LLNL-TR-648935

Trip Report

Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo (SNA + MC 2013), October 27 – 31, 2013

Monte Carlo Codes Invited Session Meeting

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Auspices

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Introduction

The Monte Carlo Codes Invited Session was hosted by the SNA + MC 2013 conference to provide international researchers and users a showcase to present and collaborate on their Monte Carlo codes and applications in nuclear criticality safety, reactor modeling, health physics modeling, and particle physic modeling. There were participants form ten countries who presented one or two posters in Monte Carlos Codes Invited Session. The NCSP supported codes COG (LLNL), MCNP (LANL) and SCALE (ORNL) were participants. COG and SCALE also provided hands-on demonstrations using laptop computers. There were approximately fifty people attending in total.

Participating Codes, their Affiliation, and Country of Origin

Monte Carlo Code	Affiliation	Country
ARCHER	RPI	USA
COG11	LLNL	USA
DIANE	CEA	France
FLUKA	INFN & CERN	Italy & CERN
GEANT4	GEANT4 Collaboration	International (CERN+)
KENO & MONACO (SACLE)	ORNL	USA
MC21	KAPL & Bettis	USA
MCATK	LANL	USA
MCCARD	Seoul National University	South Korea
MCNP6	LANL	USA
MCU	Kurchatov Institute	Russia
MONK & MCBEND	AMEC	United Kingdom
MORETS	IRSN Fontenay-aux-Ross	France
MVP2	JAEA	Japan
OPENMC	MIT	USA
PENELOPE	Barcelona University	Spain
PHITS	JAEA	Japan
PRIZMA	VNIITF	Russia
RMC	Tsinghua University	China
SERPENT	VTT	Finland
SUPERMONTECARLO	CAS INEST FDS Team Hefei	China
TRIPOLI-4	CEA	France

The Posters for the Invited Monte Carlo Codes

ARCHER$_{RT}$ — A GPU-based Monte Carlo Radiotherapy Dose Calculation Engine and its Application to Helical Tomotherapy

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[2] Medical Physics, University of Wisconsin Madison, WI, USA
[3] Molecular Imaging, Radiotherapy and Oncology, Université catholique de Louvain Brussels ,Belgium
*Email: xug2@rpi.edu Website: http://rrmdg.rpi.edu

INTRODUCTION

Monte Carlo (MC) methods provide the most accurate radiation dose distributions for many medical physics applications. Nonetheless, due to slow simulation speed, MC methods remain to be impractical for routine use. Recently the graphics processing unit (GPU) has emerged as a secure and affordable hardware for parallel computing. At RPI we have been developing a MC code **ARCHER** (**A**ccelerated **R**adiation-transport **C**omputations in **H**eterogeneous **E**nvi-**R**onments). In this paper, we describe the implementation of ARCHER$_{RT}$ (RadioTherapy) on the GPU/CUDA platform and its applications in accelerating the MC calculations for tomotherapy dose calculation.

METHODS

In ARCHER$_{RT}$, photon transport is modeled in an analog manner, in which photoelectric effect, Compton scattering and pair production are modeled. Electron transport is handled by the mixed condensed history method [1]. In this method, interactions with an energy loss greater than a preset value (hard collision) are simulated explicitly; below that preset value, the energy loss is treated with Continuously Slowing Down Approximation (CSDA).

The code is developed in the CUDA C environment. GPUs typically contain hundreds or thousands of streaming processors. With each processor simulating multiple particles, we are able to obtain high computational efficiency and reduce the simulation time significantly.

For the radiotherapy simulation, the source particles come from pre-calculated phase-space-files(PSFs)[2], CT-converted voxel phantoms are used as transport media. Typical PSF for radiotherapy is very large. To better accommodate the big data, the simulation is performed in batches. Meanwhile, the batch simulation facilitates the statistical uncertainty evaluation. To achieve desirable statistical level, the PSF may be recycled. ARCHER$_{RT}$ works for different radiotherapy modalities. In this work, application on helical tomotherapy (HT) was demonstrated.

Two clinical HT cases were considered in this study: prostate tumor and lung tumor. The prostate phantom consists of 260 × 256 × 108 voxels, with a voxel size of 0.1875 × 0.1875 × 0.3 cm^3 . The lung phantom consists of 256 × 256 × 160 voxels, with a voxel size of 0.1953 × 0.1953 × 0.2 cm^3.

The codes were tested on a system consisting of an Intel Xeon 5650 CPU with 16 GB RAM, and 1 NVIDIA Tesla M2090 GPU card.

Figure 1 shows the photo and scheme of tomotherapy.

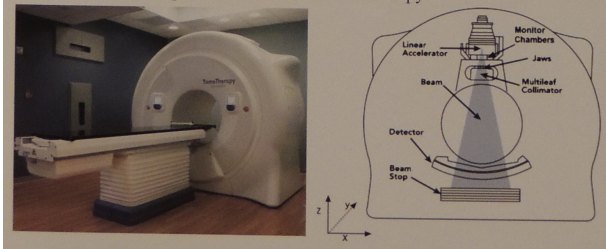


Figure 1: photo (left) and scheme (right) of tomotherapy

RESULTS: DOSIMETRIC

To validate the dosimetric accuracy of ARCHER$_{RT}$, we simulated the same cases with well established MC code GEANT4 and compared the results from both codes. For both cases ,relative statistical error (1 σ) of voxel doses in the PTV is ~ 1%. Figure 2 and Figure 3 show the Dose Volume Histogram (DVH) of two cases. The dash lines are GEANT4 results, solid lines are ARCHER results. It can be seen that two sets of DVHs agree nicely except for a slight difference in the gradient region for the PTV. Figure 4 shows the isodose map of a slice of prostate case, two dose distributions agree very well. Gamma test pass rates (2mm/2%) are 99.7% and 98.5% for prostate and lung cases, respectively.

