Basic Data, Computer Codes and Integral Experiments: The Tools for Modelling in Nuclear Technology

Enrico Sartori*

OECD/Nuclear Energy Agency, Issy les Moulineaux, France

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*sartori@nea.fr

Abstract

When studying applications in nuclear technology we need to understand and be able to predict the behaviour of systems manufactured by human enterprise. First, the underlying basic physical and chemical phenomena need to be understood. We have then to predict the results from the interplay of the large number of the different basic events: i.e. the macroscopic effects. In order to be able to build confidence in our modelling capability, we need then to compare these results against measurements carried out on such systems. The different levels of modelling require the solution of different types of equations using different type of parameters. The tools required for carrying out a complete validated analysis are:

- The basic nuclear or chemical data
- The computer codes, and
- The integral experiments.

This article describes the role each component plays in a computational scheme designed for modelling purposes. It describes also which tools have been developed and are internationally available.

The role of the OECD/NEA Data Bank, the Radiation Shielding Information Computational Center (RSICC), and the IAEA Nuclear Data Section are playing in making these elements available to the community of scientists and engineers is described.

Modelling ...

Modelling in the field of technological applications requires ***predicting*** the macroscopic behaviour of the system considered in a given situation. The role of a model is ***not forecasting***, but to predict "what-if" situations.

Systems consist of components and depending on the scale at which we analyse them, we have to look at quite different physical phenomena and aspects. The system considered might itself be a component of a system at a larger scale: e.g. a nuclear power plant is a component of the world's electricity generation system. A model of performance of an overall electricity system will not include specifically reactor physics models.

The core of a reactor in a nuclear power plant can be seen for certain aspects, as the place where the heat is produced that is required to drive the turbines for electricity generation. A model could simply concern effective ways of removing that heat and achieving efficiency in electricity generation. The heat generation or power of a reactor depends however on the size of the reactor, the detailed composition and configuration of the nuclear fuel and the neutron flux level. The behaviour of fuel, while it is burned, depends on a number of phenomena such as how well heat produced in the fission process is conducted across the fuel pellet, through the gap to the cladding and to the coolant, the release of fission gas, etc. Reactor physics on the other hand has to model among others the maintaining of balance in the neutron economy through the cycles in the reactor. The balance is determined by the different microscopic nuclear physics phenomena: e.g. capture, fission etc. The fission process in itself opens a new world of complex modelling, mostly of phenomenological nature. Reactor physics or radiation transport does not zoom into this lower level scale. They simply take up these microscopic models in the form of nuclear data and in many cases they are simply taken for granted. The nuclear cross sections themselves are obtained from nuclear models and experiments, which are independent of reactor physics. These describe the interaction of elementary particles such as neutrons or photons with nuclides of the different materials composing the system. Should we zoom in even further, we would soon reach the basic physics models concerned with the components of the nucleons.

At each given level of scale we have a relatively large set of components from the lower scale playing together. Macroscopic behaviour of a system is the result of the symbiosis and synergy of such diverse and extraordinarily large numbers of microscopic events. ***At each scale*** the models used address ***different phenomena*** which seen from the lower scale are each time macroscopic.

In fact at every different scale different physical laws are prevailing that determine the behaviour of the ensemble. In our specific case we start with the Dirac or Schrödinger equation, then with the Boltzmann equation and depending on the problem the heat-conduction -, Navier-Stokes - and constitutive equations. Objects in the physical world as they cluster in large groups get organised by different physical laws.

In practice it is not possible to predict the behaviour of a system starting from first principles at the most basic level. It is already very difficult to derive the 'macroscopic behaviour' at the next higher level starting from the lower level.

... and Measurement

The *cornerstone* of knowledge is measurement. Without it a hypothesis in a physics model cannot be proven. Measurement consists in comparing as precisely as possible with something else, and establishing a quantitative relationship with it. Measuring can also affect the measurement itself. Also measuring one aspect may destroy the ability of measuring another. Measurements are normally not really straightforward.

