1.2 ADVANCED COMPUTATIONAL TOOLS FOR PHYSICS DESIGN

- **Space-time Analysis code for AHWR**

The knowledge of the space and time dependent behaviour of the neutron flux is important for the reactor safety analysis under operational and accidental conditions.

A time-dependent diffusion theory code called ARK3 (Advanced Heavy Water Reactor Kinetics in 3-D) is being developed for the AHWR. The code ARK3 has option to use advanced Krylov subspace based solution techniques. The space-time analysis code simulates the transient, due to the disturbed reactor steady state, by numerically solving the time dependent diffusion equations. The code is coupled with a visualization tool to plot fluxes as a function of transient time, at any planar cross-section of the reactor core. It is validated against a HWR benchmark problem, which simulates power rise due to half-core coolant voiding and subsequent control action. Representative snapshot flux profiles in two central planar cross-sections when power is at a maximum value, are illustrated.

The code ARK3 is currently being used to analyze AHWR transients such as LORA, operational transient with xenon and validation of reactor physics software in AHWR simulator. This code will be coupled with the thermal-hydraulic analysis code for studying the combined effects of neutronic and thermal hydraulic behaviour.

- **ATES3 – Anisotropic Transport Equation Solver in 3-D**

An accurate prediction of the time dependent multi dimensional & multi energy group neutron flux at successive time instants, is one of the main aspects of reactor physics design. There are primarily two main approaches: deterministic (\(S_n\), Collision probability) and Stochastic (Monte Carlo). Often, the reactor core calculations are done with diffusion theory, which is an approximation of the neutron transport theory, a deterministic approach. But an exact transport theory treatment is necessary in several cases such as high leakage reactors, for fluxes at the boundary and beyond, shielding analysis, verification of the approximate methods etc.

Recently, a neutron-gamma transport theory code, called ATES3, has been developed in 3-D Cartesian geometry for steady state criticality and external source problems. Apart from conventional methods of solutions, the code makes use of a few advanced Krylov subspace based schemes. The code is written in Fortran-90 language and has modular structure. These features make it more understandable and comparatively easier to modify. The...
code ATE53 has been validated against a few international benchmarks and is being subjected for more rigorous testing. Figure below gives the material layout and the corresponding thermal flux shape for an LWR benchmark. The flux dip at the Control Rod (CR) location can be seen clearly.

As is well known, transport problems are highly memory and CPU time intensive problems, a single PC or workstation is not sufficient. Hence, it is very important to adopt the present code to parallel computers. Efforts are being made to parallelize the code on BARC’s ANUPAM parallel systems. Incorporation of methods of solutions and user-friendly advanced features like visualization tools etc. are being incorporated.

Monte Carlo Technique: Code Development and Reactor Physics Simulation

Monte Carlo, as a tool in numerical analysis has gained wide spread applicability over the past few decades. The advent of high speed computing machines has been mainly responsible for the continual development of Monte Carlo method. Used properly, Monte Carlo can give quick “first cuts” at difficult problems, that is problems which are intractable by the traditional analytical or numerical techniques.

The greatest advantage of the Monte Carlo method is the exact simulation of the geometry. In deterministic methods only some special geometry can be simulated exactly, for irregular geometry some approximations must be considered. Monte Carlo method does not take any approximations in defining geometry. For this reason Monte Carlo method is essential for reactor calculations which involves complicated geometry e.g. Secondary shutdown system of 500 MWe PHWR, hexagonal geometry of CHTR, Nuclear Power Pack, Pebble bed reactors etc. as well as for deep penetration problems.

The main objective is to develop a general geometry Monte Carlo code with burn up, which will be used for criticality calculations, safety evaluations, accelerator driven sub-critical system’s calculations, shielding calculations etc. with greater confidence and wider flexibility.

Development of Random Number Generator

Random number plays an important role in any Monte Carlo calculation. The accuracy of the results depends on the randomness of the random numbers, its uniformity and its cycle length.

To provide uniform random sequences having larger cycle length required for Monte Carlo calculations a Random Number Generator (RNG) with large cycle length \(2^{57}\) has been developed using bit manipulation technique. Some of its properties namely uniformity, Expectation Value, Variance, Frequency distribution, Auto-Correlation, Chi-square test etc. have been performed. It was compared with RANDU of PC in FORTRAN, RAND of PC in Basic, RAND of Honeywell DPS-8 System and RAN of PDP-11/23 and found to be superior among...
Correlation Coefficient of this RNG has been compared with that of different RNGs in the Table. It is seen that current RNG has been much closer to the expected value (the correlation coefficient between neighboring bits of a random sequence is expected to be zero). This RNG is ready to be used in any code, which requires large cycle of uniform random sequences.

### Development of 69-group spherical geometry Criticality Code

Monte Carlo code for criticality calculation has been developed for spherical geometry with WIMS 69 group energy treatment. This code is being extended for AHWR/PHWR lattice cell with WIMS 69 group cross-section data.

