (0.12%)
	cerb_scmcase4.input	HP-UX	400	0.998042			1.0334	6.3786E-04
		PC	296	0.998042			1.0334 (0%)	6.3787E-04 (0%)
	cerb_scmcase5.input	HP-UX	400	0.998042			1.1036	1.4399E-03
		PC	338	0.998041		·	1.1037 (0.01%)	1.4400E-03 (0.01%)

Figure 1: Relative Changes (%) Induced in Channel Powers for "SimpleCell" Case by the PC calculations, Relative to the Reference HP-UX Calculation

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
Α									0.00	0.00	-0.03	0.00	0.00	-0.03								
В						0.00	0.00	0.00	-0.02	0.00	-0.02	-0.02	0.00	-0.02	0.00	0.00	0.00					
С					-0.03	-0.02	0.00	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	0.00	-0.02	-0.03				
D				0.00	0.00	0.00	0.00	-0.02	0.00	-0.02	-0.02	-0.02	-0.02	0.00	-0.02	-0.02	-0.02	-0.02	0.00			
Ε			0.00	0.00	0.00	-0.02	0.00	-0.02	-0.01	-0.02	-0.02	-0.02	-0.02	-0.02	0.00	-0.02	-0.02	-0.02	-0.02	-0.03		
F			-0.03	-0.02	0.00	0.00	-0.02	-0.01	-0.01	-0.02	-0.02	-0.02	-0.02	-0.01	-0.01	-0.02	-0.02	-0.02	-0.02	-0.03		
G		0.00	0.00	-0.02	-0.02	0.00	0.00	-0.01	-0.02	-0.02	-0.02	-0.02	-0.02	0.00	-0.01	-0.02	-0.02	-0.02	-0.02	-0.02	-0.03	
Н		0.00	0.00	-0.02	-0.02	-0.02	-0.02	-0.02	0.00	-0.02	0.00	0.00	0.00	0.00	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	
J	0.00	-0.02	0.00	-0.02	-0.02	0.00	-0.02	-0.02	-0.02	0.00	0.00	0.00	0.00	-0.02	0.00	0.00	0.00	-0.02	-0.02	-0.02	-0.02	-0.03
K	-0.03	0.00	0.00	-0.02	0.00	0.00	-0.02	-0.02	0.00	-0.02	0.00	-0.02	-0.02	0.00	-0.02	-0.02	0.00	-0.02	-0.02	-0.03	-0.02	0.00
L	0.00	-0.02	-0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	0.00	0.00	0.00	-0.02	-0.02	-0.02	-0.03
M	-0.03	-0.02	-0.02	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	-0.02	0.00
Ν	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.02	0.00	0.00	0.00	0.00	0.02	0.02	0.00	0.00	0.00	-0.01	-0.02	-0.02	-0.02	0.00
0	0.00	0.00	0.00	0.00	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.00	0.00	0.00	0.00	-0.02	-0.02	0.00
Р		0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.00	0.00	0.00	0.00	-0.02	-0.02	
Q		0.00	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.00	-0.02	0.00	
R			0.00	0.00	0.02	0.03	0.02	0.03	0.02	0.02	0.03	0.03	0.02	0.03	0.03	0.02	0.02	0.02	0.00	0.00		
S			0.00	0.00	0.02	0.02	0.03	0.02	0.02	0.03	0.03	0.03	0.02	0.03	0.03	0.02	0.02	0.00	0.00	-0.03		
T				0.03	0.03	0.02	0.04	0.04	0.03	0.02	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.00	0.00			
U					0.03	0.03	0.02	0.02	0.04	0.02	0.04	0.02	0.04	0.02	0.02	0.00	0.03	0.04				
V						0.04	0.03	0.03	0.03	0.05	0.02	0.05	0.02	0.03	0.03	0.03	0.00					
W									0.04	0.04	0.03	0.03	0.04	0.04								