Measurements are never exact; they have associated uncertainties - confidence bounds. If they concern a single quantity, the measured values have probability distributions that can be expressed in the form of a series. A convenient way to express such distributions is the moments of distributions. The fist moment is called also the expectation value and the second moment its the variance or 'error'. In physics we deal with many variables and the measurement of each is not necessarily independent of the others. In this case the expectation of the sum of variables is the sum of expectation of each variable. However, the variance of a sum of variables is the sum of the single variables only if they are independent. If they are not independent we say also they are not orthogonal to each other. The uncertainties of sets of parameters are expressed by so called ***covariance matrices***.

Experimental data with no 'error bars' are of no use because they would assume zero variance, complete independence and that one should have absolute confidence in them. This goes against the concept of measurement. Experiments do not provide physical information, but measurements. It is the responsibility of the physicist or engineer to deduce physical information from both the measurement and the knowledge of the behaviour of the experimental setting. In other words, measurements need interpretation for extracting information. Confidence intervals can be trusted only when the rigorous procedure used to derive them is documented.

... together with Sensitivity Analysis

The models we are using depend on the scale at which we are carrying out the investigation and the context of it. Models aim at predicting *macroscopic* or *output* or *target* quantities. The models are driven by input parameters describing the specific problem we intend to tackle. The model itself describes the interrelation of or physical laws governing the 'varying' and constant parameters. The number of input parameters can vary depending on the refinement at which we wish to conduct system behaviour simulation. Once we have defined what our *'target'* quantities for our model are we may well wish to ask the question, which of the input parameters are the most influential ones in determining the output? Which ones are unimportant or negligible? Fortunately, we have a method that can help us in answering such questions and to verify that all important variation in the system are taken care of as far as our target output is concerned. This method is the Sensitivity Analysis (SA).

SA aims to ascertain how a given model (numerical or otherwise) depends upon the information fed into it. It is a powerful method to answer ***what-if*** questions. Sensitivity analysis is of particular importance to model developers for identifying those processes and parameters requiring particular attention. It is a guide for model improvement, including in our case for data improvement as well as to model simplification. Sensitivity analysis codes have been developed rather early as compared to general uncertainty analysis codes because they are very useful also without covariance data as they give important insight into model characteristics.

The scope of SA is much wider as it may be coupled to optimisation / search algorithms; by identifying the most important parameters. SA may allow the dimensionality of the space where the search is made to be reduced. Derivative-based sensitivity analysis methods have been used extensively in reactor physics and radiation transport. This method has proven effective for linear systems. However, many of the reactor physics and radiation transport models are linear.

... lead to a valid Uncertainty Analysis

Uncertainty Analysis (UA) aims at quantifying the uncertainty in what comes out of the model. Uncertainty Analysis and Sensitivity Analysis go hand in hand. Sensitivity analysis' role is also to decompose the uncertainty in model outcome according to source or input in an exhaustive fashion, i.e. without any residual variation left unaccounted for.

Many reactor physics and radiation transport calculations aim at an accurate prediction on integral design parameters of power reactors. UA in nuclear engineering is essential to determine the confidence one can place into results from design calculations and simulation of operating facilities, and to identify areas where the input data need improvement. A combination of uncertainty and sensitivity analysis is also essential in model validation.

There are several sources of uncertainty, including those due to model simplification, discretisation of variables, numerical algorithms, and finally all those related to model input data. The latter comprise both physical constants describing the basic phenomena underlying the physical processes such as interaction of cross-sections and others related to composition and geometrical dimensions of materials specific to the problem.

A number of computational tools have been developed to assess the different uncertainties. Uncertainty analysis relative to data consists of several phases:

- The data evaluation process requiring least square methods for estimating expectation values for cross-sections and their covariances, verification of their physical and mathematical properties
- Processing the cross sections and covariance matrices into a suitable form for applications (e.g. energy multi-group form)
- Sensitivity and Uncertainty analysis relative to specific target or output quantities characterising the system performance.
- A consistency analysis of the data and a possible improvement through adjustment.