### Simulations of Reactivity Induced Transients for Thermal and Fast Reactors and Stability Studies

An accurate prediction of the consequences of an accident in a nuclear reactor is vital from the reactor safety point of view. This in turn requires the solution of coupled time-dependent neutron diffusion equations, time-dependent heat conduction equations and single and two phase coolant dynamics equations. All of these require large computer memory and computational time. Present day large-sized power reactors are neutronically loosely coupled. The looseness of the coupling is further enhanced by the deliberate flattening of the power distribution. The study of the neutronic transient behaviour under accidental conditions in such reactors requires accurate methods of solution of system of coupled multidimensional multi energy group time dependent neutron diffusion equation. Two distinct approaches exist for this purpose namely; the direct (implicit time differencing) and Improved Quasistatic (IQS) approach. Both the approaches need solution of static space energy dependent neutron diffusion equations at successive time steps.

A three-dimensional computer code 3D-FAST was developed based on Incomplete LU (ILU) preconditioned Biconjugate Stabilized method. The code was parallelized on ANUPAM distributed memory parallel system. The domain decomposition technique was used to create parallelism. The parallel
A computational scheme was tested by analyzing a well-known Canadian PHWR benchmark problem, which simulates a loss of coolant accident.

The transient was simulated using two energy groups and $52 \times 52 \times 40$ meshes. Twenty-nine space and energy dependent calculations were done with time step of the order of 0.1 sec. Table presents the CPU gain due to parallelization. The code was used to analyze the inadvertent withdrawal of two control rods along with drainage of light water from the zone controller units (ZCUs) for 540 MWe PHWR. Figures show the variation of reactivity and power as a function of time for this transient.

The accident analysis of fast reactors is generally carried out in two phases. The first phase is generally called as pre-disassembly phase and the second one as disassembly phase. In pre-disassembly phase, the transient is analyzed up to coolant voiding and fuel melting. The disassembly phase calculations are carried out with reactivity rates estimated from coolant voiding and fuel slumping. These transients are terminated by the disassembly of the core, which introduces sufficient negative reactivity. The calculation of disassembly reactivity requires the solution of coupled neutronics and hydrodynamics equations. A computer code for pre-disassembly calculations, which calculates coolant voiding, fuel melting, fuel and clad deformation and molten fuel slumping, is being developed. For the disassembly phase a computer code DISA is developed. This solves point kinetics equations coupled with two

<table>
<thead>
<tr>
<th>Parallel System</th>
<th>No. of Slave processors</th>
<th>Solver CPU time (sec)</th>
<th>Speed-up by parallelisation</th>
<th>Parallel efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANUPAM-PC</td>
<td>Sequential</td>
<td>803</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>410</td>
<td>1.95</td>
<td>97.5 %</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>246</td>
<td>3.26</td>
<td>81.5 %</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>130</td>
<td>6.18</td>
<td>61.8 %</td>
</tr>
</tbody>
</table>

CPU times for Parallelised BiCGSTAB[ILU] for IQS Approach ($\epsilon = 10^{-4}$)
dimensional hydrodynamics equations. Figures show the equation of state for fuel used in DISA. The variation of net reactivity and power as function of time for a hypothetical transient in a typical fast reactor are shown in figures. It is planned to improve the neutronics model of pre-disassembly code by replacing the point kinetics calculations by multidimensional, multi energy group neutron diffusion code 3D-FAST. It is also planned to couple both phase calculations.

New concepts have emerged in the dynamics of nonlinear systems in last two decades. As part of our nonlinear studies in reactor physics we have studied some of these issues for a typical PWR. Here the dynamics refer to a single-phase coolant using point kinetics and a feedback through fuel & coolant temperature coefficient of reactivity. Typical scenario of limit cycle reactor operation were observed as a function of coolant temperature coefficient. The temporal behaviors can be identified for certain values of this parameter.

For a specific value of coolant temperature coefficient the critical state becomes an oscillatory state (limit cycle). This latter state constitutes a new operational regime for reactor dynamics. These studies contribute towards understanding safety and performance of reactors.
advanced heavy water reactor

‘XnWlup’ Software for Reactor Physics Applications

As a result of the IAEA coordinated research program entitled “Final Stage of the WIMS library Update Project” new and updated WIMS-D libraries are generated by processing evaluated nuclear data files such as ENDF/VI.6, JENDL-3.2 and JEF-2.2. These WIMS-D libraries provide knowledge about the various relevant neutron-nuclear cross sections data in the form of 69/172 neutron energy groups. In order to help the WIMS-D library users to quickly view the plots of the energy dependence of the multi-group cross sections of any nuclide of interest, a computer program ‘XnWlup’ is developed for MS-Win operating system using Microsoft Visual C++. It is also possible for the WIMS-D library users to compare the energy dependence of cross section data of various nuclides, different WIMS-D libraries and different temperatures.

The first version of this software ‘XnWlup1.0’ helps to obtain the histogram plots of the values of cross section data of an element/isotope as a function of energy. The second version of this software ‘XnWlup2.0’ is serving as an exhaustive equivalent handbook of WIMS-D cross section libraries for thermal reactor applications and used for comparing different WIMS-D compatible nuclear data libraries originating from various countries. The next version of this software ‘XnWlup3.0’ was developed to plot the cross sections of a resonant nuclide using resonance integral tabulated data of WIMS-D library for the given background dilution cross section and temperature. Also the revised software ‘XnWlup3.0’ is now capable of plotting either the resonance integral data as a function of dilution cross section for a selected temperature grid point or as a function of temperature for a selected dilution cross section grid point for a given resonance energy group.
Illustration of plots of absorption resonance integral data of $^{232}$Th at 600 K and for various background dilution cross sections.

T. K. Thiyagarajan <thiyag@barc.gov.in>