Directions in Radiation Transport

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ABSTRACT

This paper examines different directions in radiation transport covering improvements in high performance computing (HPC), multi-physics applications and advanced radiation transport modelling. HPC takes advantage of increases in clock speed and the continued evolution of parallel computer architecture and the paper provides an update of latest experience. An example is given of the speedup obtained using the ANSWERS MONK code on a BEAVRS benchmark application. The two-way transfer of data in multi-physics modelling presents a challenge and various methods for solving fully coupled, non-linear models are surveyed. Along with other examples, the paper shows a fissile solution criticality excursion application involving strongly coupled neutronics and thermal-hydraulics modelled via the Imperial College FETCH code. The paper describes the extensive work carried out on the validation and benchmarking of simulation tools, which includes broadening their range of application by replacing empirical correlations with fundamental physics, together with latest work on uncertainty quantification methods. Adaptivity methods for computational mesh refinement are under development and the paper discusses different methods of adapted spatial and angular discretization. Finally the paper considers hybrid modelling methods which involve a combination of deterministic and Monte-Carlo simulations to improve modelling performance. An example is given where performance is improved by a factor of hundreds.

1. INTRODUCTION

Radiation transport modelling has been around for a long time, for instance the WIMS, MONK and MCBEND codes were in use in the UK nuclear industry in the 1960s, with applications in the fields of reactor physics, criticality and shielding, respectively e.g. [1].

Modelling has come a long way since those early days: whereas 2D simulation was the norm, 3D models are now common; multi-group energy schemes have been replaced by continuous energy nuclear data representations in Monte Carlo models; finer multi-group schemes have evolved for deterministic codes, with hundreds or thousands of energy groups; and approximate geometries have been replaced by accurate 3D geometrical representations and geometry can be imported from CAD files.

More exciting advances are on the horizon to increase the power of simulation tools. The advent of high performance computers is allowing bigger, higher fidelity models to be created, if the challenges of parallelization and memory management can be met. 3D whole

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core transport modelling is becoming possible. Uncertainty quantification is improving with large benefits to be gained from more accurate, less pessimistic estimates of uncertainty. Advanced graphical displays allow the user to assimilate and make sense of the vast amounts of data produced by modern modelling tools. Numerical solvers are being developed that use goal-based adaptivity to adjust the nodalisation of the system to provide the optimum scheme to achieve the user requested accuracy on the results, thus removing the need to perform costly convergence studies in space and angle etc. More use is being made of multi-physics methods in which radiation transport is coupled with other phenomena, such as thermal-hydraulics, structural response, fuel performance and/or chemistry in order to better understand their interplay in reactor cores.

2. BEGINNINGS

This section describes some of the key milestones in radiation transport modelling development. Early codes developed out of post-war nuclear weapons programs [2]. Two neutron transport codes using the Monte Carlo method were the O5R code from Oak Ridge and the GEM code in the UK [3]. The GEM code was the forerunner of the MONK criticality and reactor physics code [4] that is one of the ANSWERS suite of radiation transport codes [5, 6]. The ANSWERS codes have been around for 50 years and have been in use in the UK since the 1960s e.g. [1]. In addition to the MONK criticality code the ANSWERS suite also contains the WIMS (Winfrith Improved Multi-group Scheme) deterministic reactor physics code [7] and the Monte Carlo MCBEND (M^{c}Cracken and BENDall) shielding and dosimetry code [4].

Over the intervening fifty years great improvements have been made in radiation transport modelling. It is now possible to model highly complex geometries and to import the geometry from CAD files produced when designing radioactive facilities [8]. Codes have been parallelised to allow them to run faster on modern parallel computer architectures [8]. Databases of experimental data have been compiled to facilitate validation of the increasingly complex modelling codes, such as the ICSBEP database for criticality data [9], the IRPhE database for reactor physics data [10], SFCOMPO for burnup data [11] and the SINBAD database for shielding data [12, 13].

In the field deterministic modelling codes, 1D/2D solvers have been replaced by 3D calculations [7] and the number of energy groups available for calculation has increased from several tens [1] to thousands [5]. Equivalence theory for resonance self-shielding has been replaced by a more accurate sub-group treatment [14] and lattice transport calculations coupled to whole core diffusion calculations are used to provide accurate simulations of whole core behaviour [15]. In Monte Carlo codes, a continuous energy representation of the nuclear data is used [4], allowing the full accuracy of the evaluated nuclear data files to be gained and the Woodcock tracking method [16] allows geometries of enormous complexity to be constructed in relatively short times. The use of automatically generated importance maps allows the performance (figure of merit) of shielding calculations to be improved by a factor typically of order a hundred and for criticality calculations, the use of super-history powering [17] (or equivalently Wieland acceleration [18]) reduces bias in the estimation of the multiplication factor and its associated uncertainty.

The impressive progress made over the last fifty years is set to be eclipsed by research currently underway in numerous areas, some of which are discussed below.

3. HIGH PERFORMANCE COMPUTING

HPC developments are crucial in realizing efficient radiation transport simulation. One of the main drivers for code development at the current time is the continued evolution of parallel computer architecture. When computer speedup was driven by increases in clock speed, a computer program could remain unaltered and still benefit from an upgrade to a faster computer. Now that computer speedup generally results from increased parallelism, upgrading to a faster computer will not automatically result in improved performance of a program, unless it has been written to take advantage of parallel architectures and distributed memory. As noted in Section 2, older software has had to be rewritten in recent years to take advantage of parallel architectures, but this is only a start as computer architectures continue to evolve. For example, consider a MONK calculation employing MPI (message passing interface) to distribute the calculation over multiple nodes of an HPC. Figure 1 shows an example of such a calculation for the BEAVRS benchmark. The original scaling results on the INDY HPC show approximately linear scaling for high numbers of processors (only roughly 50% efficiency is obtained as this calculation was performed without the use of a parallel fission bank algorithm). Re-running the scaling study on a more modern computer with similar architecture using faster processors (Enigma) it is seen that the performance saturates above about 100 cores. Thus parallel algorithms that appear to be taking full advantage of parallel architecture at one time may be found to be in need of improvement when the next generation of computers arrives.

Typical HPC architectures consist of a number of nodes with multiple processors on each node and a standard way of taking advantage of such architectures is to use MPI to distribute the calculation across many nodes and multi-threading (such as OpenMP) to distribute the calculation between the different processors on each node while sharing the memory on each node, i.e. hybrid MPI/OpenMP [19]. Even then further improvements may be obtained by careful memory management, ensuring that the required data are close to the processor when needed, to minimise communication costs. Further steps may be needed to take full advantage of distributed memory. Large calculations requiring more memory than there is available on an individual node, can often be achieved by employing some form of domain decomposition [20] in which the problem data are divided between multiple nodes. Modern massively parallel computers continue to increase the number of processors available, though the memory does not increase in proportion to the number of processors. Typical modern architectures may contain a mixture of “fat Cores” with associated high capacity, low bandwidth memory and “thin cores” with associated low capacity, high bandwidth memory [21]. Codes must be optimised to take full advantage of such heterogeneous architectures. This may place a significant burden on code developers and therefore some institutions are developing high level languages to be used by the code developers, which use lower level libraries to allow the code to be compiled on different computer architectures. An example is Imperial College’s Firedrake project for the solution of PDEs using the finite element method [22] which makes use of the OP2 project at Oxford University which is developing a framework for applications on clusters of CPUs or GPUs [23].