Uncertainty Analysis (UA) and Sensitivity Analysis (SA) of model output can assist both in model verification and validation. Verifying that the model does not exhibit unexpected strong dependencies upon expected non-influential parameters is a valuable element of quality assurance. Likewise, by assigning a range of uncertainties to the input parameters, the mean value of the model prediction can be estimated and compared with observation. Unacceptably high deviations can be tracked back to unrealistic parameter value ranges with an iterative procedure, which allows model and data to be verified.

... and to a Consistency Analysis

When experimental values corresponding to output or target quantities exist, consistency analyses between the observations and the parameters used together with parameter adjustments can be carried out with the help of the sensitivity and covariance information. In the adjustment procedure in addition to the adjusted parameters, new covariance information is produced containing the new variances and correlations. It is very important that the right covariance information is used for the different situations.

The purpose of ***data adjustment*** is improved agreement between computer model results and measurements made in the system investigated or specific experiments or mock-ups devised to resemble it. Data adjustment is often also criticised as it may well improve agreement with available measured target quantity data but lead to unphysical changes in the parameter data and disagreement with unmeasured, and frequently more important model output data. Adjustment methods always indicate where the input parameters need change or improvement to predict measured macroscopic effects. However adjustment, if not used with care and detailed analysis, may simply correct deficiencies in the computational models used, like insufficient fine mesh in energy, space and angle, deficiencies in the basic data reduction methods adopted, geometrical approximations and insufficient knowledge of material compositions. Data adjustment methods are however the tools that provide a useful feedback to basic data evaluators. It also provides a wealth of information on the quality of the input data and the model used.

Comprehensive codes devoted to SA and UA analyse the consistency of a set of differential and integral nuclear data, adjust the differential nuclear data to improve agreement with integral observations, and identify inconsistent data. Linear perturbation theory is used for the sensitivity calculations. Data consistency and adjustment computations use least squares techniques.

Tools Required for Modelling

The three basic components required for modelling in nuclear energy applications are:

1. **basic nuclear data, material properties data, chemical-thermodynamics data and derived**
   application data libraries, group constants, continuous energy data. The basic particle interaction data is described in numerical form in ***evaluated nuclear data*** libraries such as ENDF/B-VI, JEF-2, JENDL-3 and others. These libraries are very general and describe within the energy range considered (10^{-5} - $2{\cdot}10^{7}$ eV) all basic phenomena (neutron interaction cross-section, photon production, photon interaction cross-section, fission yields and radioactive decay data). These contain information in great detail and in a form not directly usable by computer codes. There is consequently a need to filter out relevant information and to condense it to a form

appropriate for applications (e.g. multi-group cross-section libraries, continuous energy cross-section libraries, etc.). The computer code system most widely used for that purpose is NJOY.

Detailed information on these data can be found for example by visiting the following Web sites:
USA:
http://www.nndc.bnl.gov/ (National Nuclear Data Center- Brookhaven - NNDC)
http://epicws.epm.ornl.gov/rsic.html (RSICC)
http://t2.lanl.gov/data/data.html (LANL)

Europe:
http://www-nds.iaea.or.at/ (Nuclear Data Centre IAEA)
http://www.nea.fr/html/dbdata/ (OECD/NEA Data Bank)
http://csnwww.in2p3.fr/amdc/ (Atomic Mass Data Centre)

Japan:
http://cracker.tokai.jaeri.go.jp/index.html (JAERI Nuclear Data Center)