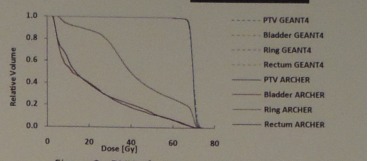


Figure 2: DVH of prostate case

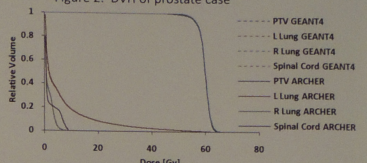


Figure 3: DVH of lung case

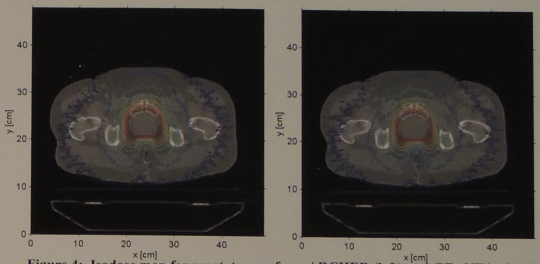


Figure 4: Isodose map for prostate case from ARCHER (left) and GEANT4 (right)

RESULTS: TIMING

The simulation timing information is listed in Table 1. Since the PSF Reading (one CPU) and MC simulation (on GPU) can be done simultaneously, the total execution time is less than the sum of all parts. It can be found from the table that the clinical HT case MC simulation can be done in 1 min. With multiple GPUs, the time can be squeezed further. For comparison GEANT4 needs many hours or days for the same task.

Table 1: ARCHER$_{RT}$ execution time for clinical cases

Clinical cases	# of particles simulated	GPU time [s]	Reading PSF time [s]	Reading CT phantom and misc [s]	Total execution time [s]
Prostate	600 million	60	38	~10	69
Lung	530 million	50	11	~8	58

CONCLUSION

ARCHER$_{RT}$, a GPU-based fast and accurate dose calculation engine, has been under extensive development and was applied to tomotherapy tests. Two clinical TomoTherapy® treatment plans were used to show the clinical utility. ARCHER$_{RT}$ agrees very well with GEANT4 in terms of dosimetric accuracy and it runs much faster: with a single GPU, a full clinical treatment plan can be simulated in one minute.

REFERENCES

[1] M. J. Berger, "Monte Carlo Calculation of the penetration and diffusion of fast charged particles", Methods in Comput. Phys., vol 1, p 135 – 215, Academic, New York, 1963
[2] E. Sterpin, et al, "Monte Carlo simulation of helical tomotherapy with PENELOPE,". Phys. Med. Biol., 2008. **53**: p. 2160

The GPU programming tools were developed using funding by the National Institute of Biomedical Imaging and Bioengineering (Grant number R01EB015478).

COG11.1 – New Features, Data, V&V

Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
Lawrence Livermore National Laboratory, 7000 East Avenue, L-198, Livermore, CA, 94550, USA
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

New Features

CritDetVR – Enables hybrid criticality/shielding calculations for variance reduction of detector scores with no bias in the keff calculation.
DFG – Simulates delayed gamma emission from the fission product decay.
NRF – Simulates nuclear resonance fluorescence reactions for nuclear photon absorption and emission.
RadSrc – Automatic photon source calculation for gamma emission from α-decay at a user-specified time (age).
COGLEX – Update includes dictionary entries for compounds with thermal scattering law.

New Data Libraries

NRF Library (Dr. Jim Hall, LLNL):
COGNRF
RadSrc Library (Dr. Ed Lent, LLNL):
COGRS
DFG Libraries (Dr. Ed Lent, LLNL):
DFG.ENDFB7R1
DFG.JEFF3.1.1
DFG.JENDL4
Neutron Libraries:
ENDFB7R1, **PT.ENDFB7R1**, **T.ENDFB7R1**
JEFF3.1.2, **PT.JEFF3.1.2**, **T.JEFF3.1.2**
JENDL4
Dosimetry Library:
IRDFF1.02
Supported Library Formats:
ENDL, **ENDF**, **ACE**
GND (in progress)
Many, many older data libraries continue to be supported (e.g., JEF2.2, ENDF/B-V).

MC-to-S_N

ARDRA – COG geometry package is included in LLNL's modern massively parallel S_N code with automatic meshing features.