On a smaller scale, the humble laptop or desktop also benefits from increased numbers of processors on the mother board with high capacity memory and significant processing power on the graphics card in terms of GPU cores with low capacity memory. Making use of both of these resources could result in significant performance improvement for desktop users.

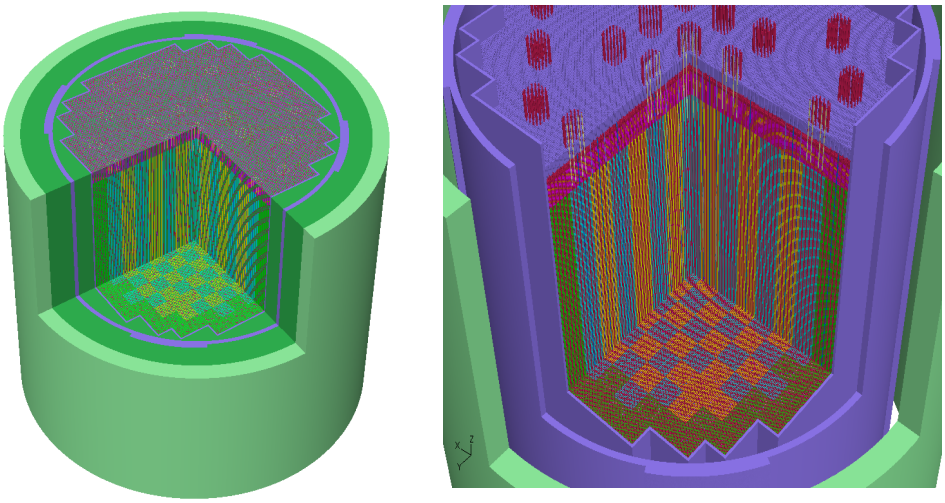


Figure 1a: MONK BEAVRS Model

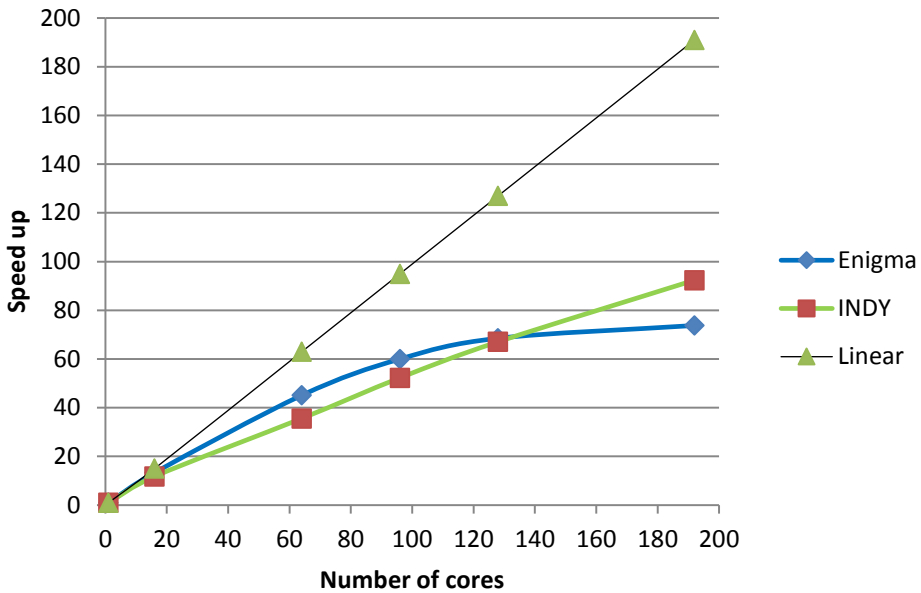


Figure 1b: MONK Scaling for BEAVRS Calculation

4. MULTIPHYSICS

Holistic simulation of nuclear plant performance is an increasing requirement from reactor designers, operators and regulators. The simulation of various parts of a nuclear power plant can require models of a range of physical and/or chemical process, such as: neutronics/radiation transport, thermal-hydraulics, structural response, fuel performance and chemistry. In the UK, EdF Energy have developed a suite of codes to model gas-cooled

reactors, including: PANTHER (Pwr and Agr Neutronics and Thermal-Hydraulics Evaluation Route) [15] for coupled neutronics and thermal-hydraulics, FEAT (Finite Element Analysis Toolbox) [24] for coupled thermal-hydraulics and structural response, ENIGMA [25] for fuel performance and GKM (Gas Kinetic Model) [26] for gas circuit chemistry. A number of the codes (including WIMS, PANTHER, VIPRE and ENIGMA) can be accessed via the RPW (Reactor Physics Workbench), which provides an interactive user interface and a sophisticated data management system [27]. PANTHER contains built-in subchannel thermal-hydraulics models for GCRs, PWRs and BWRs, and it can be coupled to VIPRE for DNBR and post dryout heat transfer or to RELAP for whole plant thermal-hydraulics. It can also be interfaced to ENIGMA, a generic UO2 fuel performance code to predict fuel temperatures, clad stresses and strains and fission product release.

When the interaction between phenomena is significant in only one direction the computer models for the phenomena need only be interfaced, passing data from one model to the other, usually via a file. On the other hand, if there is two way feedback between the models then full coupling is required in both directions. This is shown to be the case for core neutronics and thermal-hydraulics in [28]. This is why PANTHER has built-in, couple sub-channel thermal-hydraulics and full coupling is provided to the VIPRE and RELAP codes.

In addition, fluid drag, heat transfer and thermal expansion result in deformation of the solid structures that can feedback on the fluid flow. Therefore EdF Energy's FEAT code provides a CFD calculation of thermal-hydraulic behaviour with coupled structural response. For example, Figure 2 shows part of a boiler simulation, with 2a showing the predicted gas velocities and temperatures, 2b the structure temperatures, 2c the resulting structural deformation (greatly exaggerated to aid visibility) and 2d the resulting hoop stresses.