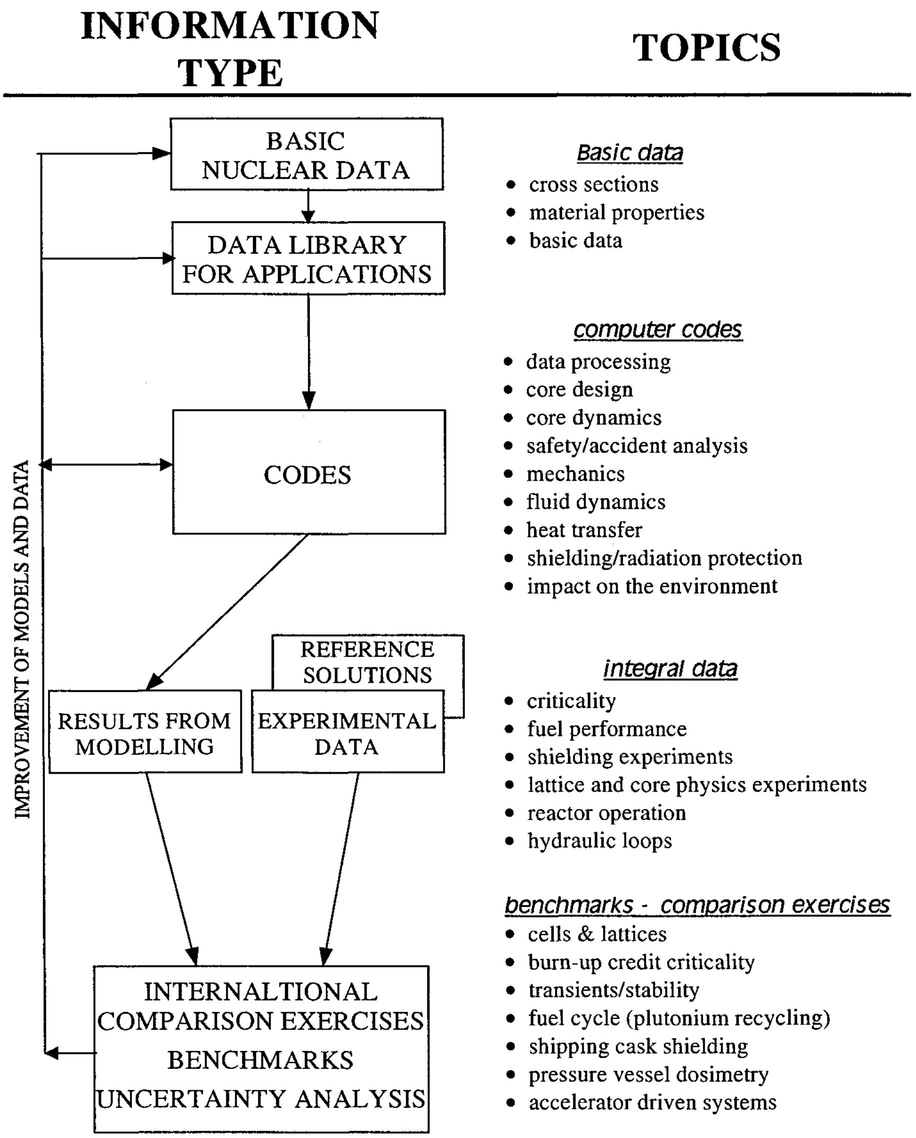
Other basic data such as TDB (***chemical thermodynamics*** data needed for speciation studies - http://www.nea.fr/html/dbtdb/) and MATPRO (http://www.nrc.gov/RES/SCDAP/nrc.html) for ***material properties*** are available. Many other basic data are distributed together with the computer codes using them.

2. **computer codes carrying out different modelling aspects such as:**

- nuclear models
- experimental data processing
- basic and evaluated data processing,
- spectral calculations, reactor cells and lattices
- multi-dimensional radiation transport, criticality , power distributions
- radiation shielding, heating and damage
- isotopic inventories, burn-up and build-up
- in-core fuel management, economic aspects of the fuel cycle, optimisation
- reactor dynamics, coupling of neutronics and thermal-hydraulics
- heat transfer and fluid flow,
- fuel behaviour
- deformations, stress and structural analysis,
- radiological safety, hazard and accident analysis
- environmental impact, confinement and dispersion in geosphere, biosphere and atmosphere

The computer codes used in most nuclear applications have the role of bridging the gap between the underlying microscopic phenomena and the macroscopic effects. They also accumulate, in a readily usable way using a mathematical and algorithmic language, the wealth of physics knowledge that science and technology have acquired during the last half century. In many cases these computer codes can have a relatively complex structure: in addition to several modular codes they also contain associated data libraries (for generic applications or project oriented), application dependent code/data sequences, test problems, etc.