LLNL-POST-644394

V&V

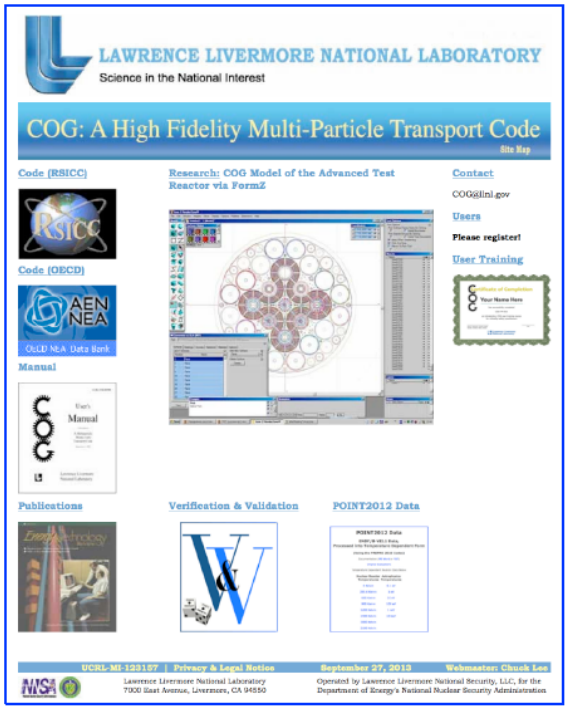
COG11BETA2 has been extensively tested using the following test suites:
Regression tests (11 cases)
ICSBEP criticality benchmarks (501 cases)
NRF tests (3 cases)
SINBAD shielding benchmarks (9 cases)
SILENE Activation benchmarks (11 cases)
PHOTONUCLEAR benchmarks (16)
KOBAYASHI exact solutions (in progress)
CRITCYL exact solutions (in progress)

Automation

LLNL is automating V&V code/data testing as described by M.-A. Descalle at ND2013. BNL is involved in a similar effort.

Website/Email

Please visit our website at http://cog.llnl.gov and contact us at COG@llnl.gov.



COG11.1 – Practical Applications

Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent

Lawrence Livermore National Laboratory, 7000 East Avenue, L-198, Livermore, CA, 94550, USA

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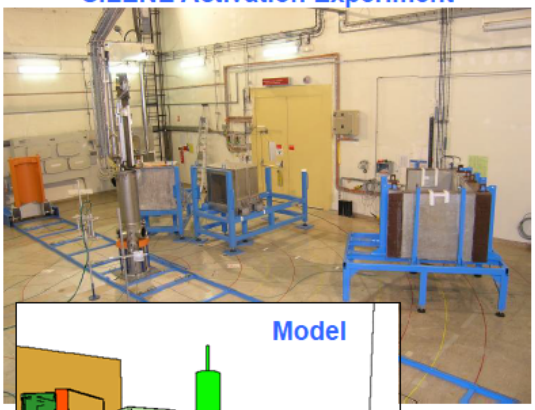
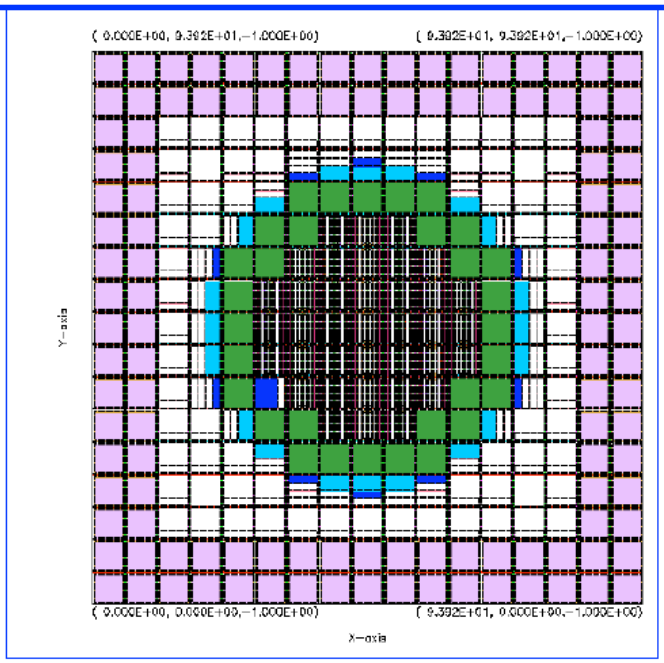
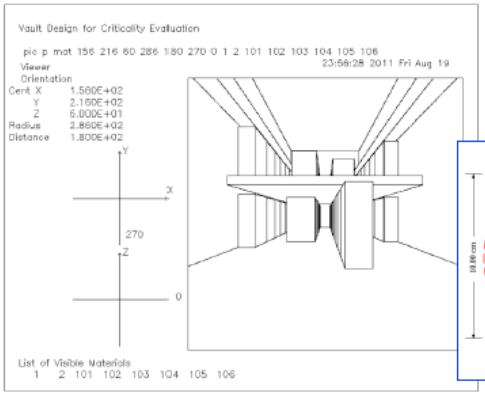
SILENE Activation Experiment

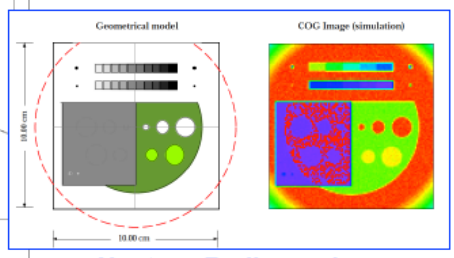




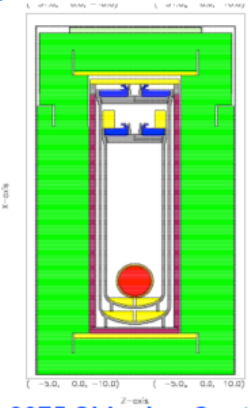
Detailed Model of ZPPR-21F
Reactor Physics