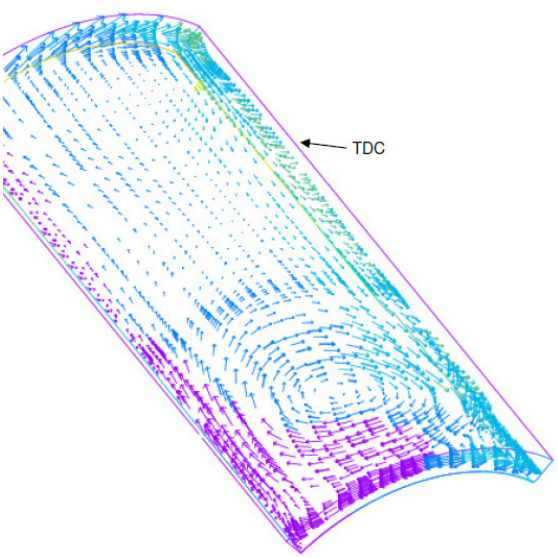


Figure 2a: FEAT CFD: Velocity vectors and fluid temperature

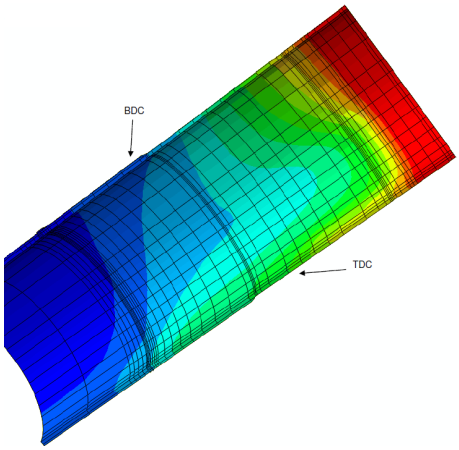


Figure 2b: FEAT Structure temperatures

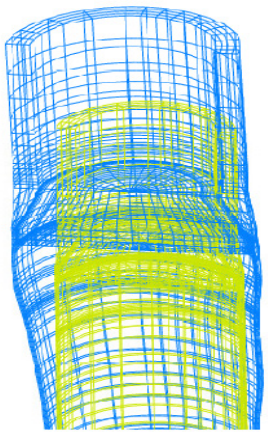


Figure 2c: FEAT mesh distortion (greatly magnified)

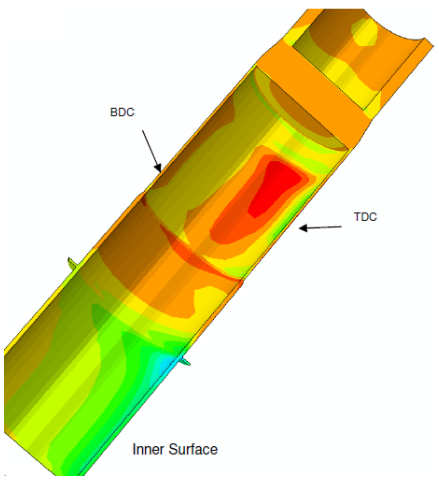


Figure 2d: FEAT Hoop stresses

The Imperial College FETCH code [29] consists of a coupling of the EVENT radiation transport code [30] to the FLUIDITY CFD code [31]. This has a wide range of application to strongly coupled systems, including criticality excursions in fissile solutions such as the Y12 [32] accident. Figure 3 illustrates the application to a fissile solution criticality excursion in the TRACY facility [33]. This involves strongly coupled neutronics and thermal-hydraulics, including advection of delayed neutron precursors, the chemistry of radiolysis of the solution, radiolytic gas bubble production, buoyancy effects of bubble production and thermal expansion, and advection of the bubbles.

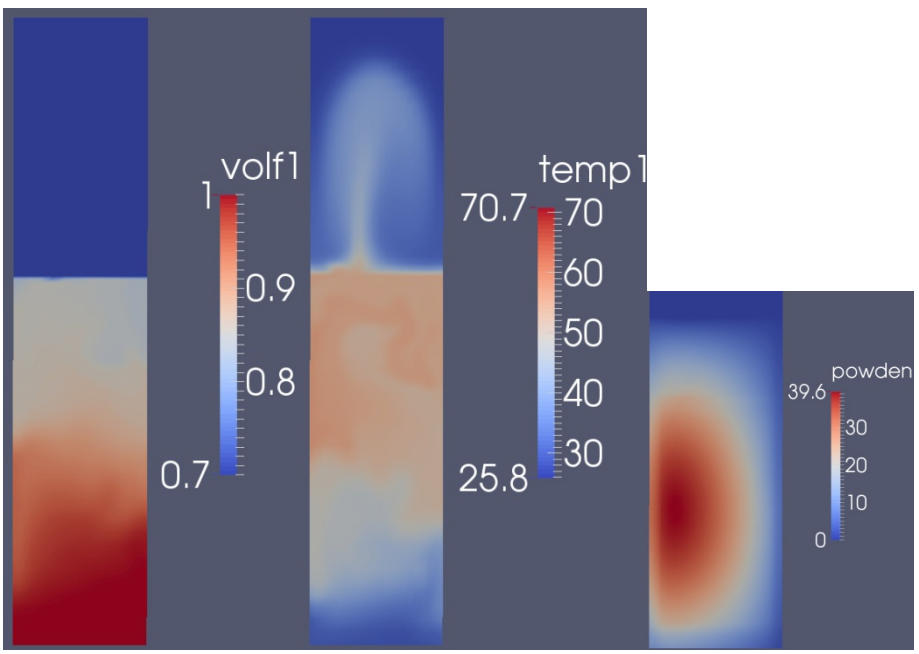


Figure 3: FETCH Results: volume fraction of liquid, temperature and power density

Multi-phase FLUIDITY is being developed to include two-way fluid-structure interactions via FEMDEM to model structure deformation and fragmentation and incorporating fluid interaction using the immersed body method [34]. In this approach, the Finite Element Method (FEM) is used to calculate the stresses and strains in the solid components and the Direct Element Method (DEM) is used to track the movement of individual solid components, incorporating interaction with the fluid via the immersed body approach.

With the advance of high performance computing, high fidelity simulation becomes possible in which empirical correlations are replaced by more fundamental physics, finer resolution of complex phenomena is possible and coupling of more phenomena can be achieved. To facilitate the coupling of multi-physics phenomena, a series of EU projects was set up to produce a platform for coupling existing codes. The NURESIM, NURESP, NURNEXT and NURESAFE [35] projects ran is series and resulted in the production of the SALOME platform [36], which is open source software distributed under the terms of the GNU LGPL licence. SALOME allows the user to create, modify and mesh CAD models

or import existing meshes, handle physical properties and quantities attached to geometrical items, perform coupled calculations using one or more external solvers and display the results.

In the USA, the Consortium for Advanced Simulation of Light water reactors (CASL) is developing the Virtual Environment for Reactor Analysis (VERA) with the aim of improving the performance of the current generation of LWRs [37]. The development is driven by a set of Challenge Problems that are important to the nuclear industry. Examples include crud induced power shift and accelerated corrosion, which are multi-physics problems involving neutronics, thermal-hydraulics, fuel performance and chemistry. VERA3.3 includes Method Of Characteristics (MOC), Sn, SPn and Monte Carlo radiation transport models, subchannel thermal-hydraulics, fuel performance and coolant chemistry capabilities. Coupled physics modules include MOC, Sn or SPn with subchannel thermal-hydraulics and MOC with subchannel thermal-hydraulics and fuel performance.