Fig. 1: Procedures, Data and Computer Codes for Model Validation and Improvement



Basic data

- cross sections
- material properties
- basic data

computer codes

- data processing
- core design
- core dynamics
- safety/accident analysis
- mechanics
- fluid dynamics
- heat transfer
- shielding/radiation protection
- impact on the environment

integral data

- criticality
- fuel performance
- shielding experiments
- lattice and core physics experiments
- reactor operation
- hydraulic loops

benchmarks - comparison exercises

- cells & lattices
- burn-up credit criticality
- transients/stability
- fuel cycle (plutonium recycling)
- shipping cask shielding
- pressure vessel dosimetry
- accelerator driven systems

Many computer codes for nuclear applications are in the public domain, but there is also proprietary software that is widely used. The best sources for computer codes in the nuclear energy fields are as follows:

USA:
ESTSC (Energy Science and Technology Software Center – DOE-OSTI Oak Ridge)
http://www.osti.gov/estsc/

RSICC (Radiation Safety Information Computational Center – ORNL Oak Ridge)
http://www-rsicc.ornl.gov/rsic.html

International:
OECD/NEA Data Bank – France (http://www.nea.fr/html/dbprog/)
A computerised and searchable program abstracts database is available free of charge on CD-ROM.

These codes, before they are released, are subject to a series of tests, model validation and benchmarking. Their scope includes practically all the important aspects of modelling in nuclear technology applications.

3. integral experiments data bases

- shielding experiments
- criticality experiments
- reactor core and lattice experiments
- data from reactor operation
- fuel behaviour experiments
- thermal hydraulic loops experiments
- seismic and material strength data bases

Integral experiments are the references needed for model development, verification, and validation.

International Benchmark Studies

What is a benchmark?

The term means a fixed 'point of reference' used in comparisons. For our purpose it can take two different forms:

1. ***theoretical benchmark***, an 'exact' reference to a specified precision, obtained by solving mathematical equations describing a physical phenomenon or process. While a theoretical benchmark is an exact solution to a mathematical problem, it does not make statements about the precision in predicting the physical phenomenon itself. It simply asserts what the measure of the physical phenomenon would be if the equations represented exactly the

physical world. Theoretical benchmarks are used essentially to validate approximations inherent to algorithms used in large computer codes and their correct coding,

2. ***experimental benchmark***, a well designed and instrumented measurement, addressing a well-defined physical phenomenon or aspect thereof. Some of them are called 'clean' because the experimental set-up used contains few and relatively simple components, which facilitates meeting the objective of unfolding the requested data. It consists of a precise description of the apparatus, geometrical set-up and data analysis tools. The experimental benchmark data have associated uncertainties, the derivation of which is precisely documented. Experimental benchmarks are needed to validate the physics models used in the computer codes together with the associated basic data used to describe for instance the microscopic phenomena underlying the macroscopic behaviour. They are normally used to check the correct ***integral*** behaviour of algorithms and the basic data working together.

Both types of benchmarks are widely used. They have a complementary function. Theoretical benchmarks often cover also aspects, which would otherwise be difficult or too expensive to measure. The community concerned with establishing well qualified computing tools for the design and operation of nuclear technology facilities has established international co-operations to facilitate the comparison of their methodologies. International comparison exercises (called also standard problems) have been designed covering the diverse needs of methods validation. The purpose of such comparison exercises is twofold:

- familiarisation with working methods and assumptions made by experts from different teams
- assessing the own skills in modelling, gaining experience and building confidence in the methods used

Role of code comparison and benchmarks

Essentially three elements are required to ensure modelling tools meet the requirements of nuclear industry and licensing needs:

- state of the art computer code design and programming according to quality assurance principles
- quality assurance in maintenance of the code
- model assessment and validation of codes through benchmarking and code comparison exercises.