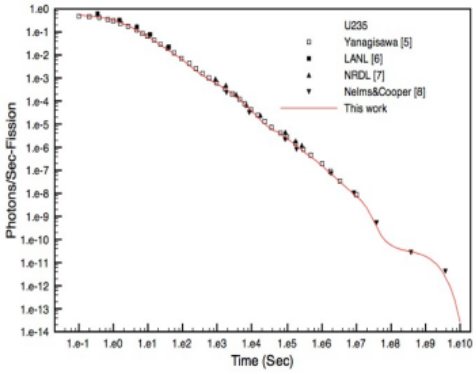
Storage Vault Model
Shielding & Criticality Safety



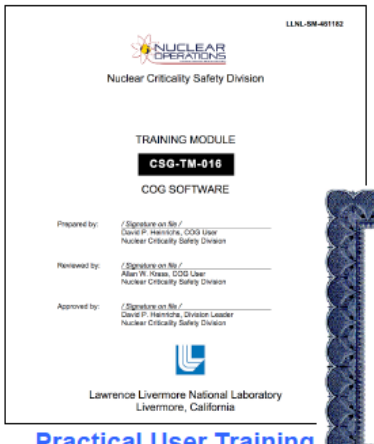
Neutron Radiography



9975 Shipping Container
Shielding & Criticality



Fission Product Decay Gammas
Dose Assessment



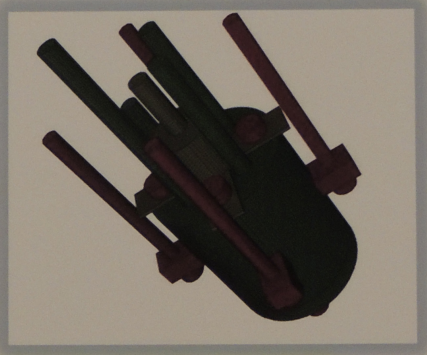
Practical User Training

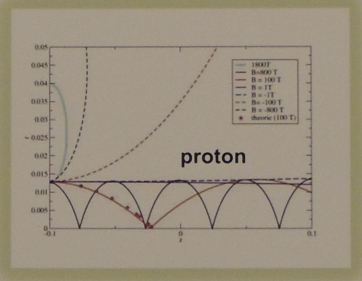
LLNL-POST-644395

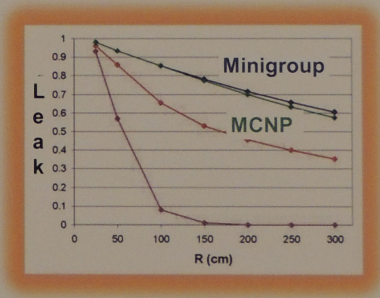
Diane multiparticle Monte Carlo transport code

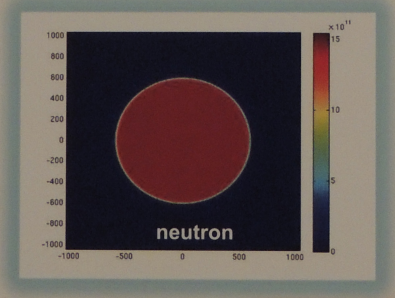
M.Caillaud, S.Lemaire, S.Ménard, P.Rathouit, J.C.Ribes, D.Riz
CEA DAM (Bruyères-le-Châtel)

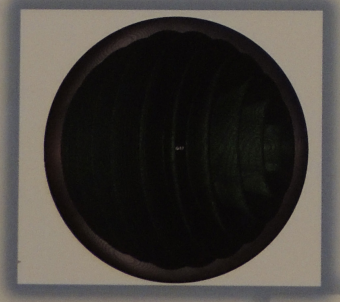
- **Geometry**
  - ✓ 3D
  - ✓ Internal or MCNP input cards
- **Multigroup cross sections**
  - ✓ ZADIG code process ENDF data
  - ✓ All the reactions for n, γ, e^-, e^+ (in-flight annihilation, fluorescence, bremsstrahlung)
  - ✓ Light charged particles
- **Thermalization** : in-flight or cross section
- **Particles transported** : n,γ,e^-,e^+,p,d,t,α
  - e^-/e^+ : 2 models, detailed transport or SSB model in ZADIG (secondary Bremsstrahlung photons are produced)
- **Transport**
  - ✓ Analog, Woodcock, mix
  - ✓ Forward, adjoint
  - ✓ Automated variance reduction techniques
  - ✓ Electromagnetic fields
  - ✓ Parallelized (MPI) code : 140 000 cores of TERA 100
- **Tallies**
  - ✓ K_{eff}, α, point detector, surface flux, radiographic and mesh tallies, energy deposition
- **3D mesh vizualisation**



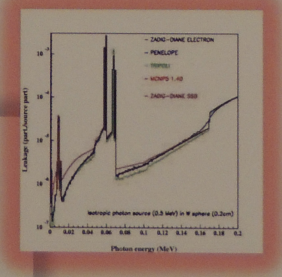


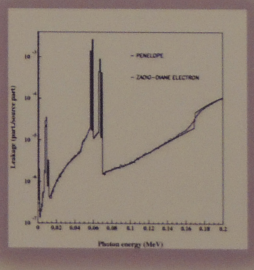


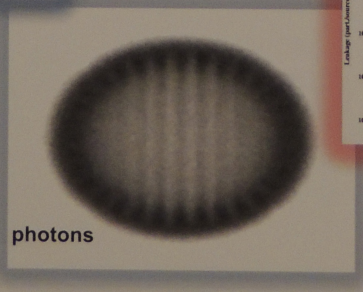




Atomic relaxation (X-rays, Auger e-) after photoelectric effect







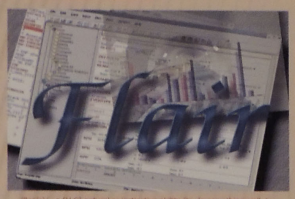
FLAIR: Fluka advanced graphical interface