Another initiative for solving multi-physics equations is the Multiphysics Object Oriented Simulation Environment (MOOSE) being developed at INL to simplify the creation of fully coupled, nonlinear, multiphysics applications [38]. MOOSE has been developed to solve systems of coupled partial differential equations (PDEs) using Jacobian-free Newton-Krylov solution methods. More than thirty MOOSE-based applications have been created to date, including examples based on the KAIST-3A benchmark core, as well as a simplified Westinghouse AP-1000 configuration, to demonstrate this new framework for simulating coupled whole core reactor phenomena such as CRUD-induced power shift and fuel shuffle.

5. VALIDATION

The complexities of modelling nuclear plant response, particularly under accident conditions can be very great. Validation of modelling tools and their range of application is therefore a key requirement. As noted above, established databases of certified experimental data have been produced for validating and benchmarking modelling and simulation tools in the fields of criticality, reactor physics, burnup and shielding. With the growth in multi-physics capability there is a need to extend the range of validation and benchmarking to include thermal-hydraulics, fuel performance, structural response and chemistry. In some areas, such as thermal-hydraulics, a wealth of relevant experimental data has been generated, including data specific to nuclear applications. Organising available data into databases of certified data, like the ICSBEP. IRPhE, SFCOMP and SINBAD databases, would be of significant benefit to the modelling and simulation community. In addition, experimental data on coupled physical phenomena, i.e. multi-physics experiments, are required to validate multi-physics modelling and simulation tools.

Under the guidance of the OECD-NEA Nuclear Science Committee, the Expert Group on Multi-Physics Experimental data, Benchmarks and Validation (EGMPEBV) has been established [39] to advise on processes and procedures for using data and benchmark models for validation of modelling and simulation tools and data; in particular, for providing guidelines and consensus recommendations for validating multi-physics simulations. The group aims to provide member countries with guidance and processes for certifying experimental data for benchmarking or testing of modelling and simulation tools and access to certified experimental data from the contributions of individual member countries. The project aims to provide member countries with: guidance and recommendations for developing benchmark models from certified experimental datasets, access to standardized

benchmark models with detailed uncertainty evaluations and uncertainty methodology guidelines, recommendations and guidelines for the range of applicability of the certified experimental datasets and a limited number of demonstrations of the validation recommendations.

Alongside the move to multi-physics simulation is the move to high fidelity simulation, including broadening the range of application of models by replacing empirical correlations with fundamental physics. In 2012, an Engineering and Physical Sciences Research Council (EPSRC) Programme Grant was awarded to harness the synergy between research groups at Imperial College London (IC), University College London (UCL) and the Universities of Birmingham (UB) and Nottingham (UN) to carry out the next generation of research into Multi-scale Examination of MultiPHase physIcs in flowS (MEMPHIS) [40]. The Programme aims to develop a modelling framework utilising massively parallelisable numerical methods to resolve multi-scale, multiphase phenomena while minimising the reliance on empirical correlations. The theoretical developments are supported by model-driven experiments to guide the developments and validate the simulation tools.

The laboratories are equipped with a range of measurement techniques which are applied to characterise interface shape as well as the properties of the bulk flow field with an emphasis on regions close to surfaces and interfaces. This allows phenomena such as wave generation at interfaces and fluid interactions with droplets to be studied in detail. A wide range of measurement techniques is available at the participating laboratories including:

WMS/MFS, Wire Mesh and Multi-Film Sensors;
ECT/ERT , Electrical Capacitance/Resistance Tomography;
GRD/XRD, Gamma/ X-ray Ray Densitometry;
CP, Local conductivity probes;
LIF, Laser Induced Fluorescence;
LDA/PDA, Laser/Phase Doppler Anemometry; and
(μ)PIV, (micro-)Particle Image Velocimetry.

These allow fluid dynamic processes to be studied on a wide range of length and timescales, as illustrated in Figure 4.

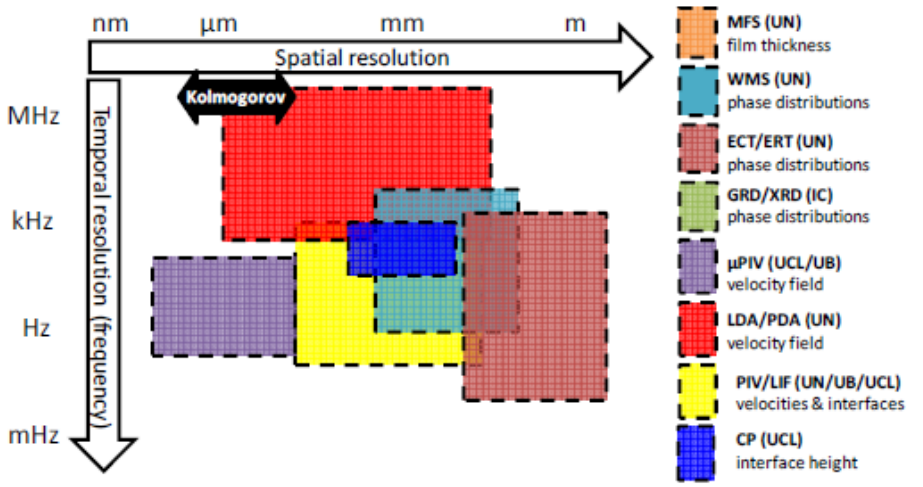


Figure 4: Resolution of available Measurement Capabilities in MEMPHIS laboratories.

The resulting experimental data will provide a valuable resource for validating aspects of high fidelity thermal-hydraulics models.

6. GRAPHICAL DISPLAY

High fidelity graphical display is important in interpreting outcomes of simulations but also in providing quality assurance of correct plant representation. With the advent of HPCs, the amount of data that can be generated by modelling and simulation tools has increased enormously. This raises the issue of how to present the data to allow the user to assimilate the important results on a practicable timescale. The Visual Workshop Integrated Development Environment (IDE) has been developed for use with the ANSWERS codes and includes numerous displays to visualise calculational results [8]. Reference 8 shows a number of ways in which sections of the domain can be visualised and results can be superimposed on the system geometry, including contour maps and colour coding; examples are shown in Figure 5. With the aid of 3D glasses, the results can also be displayed in 3D, allowing the user to walk through the geometry and follow individual particle tracks, for instance. Such multi-dimensional immersion graphics are an invaluable aid for understanding large quantities of data.