There is a further element of different nature. Even though a code has undergone the best development and validation praxis, the quality of the results depend in the end from the user. Therefore user qualification through training courses is essential. One of the best training methodologies is benchmarking and comparison with others. In such a procedure much is learned about how a well-defined problem can be translated into input to a code. The sensitivity and uncertainty analysis that normally goes with benchmarks give much insight into the role basic data used, the implication of their uncertainty onto the results, in other words a wealth of understanding is achieved.

Over the years the OECD/NEA NSC has organised a large number and comprehensive set of international comparison exercises. A list is provided as Annex I. They have been instrumental for achieving model improvements and ensure a common understanding of modelling issues.

Integral Experiments Data Bases

A large series of essential experiments concerned with nuclear energy and technology have been carried out during the last several decades in different research laboratories. This has required a large investment in terms of infrastructure, expertise and cost. Results from these experiments remain of great value today as they provide the record and the basis for the development and validation of methods and represent a significant collection of data for past, present and future research. Data reports also document measurement methods and techniques that have been developed over the years. It is also unlikely that any of these experiments will be repeated again in the future.

Integral experiments concern measurements on a system consisting of different components. The measured values are the macroscopic behaviour of the system (e.g. attenuation of dose through a complex shield, level of reactivity of a reactor or a spent fuel transportation cask, decay heat, level of burnup, etc.). They allow to gauge the combined use of computational methods and basic data used to the real world values. At the beginning of nuclear reactor development, computational methods were still in their infancy, the models used did not include sufficient knowledge to make reliable predictions. Integral experiments were then 'the reference' to be used for any design.

Integral experiments come with clearly stated and documented uncertainties in the form of confidence bounds of the measured values and a correlation matrix describing the relative independence of the measurements carried out. An integral experiment is complete if it includes a final phase of interpretation of the results. The interpretation is the part that gives insight into the phenomena and into the way they are appropriately modelled.

Computer codes and basic nuclear data have been thoroughly checked on a number of cases, be it known reference solutions or experiments. However, the number of possible combinations of their use is so big that a large and possibly comprehensive database of well-characterised experiments is needed. With such databases sufficient confidence can be built that methods and procedures used for design, operation and safety analysis are adequate.

Nuclear industries and licensing authorities need to be able to rely on the good performance of computer programs and nuclear data in all important nuclear energy calculations. It is important that the methods and data issued should be internationally accepted. This is best achieved by validation and benchmarking on an international scale, with all countries concerned participating in the testing.

List of different integral databases

In the following a few integral databases are described that have been established through the OECD/NEA:

FUEL BEHAVIOUR

A Public Domain Database on Nuclear Fuel Performance or the Purpose of Code Development and Validation (IFPE)

Visit → http://www.nea.fr/html/science/fuel/ifpelst.html

CRITICALITY SAFETY

International Criticality Safety Benchmark Evaluation Project (ICSBEP)

Visit → http://icsbep.inel.gov/icsbep/

Spent Fuel Isotopic Composition Database (SFCOMPCO)

Visit → http://typhoon.tokai.jaeri.go.jp/sfcompo/index.html

Fission Product Decay Heat Data

Visit: → : http://www.nea.fr/abs/html/nea-1606.html

Basic Minimum Values of Criticality

Visit → http://www.nttl-net.ne.jp/nais/data/data.htm

Fuel Burnup Profiles

Visit → http://www.nea.fr/abs/html/nea-1607.html

THERMAL HYDRAULICS IN NUCLEAR POWER PLANT

CSNI Code Validation Matrix of Thermal-Hydraulic Codes for LWR LOCA and Transients (CCVM)

Visit → http://www.nea.fr/html/dbprog/ccvm/

REACTOR PHYSICS

Reactor lattice and core experiments

Project initiated in 2000

Data from Reactor Operation

http://www.nea.fr/abs/html/nea-1454.html and http://www.nea.fr/abs/html/nea-1551.html