SNA+MC 2013, Paris, France 27th – 31st Oct, 2013

www.fluka.org/flair

Abstract. FLAIR is an advanced user friendly graphical interface for FLUKA. Greatly facilitating the user to build an error free input, run, process, and analyze the results. All steps performed with a few clicks from a single GUI environment

0. Interface



/fleə(r)/ n [U,C] natural or instinctive ability (to do something well, to select or recognize what is best, more useful, etc.
[Oxford Advanced Dictionary of Current English]

is more than a graphical Interface
→ is a complete integrated working environment for FLUKA

Without hiding the inner functionality of FLUKA, **flair** offers all tools for:

Front-end
- Fully featured Input file Editor;
- Geometry: interactive visualization editing, and debugging;
- Compilation of the FLUKA Executable;
- Running (Spawning on multi-core) and monitoring of the status of one/many run(s)

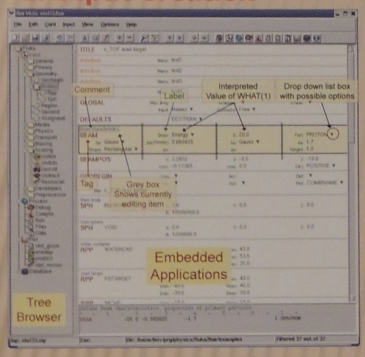
Back-end
- Post processing of FLUKA output
- Plot generations with gnuplot
- Photorealistic 3D plots with USRBIN data superimposed

Import/Export
- MCNP (Import/Export)
- GDML (Import)
- DICOM (Import)
- DXF, Povray, STL..

Other
- Database of Materials, Isotopes
- FLUKA hypertext manual

...and many more...

1. Input Creation



FLAIR main application window

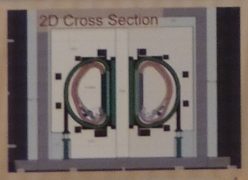
Input Editor
With the input editor the user can manipulate the input cards.
- Add card to input
- Edit & modify existing ones
- Copy & Paste
- Clone (Duplicate)
- Import from other input files
- Validate the correctness of the cards
- Error filtering
- Rearrange order

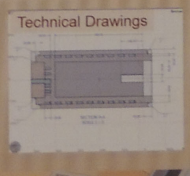
The editor will always try to rearrange the input cards (only if needed) to create a valid FLUKA input file.
e.g. body cards outside the GEOBEGIN..GEOEND will be moved inside

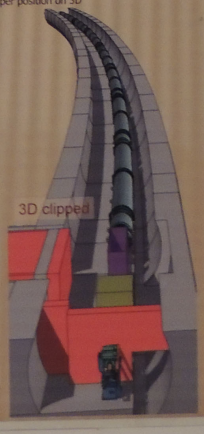
Extended Cards
Flair has introduced a few special cards to homogenise the FLUKA input file:
- REGION, referring to a region declaration in geometry
- COMPOUND, all compound cards related to one material are joined in one card

2. Graphical Geometry Editor/Debugger

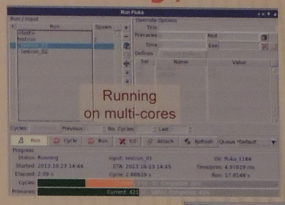
- Interactive visual editing in 2D;
- Fast/realtime 3D raytraced rendering;
- Numerically robust and use of multi-core architectures;
- Use real surface expression of bodies: NO conversion to vertices/edges;
- Debugging bodies/**zones**/regions in a graphical way;
- Graphical editing of the bodies with snapping mechanism (on intersections of body conics) to generate accurate coordinates;
- Visual selection and editing of zones w/o the need to know the orientation of bodies;
- Interactive debugging with information of problematic bodies, regions and/or zones;
- Visual setting (painting) of materials, importance's and transformations
- Fully customizable layers;
- Super position on technical drawings
- Graphical display of input/card parameters (thresholds, biasing, material properties...)
- FLUKA output (USRBIN) super position on 3D
- ... and many more...