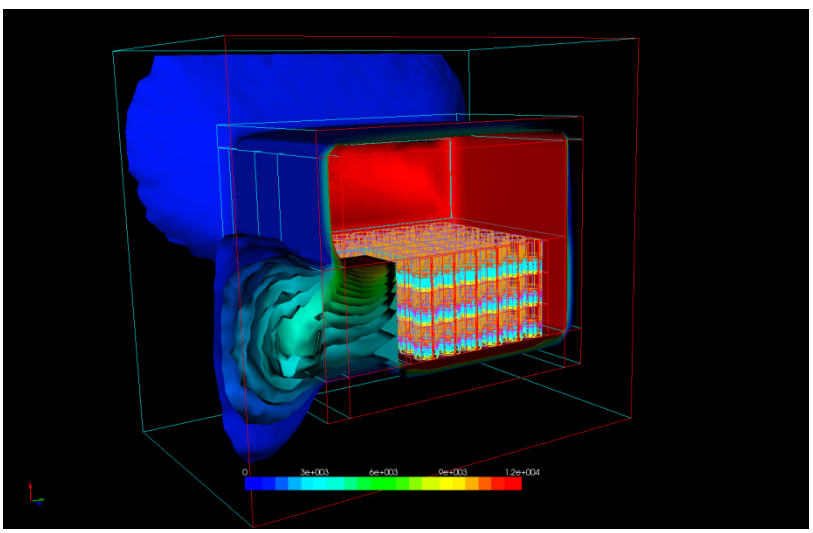


Figure 5: Dose Rate Contours superimposed on Geometry

The Data Science Institute at Imperial College acts as a focal point for the development of data management and analysis technologies and services for supporting data driven research in the College [41]. Housed within the Data Science Institute is the KPMG Data Observatory (DO) which is the largest of its kind in Europe. The observatory features an enveloping circular wall of 64 monitors powered by 32 computers providing 313 degrees of surround vision. The DO was opened in November 2015 and provides the means for users to visualise data in a way that uncovers new insights and promotes the communication of complex data sets and analysis in an immersive and multi-dimensional environment, for example see Figure 6.

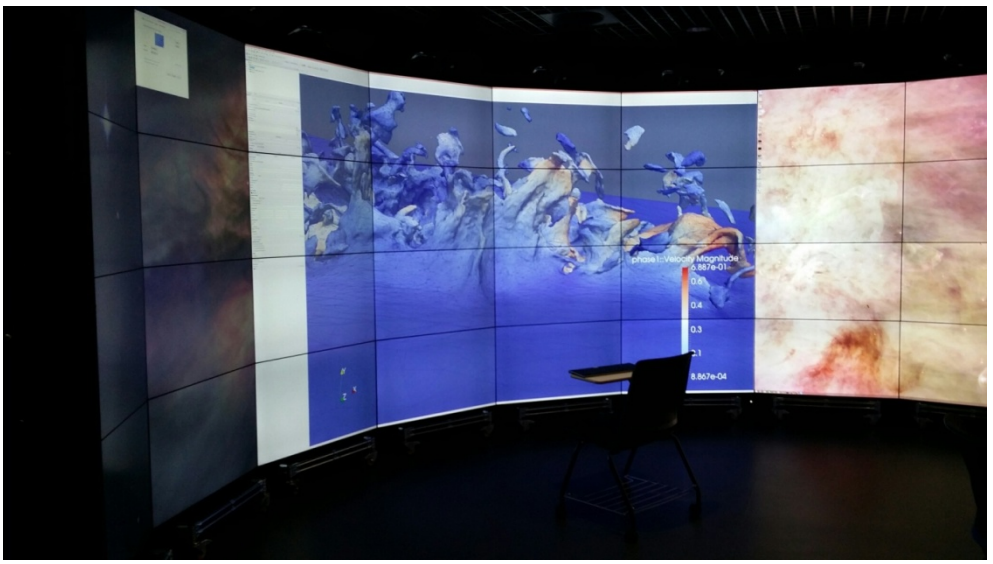


Figure 6: Data Observatory Display

7. UNCERTAINTY QUANTIFICATION

When calculating a physical quantity, it is important to have an estimate of the uncertainty associated with the calculated value. This is required in optimising plant performance and for avoiding excessive pessimism in ensuring sufficient safety margins. This is an area of intense international research in the nuclear industry at present. An overview of the uncertainty quantification tools developed for use with the ANSWERS suite of software was given at the ICNC 2015 conference [42]. A sampling approach is used to provide an estimate of the overall uncertainty. This is achieved by sampling input parameters from appropriate statistical distributions, using Monte Carlo, stratified or Latin Hypercube sampling to define and run a set of calculations. A set of sampled nuclear data libraries has also been produced to allow the uncertainty due uncertainty in the nuclear data libraries to be included in the evaluation. If factor analysis is required, to determine the main causes of uncertainty, a combination of sensitivity analysis [43] and response surface fitting is offered. Response surface fitting can include traditional techniques such as least squares fitting or methods currently being researched, such as high dimensional model representation and non-intrusive polynomial chaos [44].

A number of OECD NEA expert groups have been established to address issues related to uncertainty quantification. The expert group on Uncertainty Analysis for Criticality Safety Assessment (UACSA) was established to address issues related to Sensitivity/Uncertainty (S/U) studies for criticality safety calculations [45]. This has coordinated benchmark exercises on the evaluation of uncertainty arising from manufacturing tolerances and from nuclear data uncertainties. The current benchmark exercise addresses issues arising from correlated uncertainties resulting from multiple experiments performed in the same facility.

The expert group on Uncertainty Analysis in Modelling (UAM) was established to address uncertainty analysis in modelling of coupled multi-physics analysis for different reactor systems and scenarios [46]. The main activity is focused on uncertainties in

modelling LWR systems under steady-state and transient conditions, quantifying the impact of uncertainties on the multi-physics analysis, i.e. neutronics, thermal hydraulics modelling and fuel behaviour. The Phase I of the UAM Benchmark for BWR, PWR and VVER addressed core neutronics and Phase II addresses core thermal-hydraulics; Phase III will address coupled system thermal-hydraulics/core 3D kinetics. As noted in the previous section, the MPEBV expert group will also address issues associated with the propagation of uncertainties in multi-physics systems [39].

A topic of great importance is how to use validation data in an optimal way in order to minimise the resulting estimate of uncertainty and a number of different approaches are being pursued in this respect. For example, Monte Carlo sampling combined with Bayesian updating is used in MOCABA for the prediction of keff or nuclear reactor power shape, using validation data to reduce uncertainty [47]. This approach can handle non-linear behaviour and reduces to the generalised linear least squares method in the linear limit. An alternative approach is the use of artificial neural networks, which unlike other methods, are non-parametric [48]. The individual ANN workflow is segregated into training, validation and testing sets, where the latter encompasses the network predictive properties.