RADIATION SHIELDING EXPERIMENTS (SINBAD)

Visit → http://www-rsicc.ornl.gov/benchmarks.html and
For reactor shielding: http://www.nea.fr/abs/html/nea-1517.html
For fusion neutronics: http://www.nea.fr/abs/html/nea-1553.html
For accelerator shielding: http://www.nea.fr/abs/html/nea-1552.html

Conclusions

Apart from well-defined procedures and measures designed to facilitate interfacing the control of the machine through human activity, economical and safe operation of nuclear installations also require a set of well validated and quality assured analytical tools. Integral experiments and benchmarks are essential, basic components of validation and quality assurance procedures for modelling systems in nuclear technology applications. Without them it is not possible to built confidence in the computational methods and associated basic data used. The benchmarking exercises based on integral experiments in addition provide an effective means of self-assessment, self-training and building confidence in the capacity of translating an experimental set-up into a model-input for computational tools..

International centres have been established to facilitate the sharing of such tools worldwide. Such data are available at international level from the OECD/NEA Data Bank and other co-operating organisations

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Annex - List OECD NEANSC Benchmarks

General Benchmark Topics

- *Reaction Cross-sections/Reaction-yields Data*
    - for evaluated nuclear data file production - filling gaps
    - experiments: EXFOR Data Base - 40 years of measurements

- *Reactor Physics*
    - reactor cells and lattices
    - cores
    - recycles

- *Core Transients*
    - neutronics - thermal-hydraulics - coupling

- Radiation Shielding
    - PV dosimetry
    - shipping casks

- *Criticality Safety (away from reactor)*
    - Handling
    - storage
    - transportation
    - fuel dissolution

- *Fuel Performance*
    - basic phenomena - normal operating conditions
    - experiments data base

REACTOR PHYSICS BENCHMARKS

- *Power Distribution Within Assemblies (UOX, MOX configurations)*
    - Pin Power Reconstruction Methods
    - Comparison of Production Codes including Data Reduction

- *High Conversion Light Water Reactors*
    - MOX fuelled - tight lattice
    - cells and void reactivity coefficients

- *Physics of Plutonium Fuels, Innovative Fuel Cycles*
    - MOX Pin cell arrays (recycle 1 and 5) (PWR)
    - Void reactivity coefficient (recycle 1 and 5) (PWR)
    - MOX Burnup, 1st cycle (FR)
    - Metal Pu Fuel recycling (FR)

  - Multiple Pu Recycling in Standard and Advanced (High Moderation) PWR
  - BWR MOX benchmark
  - VENUS-2 benchmark experiment
  - KRITZ benchmark experiment
  - Accelerator driven system for actinide and fission product burning

- *3D Radiation Transport (Control Rod Worth) (Takeda)*

RADIATION SHIELDING BENCHMARKS

- Reactor Shields
- Reactor Pressure Vessel Dosimetry (VENUS-1 & 3)
- Shipping Cask Shielding
- 3D Deterministic Transport Theoretical Benchmark
- Experiments Data Base (SINBAD) (fission, fusion, accelerators)

CRITICALITY SAFETY BENCHMARKS (away from reactor)

- Storage (wet - dry)
  - Burnup Credit

- Transport - Shipping Casks
  - .Burnup Credit (Safety Margins, burnup profiles)
  - PWR, BWR, MOX spent fuel

- Minimal Critical Masses

- Criticality Safety Experiments Handbook (ICSBEP)
  (2000 critical configurations - CD-ROM, WWW)

CORE TRANSIENTS BENCHMARKS

- Rod Ejection (PWR)
- Cold Water Injection / Pressurisation (BWR)
- Rod Withdrawal at Zero Power (PWR)
- BWR Stability - Ringhals1
- Time Series (BWR) Forsmark 1 & 2
- Main Steam Line Break (PWR)
- BWR Turbine Trip benchmark