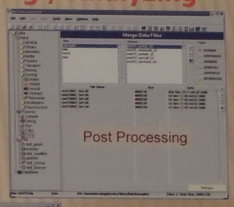


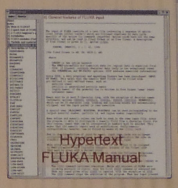


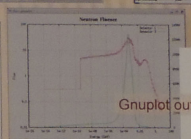


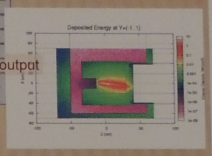
3. Running / Processing / Analyzing



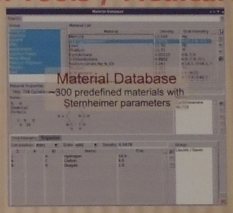


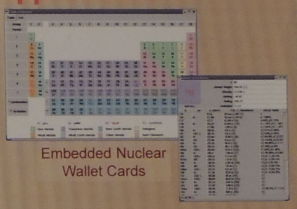




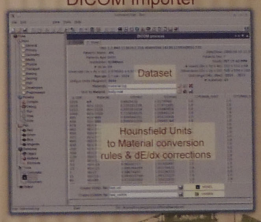


4. Tools / Medical Applications

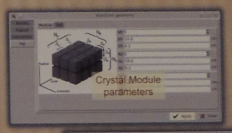




DICOM Importer



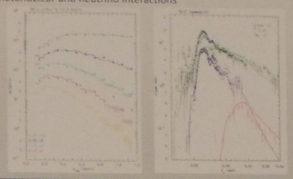
PET Geometry Generator



DICOM + p+ 200MeV simulation

Hadronic interactions

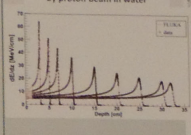
- Different models depending on the energy (*e.g.*, Dual Parton Model)
- Generalized intra-nuclear cascade, with pre-equilibrium emission and coalescence
- Evaporation, fission, Fermi break-up
- Energy range: from **threshold up to 10000 TeV**
- Photonuclear and neutrino interactions



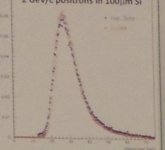
Electromagnetic interactions

- wide energy range **electrons: 1 keV – 1000 TeV**
  photons: 0.1 keV – 10000 TeV
- Compton effect with Doppler broadening
- Landau-Pomeranchuk-Migdal pair production suppression effect
- Full coupling with hadronic interactions

Depth-dose distribution induced by proton beam in water

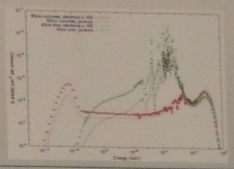


Energy deposition spectra for 2 GeV/c positrons in 100μm Si



Low-energy neutrons

- Multigroup transport technique
- 260 energy groups 0.01 meV and 20 MeV
- 31 thermal groups, 42 gamma groups
- Point-wise cross sections for few elements



Biasing

Powerful biasing techniques available:

- Region importance biasing
- Weight windows
- Leading particle biasing
- Multiplicity tuning
- Interaction length biasing
- Decay length biasing
- User-defined neutrino direction biasing
- User-defined step-by-step importance biasing

Ion interactions

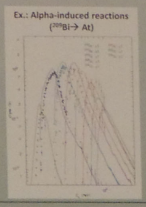
Simulation of arbitrary configurations by different models depending on the energy:

E > 5 GeV/n
Dual Parton Model
DPMJET-III

0.1 GeV/n < E < 5 GeV/n
Relativistic Quantum Molecular Dynamics Model
RQMD-2.4

E < 0.1 GeV/n
Boltzmann Master Equation
(BME)

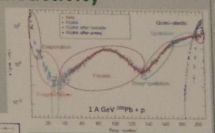
Ex.: Alpha-induced reactions (^{209}Bi→ At)

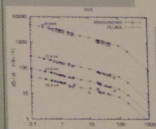


Calculation of electro-magnetic dissociation

Radioactivity

Production of radioactive nuclides based on microscopic models





- Calculation of radioactive build-up and decay
- Generation and transport of decay radiation

Residual dose rate benchmark

An international collaboration

Jefferson Lab · Uppsala University · Universität Siegen · INFN · fondazione CNAO · HIT · CERN · SLAC · NASA · AIT · Universitat de València · Paul Scherrer Institut PSI · Université de Genève · Ospedali Riuniti di Bergamo · Forschungszentrum Rossendorf

FLUKA

http://www.fluka.org

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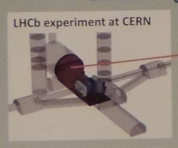
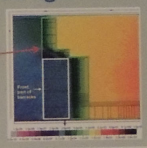
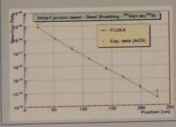
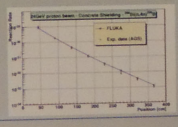
Shielding design

LHCb experiment at CERN

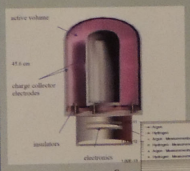






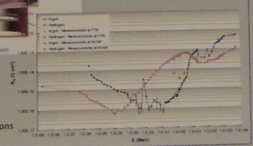


Dosimetry



Detector response calculations

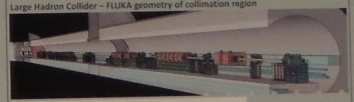
- IG5 (Centronics) high-pressure ionization chambers (5.2 l, 20 bar)
- hydrogen or argon gas filling

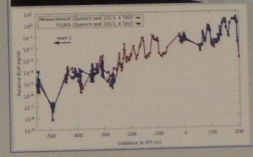


Detector response to mono-energetic neutrons

Accelerator design

Large Hadron Collider – FLUKA geometry of collimation region





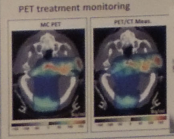
Comparison of FLUKA predictions and beam loss monitor measurements in the LHC collimation region

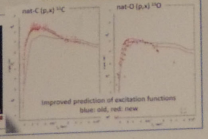
Hadron therapy

FLUKA model of human head

Dose prediction

PET treatment monitoring

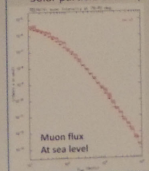




Improved prediction of excitation functions

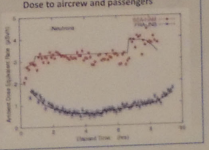
Space radiation

- Primary cosmic ray spectra and interplanetary modulation according to measured solar activity on a day-to-day basis
- Primary energies up to 500 TeV/n
- Earth atmospheric model incl. geomagnetic field
- Solar particle event spectra available