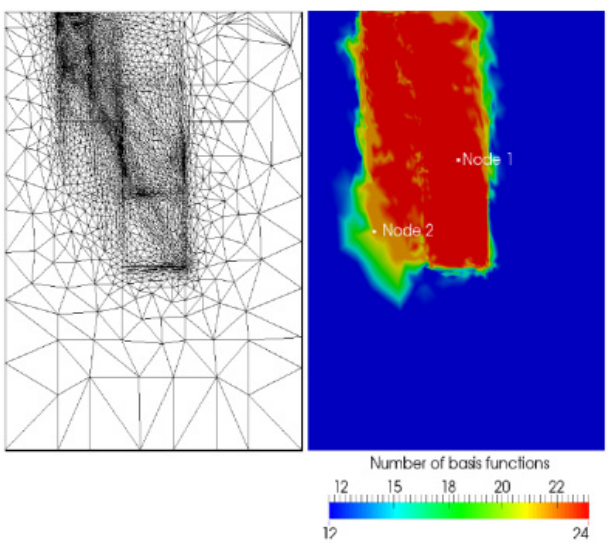
In 2009, the OECD NEA Working Party on International Nuclear Data Evaluation Cooperation (WPEC) established subgroup 33 on "Methods and issues for the combined use of integral experiments and covariance data". One of the conclusions from their 2013 report is that adjustment of the nuclear data can significantly reduce the uncertainties arising from validation against integral experiments [49]. This process of data assimilation provides a rigorous method for adjusting the (nuclear) data in line with the reported uncertainties to optimise agreement with integral experimental data, taking into account the experimental uncertainties [50]. This method can be applied to adjust the nuclear data to minimise the uncertainty of predictions over a defined application domain, though some refinement is necessary if a Monte Carlo simulation tool is used. A method for applying data assimilation to Monte Carlo criticality codes was developed by James Dyrda and is reported in his Engineering Doctorate thesis [51]. The process requires reliable covariance data from the evaluated nuclear data files and at present no individual file contains a complete set of covariances. Therefore covariance data are usually compiled from a number of different sources, including JEFF, ENDF/B, JENDL, CENDL and TENDL files [42]. The need for a consistent set of covariance data is driving current research in nuclear data, such as the ongoing efforts at Oak Ridge National Laboratory, presented at ICNC 2015 [52]. Data assimilation is a thriving area of research and a Data Assimilation Laboratory has recently been established at Imperial College to apply the latest developments in data assimilation to complex modelling and simulation tools in the UK and beyond [53].

8. ADAPTIVITY

All numerical simulations must demonstrate a required level of mesh independence. Carrying out convergence studies to prove that the mesh is sufficiently fine and that sufficient angle and energy groups are being used to obtain the required accuracy on a calculation can be a costly and time-consuming business. Ultimately the user would like to specify the required accuracy on a calculation and let the software refine the mesh, number of angles and number of energy groups to achieve the requested accuracy in the most efficient manner. This is the aim of goal-based adaptivity methods that are widely used in CFD codes to adjust the mesh, especially in transient calculations where areas of interest may be advected with the flow. These techniques have been applied to radiation transport

at Imperial College to provide automated mesh adaptivity to achieve user defined accuracy [54]. This technology has the added advantage that the user need only generate a simple mesh that conforms to the problem geometry and the code will then adjust the mesh to an optimal one for the user's requirements. The technique has been extended from spatial mesh adaptivity to angular adaptivity [55]; in this context, the order of the angular representation can vary spatially to provide more efficient calculation than is possible with a fixed angular representation.

Popular angular discretisations for the Boltzmann transport equation include spherical harmonics (Pn) and discrete ordinates (Sn) [56]. Both methods have well documented disadvantages, in particular the Pn method struggles with streaming effects in optically thin media and the Sn method suffers from ray effects [56]. Wavelets are mathematical functions used to divide data into different frequency components and study each component with a resolution appropriate to its scale [57]. Wavelets can be used to provide an alternative, hierarchical, angular representation of the Boltzmann transport equation [58]. The wavelet representation has certain advantages over the Pn and Sn representations in that streaming is not an issue and ray effects are less evident. Methods have been developed for goal-based space-angle adaptivity as illustrated in Figure 7 [59, 60]. Figure 7a shows the adapted spatial mesh and how the order of the wavelet angular discretisation varies with spatial position. Figure 7b depicts the wavelet discretisation at nodes 1 and 2, mapped onto an octahedron. It illustrates how the wavelet representation is concentrated round the streaming directions at the nodes, which is not possible using discrete ordinates or spherical harmonics. Finally, Figure 7c shows how the goal-based adaptivity improves the accuracy by roughly two orders of magnitude for a given order of representation of space-angle, for the example calculation. This illustrates the potential for goal-based adaptivity to greatly improve the efficiency of deterministic calculations in the future and remove the need for expensive and time-consuming convergence studies.



(a) Adapted mesh. (b) Adapted angular resolution.

Figure 7a: Adapted Spatial and Angular Discretisation. Reproduced with permission from author

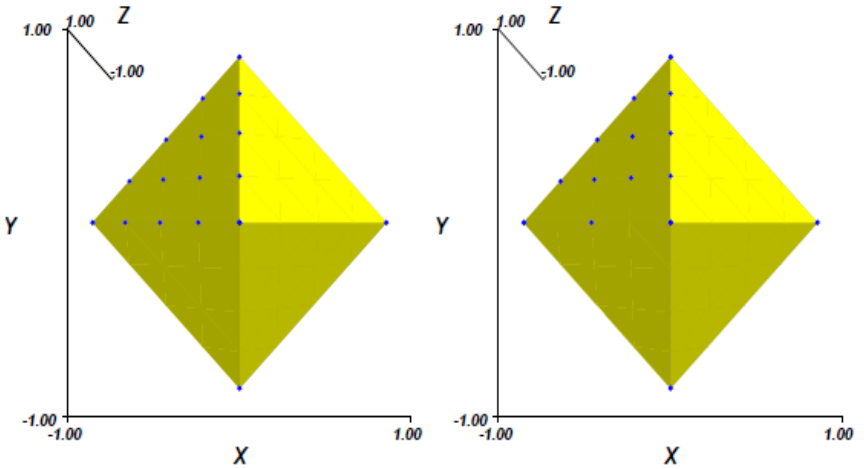


Figure 7b: Wavelet Discretisations at Nodes 1 and 2. Reproduced with permission from author

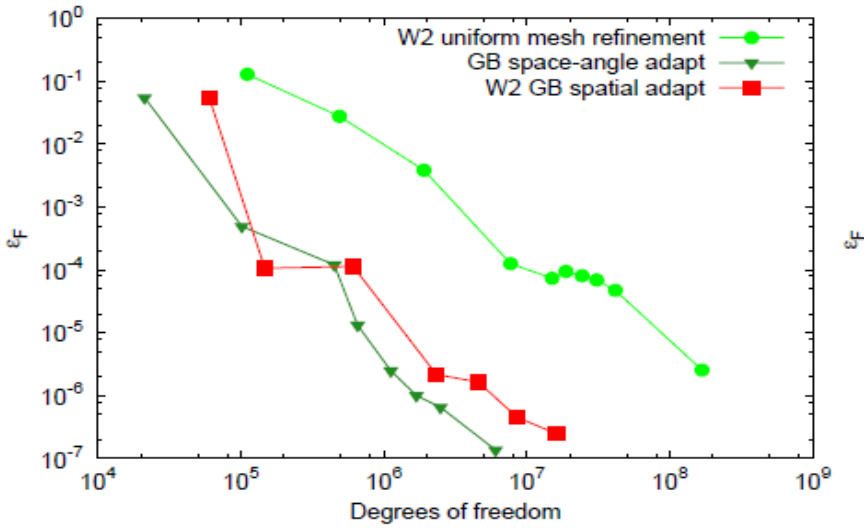


Figure 7c: Improvement in Accuracy from Goal-Based Adaptivity. Reproduced with permission from author

9. REDUCED ORDER MODELS

As noted in Section 4, high fidelity simulation tools are becoming increasingly popular, especially with the advance of high performance computing facilities. However, as such tools progress and the expansion of HPCs makes them more accessible, high fidelity tools are still computationally expensive. In addition, the requirement for uncertainty quantification drives an incompatible need for the rapid execution of large numbers of calculations. This has led to research into simulation techniques that retain the essential physics and dynamics captured by a high fidelity model but at a much lower computational

cost. This growing area of research is termed Reduced Order Modelling (ROM), also called Model Reduction. The basic idea is to use a relatively small number of solutions generated by a high fidelity model to construct a computationally cheaper model. In order to be successful, the Reduced Order Model must be predictive across the domain of parameter space of interest.

ROMs have been applied with great success to computational fluid dynamics for example [61]. Some forms of ROM require extensive modification to the simulation software to achieve model reduction. However, non-intrusive methods are available, based on the use of proper orthogonal decomposition (POD) to construct an optimal set of functions to represent the results of a number of calculations performed using the high fidelity code [61]. POD provides a rigorous framework for constructing the optimum set of functions to represent the high fidelity behaviour for a given order of approximation. This leads to very fast running calculations that are capable of faithfully reproducing detailed behaviour resulting from high fidelity simulations, potentially reducing the running costs by a factor of thousands [62].

Such reduced order methods are now being applied to the Boltzmann transport equation. In [63], it is shown that POD can be used to derive a set of angular basis functions that are capable of reproducing the detailed angular dependence of the flux with much greater accuracy than a spherical harmonic representation of the same order. Figure 8 shows the comparison with the exact solution for the Adam's pin cell. This shows that the POD solution gives good agreement with the exact solution when using only 10 basis functions and the POD solution with 55 basis functions is indistinguishable from the exact solution to the eye. On the other hand, the spherical harmonic solution using 55 functions is still a poor approximation to the exact solution. This indicates the enormous potential benefits that may be gained from the use of reduced order models.

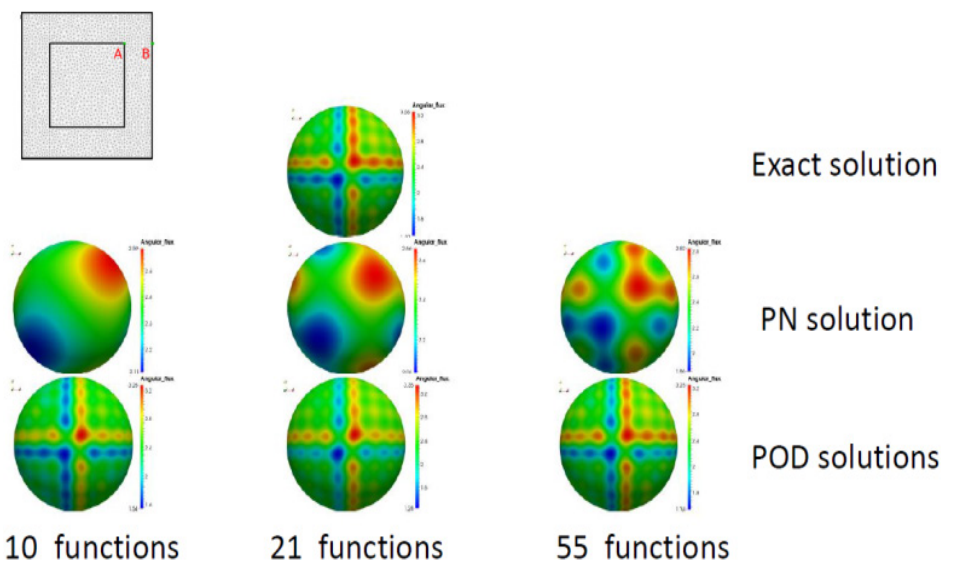


Figure 8: Comparison of POD Angular Basis Functions with Pn. Reproduced with permission from the Journal of Computational Physics.

10. HYBRID METHODS

This section describes how Monte Carlo and deterministic methods can be used in conjunction to produce significantly accelerated performance. The Monte Carlo method is a highly efficient method for solving the Boltzmann transport equation for integral parameters such as the neutron multiplication factor, or for values at isolated points such as dose rates at a small number of detectors [4]. Monte Carlo methods are increasingly being used to model distributed parameters, such as power shapes for reactor physics calculations, or variations in fuel isotopic composition across the core for burnup credit analysis [28]. Estimation of distributed parameters requires some form of nodalisation of the system on which to represent the distribution. Scoring a large number of tallies defined by the nodalisation requires a large number of samples in order to obtain acceptable statistics on all of the tallies. Methods are therefore sought to reduce run times to acceptable levels. Methods involving deterministic simulations or ideas from deterministic modelling can take many forms including: simple interfacing, use of deterministic solutions for variance reduction or bias reduction, and use of analogues of deterministic methods. A few of these are briefly discussed below.

One of the simplest ideas is to perform fast deterministic calculations for initial investigations to obtain an approximate answer and then run a Monte Carlo calculation to refine/confirm the answer and obtain accurate results. For example, the MCBEND Monte Carlo shielding code has a built-in diffusion solver that can be used for initial shield design studies [64]. This requires the user to superimpose a mesh on the geometry in order to perform fast running approximate calculations. The user can then run a Monte Carlo calculation with the same geometry and materials to confirm/refine and display the results with minimal effort [65].

Deterministic solutions have been used for some time to accelerate Monte Carlo solutions. For example, the diffusion solver within MCBEND can be used to automatically generate an importance map [66]. When a particle enters a region of high importance it splits into multiple particles (of reduced weight, so as not to bias the results) in order to give better coverage of important regions. Conversely a particle entering a region of low importance will undergo Russian roulette, whereby a coin is tossed and for tails the particle is terminated but heads the particle continues on its way (with increased weight so as not to bias the answer). In this way fewer particles are tracked in unimportant regions. Figure 9 shows an importance map generated using the Magic module in MCBEND for an analysis of an ASPIS shielding experiment from the SINBAD validation database [13]. The improvement in performance for detectors placed at a variety of locations is displayed in Table 1, in terms of the ratio of the figure of merit (FOM – a standard measure of shielding code performance) for the accelerated to un-accelerated calculations. Scoring regions 49 to 51 are close to the source and so the method offers no improvement at these locations. However, at locations around 60 and above the performance is improved by a factor of between 100 and 1000. The magic calculation took 0.023 s in this instance and the MCBEND calculation took around one hour. Thus it is seen that the method can improve performance by a factor of hundreds at effectively no computational cost.

For criticality calculations, a set of initial Monte Carlo stages is required to allow the fission source to converge sufficiently before scoring begins to avoid biasing the results. Reducing the number of such, so-called “settling stages” results in a corresponding reduction in the run time of the calculation. Various deterministic calculations have been used to reduce the number of settling stages required, including the use of a fission matrix

[67] or a coarse mesh finite difference (CMFD) solution [68]. More accurate deterministic solutions may be used and there is a trade off between the accuracy of the deterministic solution and the run time.