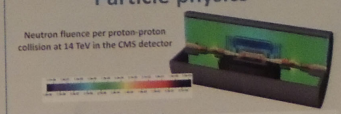
Muon flux
At sea level

Dose to aircrew and passengers

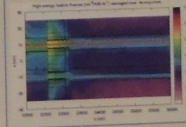


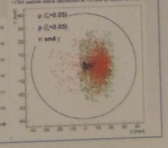
Particle physics

Neutron fluence per proton-proton collision at 14 TeV in the CMS detector



Particle fluence studies for LHC forward detectors (TOTEM)





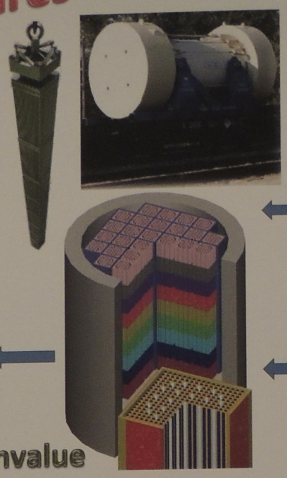
scale Monte Carlo Capabilities of

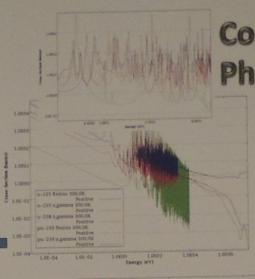
B. T. Rearden[1*], L. M. Petrie[1], D. E. Peplow[1], K. B. Bekar[1], D. Wiarda[1],

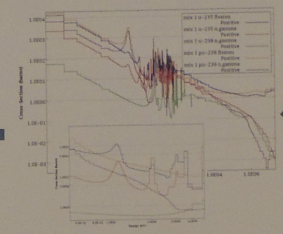
Nuclear Systems Modeling & Simulation

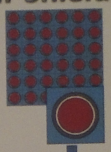
Established Features

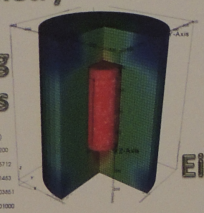
- Efficient KENO V.a Geometry
- Flexible Generalized Geometry
- Shielding Analysis
- Eigenvalue Analysis
- Continuous-Energy Physics
- Resonance Self-Shielding
- Multigroup Physics

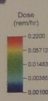




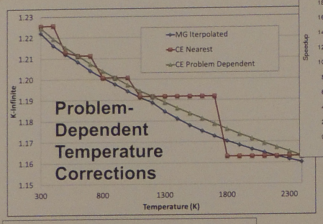




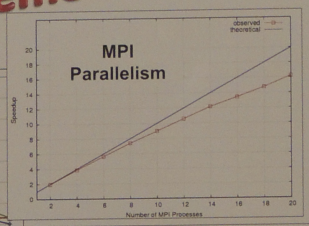




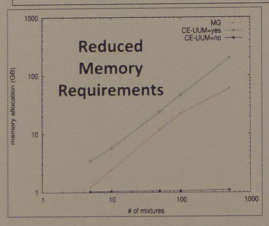
KENO Enhancements



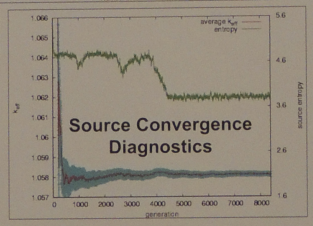
Problem-Dependent Temperature Corrections



MPI Parallelism

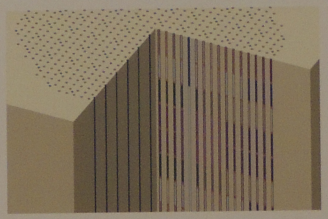


Reduced Memory Requirements



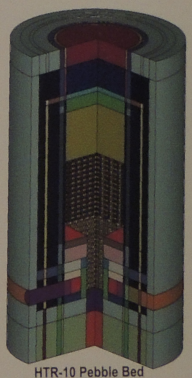
Source Convergence Diagnostics

Depletion

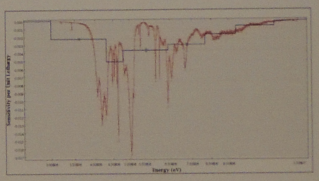


Graphite Reactor Benchmark

- 7,930 depletion zones
- ~10,000 units, ~32,000 regions
- 1.2GB memory
- 50M histories
- Total problem time: 72 hours