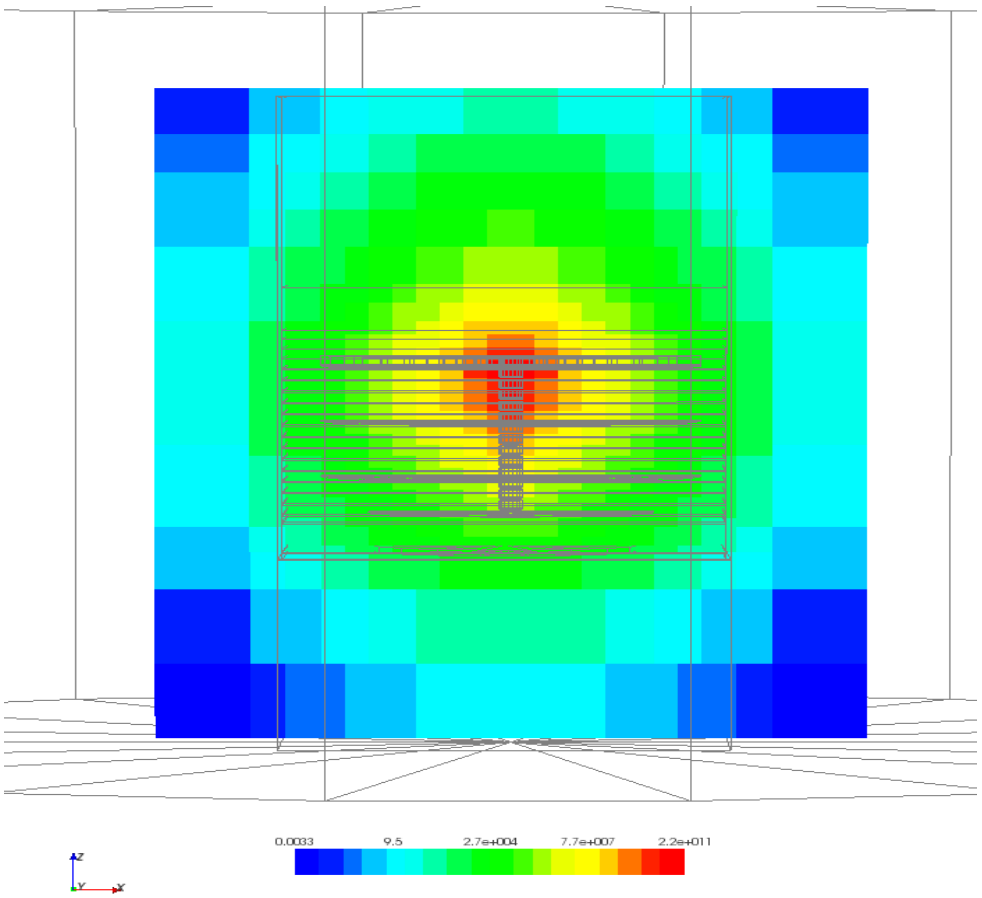


Figure 9: MCBEND Importance Map

Table 1: FOM Ratios for Accelerated to Un-accelerated Calculations by Scoring Region

Scoring Region	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63
FOM ratio	0.2	0.3	0.5	1.2	2.7	6.1	13	31	60	103	268	605	994	464	722

A common nodalisation scheme in a Monte Carlo code is to superimpose a mesh on the geometry and score the quantities of interest in the mesh elements to produce a 3D histogram to represent the distribution, for example using a unified tally (UT) mesh in MONK or MCBEND [4]. So far there has been little effort devoted to the optimisation of the nodalisation scheme. One exception is the use of functional expansion tallies to score the coefficients of an expansion of the desired parameter in terms of a set of basis functions,

such finite element basis functions are shown in [69]. This allows a smoother representation of distributed parameters by using linear, quadratic or higher order basis functions. This is a relatively untapped area with scope for significant improvement of nodalisation schemes in the future.

There are other areas where methods from deterministic modelling may lead to significant advances in "Monte Carlo" methods. For instance, the use of a deterministic set of quadrature points rather than pseudo-random numbers is able to achieve a more uniform coverage of the parameter space. In some situations, quasi-random numbers based on deterministic sequences may significantly out-perform Monte Carlo sampling in terms of the computation required for a user-specified accuracy (standard deviation). This has been found to be the case for modelling fluid flow in a porous medium, which is a material with stochastic properties. Calculations using quasi-random numbers have been found to be much more efficient than Monte Carlo sampling in this case [70]. Replacing pseudo random sequences by more regular though correlated sequences has had a large impact in some fields in recent years and offers the potential for exploitation in radiation transport modelling.

Another deterministic method that has recently spawned a stochastic analogue is the multigrid method. With the multigrid method, an initial fine mesh is progressively coarsened to provide a series of fast-running approximate solutions that converge longer wavelength components of the solution with increased speed. The solver typically moves down and up the coarsened models in a V sequence to converge all wavelength components of the solution much faster than a single grid solver. This method has been successfully applied to the Boltzmann transport equation [71]. An analogous technique referred to as Multilevel Monte Carlo has been developed for solving stochastic problems. With this method, a series of progressively more approximate, faster-running problems is devised such that the variance of the difference between successive approximations is small. With Monte Carlo simulations, the variance of the solution reduces as N-1/2 where N is the number of samples. With the multilevel Monte Carlo method, many of the calculations are performed with the faster running approximate models, thus reducing the computational cost of achieving a given accuracy (variance). The technique has been successfully applied to problems such as fluid flow in a porous medium, which is a material with stochastic properties [72]. This is another promising technique, which has yet to find significant application in radiation transport modelling.

11. CONCLUSIONS

Much progress has been made over the last fifty years in improving modelling tools for radiation transport and more exciting advances are on the horizon to further increase the power of simulation tools. A number of areas have been identified that are likely to lead to significant developments in the near future.

The inexorable progress of high performance computing will continue to drive progress and pose challenges for parallelization and memory management. This will allow more comprehensive and realistic simulation tools to be developed, with particular emphasis on multi-physics tools to address a wider range of nuclear reactor issues.

A range of options is now available for coupling physical models to produce multi-physics tools and an NEA expert group has been recently established to address the issue of validation of such tools. The huge amounts of data generated by high fidelity multi-physics models require corresponding advances in graphical display to allow the user to

assimilate the results of complex calculations.

Uncertainty quantification is improving with large benefits to be gained from more accurate, less pessimistic estimates of uncertainty and the issue of propagation of uncertainties through multi-physics models is being addressed.

New solver technologies are allowing spatial and angular discretisations to be automatically optimised to meet user-specified accuracy requirements and to facilitate the generation of accurate fast-running models, while hybrid deterministic – Monte Carlo methods offer additional avenues for progressing modelling tools.

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