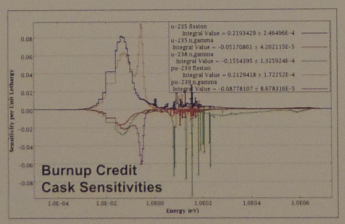


HTR-10 Pebble Bed Reactor Benchmark

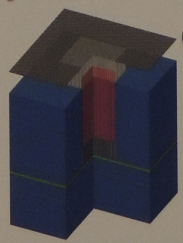


Sensitivity and Uncertainty Analysis

Established Multigroup Methods

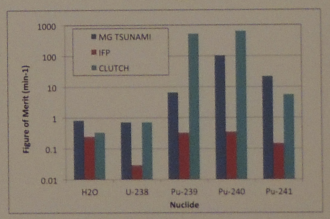


Burnup Credit Cask Sensitivities

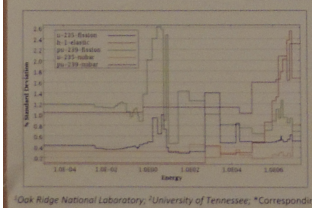


MIX-COMP-THERM-004 Critical Experiment

Continuous-Energy Methods



Sensitivity	Reference	MG TSUNAMI	CE TSUNAMI IFP	CE TSUNAMI CLUTCH
H_2O	0.2935 ± 0.0179	0.2805 ± 0.0088 (-0.65 σ_{eff})	0.2733 ± 0.0052 (-1.08 σ_{eff})	0.2793 ± 0.0065 (-0.75 σ_{eff})
^{238}U	-0.0061 ± 0.0003	-0.0050 ± 0.0002 (2.80 σ_{eff})	-0.0055 ± 0.0003 (1.16 σ_{eff})	-0.0057 ± 0.0001 (1.14 σ_{eff})
^{239}Pu	0.1262 ± 0.0087	0.1264 ± 0.0014 (0.02 σ_{eff})	0.1188 ± 0.0020 (-0.83 σ_{eff})	0.1190 ± 0.0001 (-0.83 σ_{eff})
^{240}Pu	-0.03777 ± 0.00350	-0.03750 ± 0.00011 (0.08 σ_{eff})	-0.03738 ± 0.00060 (0.11 σ_{eff})	-0.03743 ± 0.00002 (0.10 σ_{eff})
^{241}Pu	0.00589 ± 0.00042	0.00599 ± 0.00004 (0.24 σ_{eff})	0.00567 ± 0.00014 (-0.50 σ_{eff})	0.00579 ± 0.00003 (-0.24 σ_{eff})
Memory Requirements (increase from Eigenvalue Analysis)		13 GB	11 GB	63 MB



Covariance Data

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{239}Pu nubar	^{239}Pu nubar	4.0332E-01 ± 2.5625E-06
^{238}U n,gamma	^{238}U n,gamma	1.9457E-01 ± 1.2387E-05
^{239}Pu fission	^{239}Pu fission	1.5501E-01 ± 1.0834E-05
^{235}U nubar	^{235}U nubar	1.3981E-01 ± 5.0038E-07
^{239}Pu fission	^{239}Pu n,gamma	1.2261E-01 ± 4.3564E-06

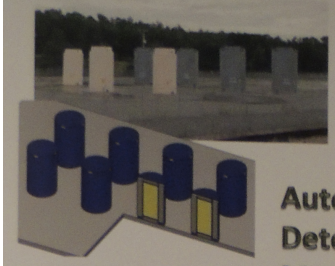
[1]Oak Ridge National Laboratory, [1]University of Tennessee, *Corresponding Author, E-mail: reardenb@ornl.gov

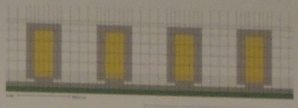
the SCALE Code System

C. Celik[1], C. M. Perfetti[1], A. M. Ibrahim[1], S. W. D. Hart[2], and M. E. Dunn[1]

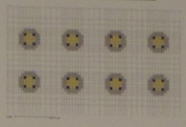
OAK RIDGE National Laboratory

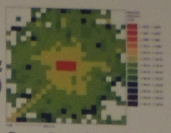
Hybrid Shielding Methods

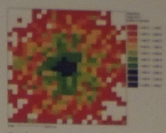




Automated Deterministic Model Setup

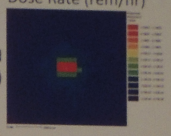


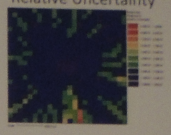




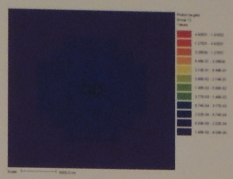
Dose Rate (rem/hr)

Relative Uncertainty





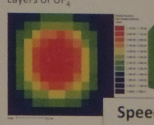
Biased Source



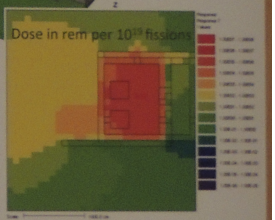
Importance Map

Criticality Accident Alarm System Modeling

West wing of the ORCEF, building 9213



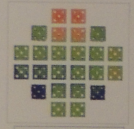
Speedups of 3000 to 4500

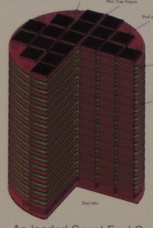


KENO Fission Source

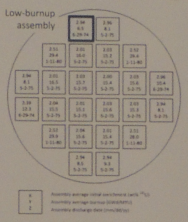
Hybrid Shielding for Detector Response

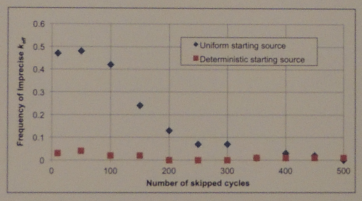
Hybrid Criticality Methods





As-loaded Spent Fuel Cask





Deterministic Fission Source Specification

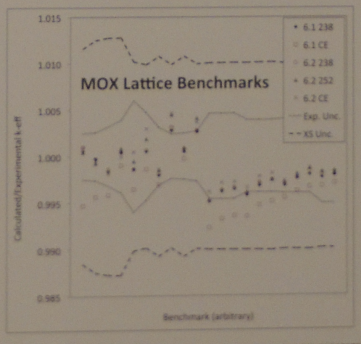
V & V

Validation

400 Criticality Benchmarks
Shielding Benchmarks

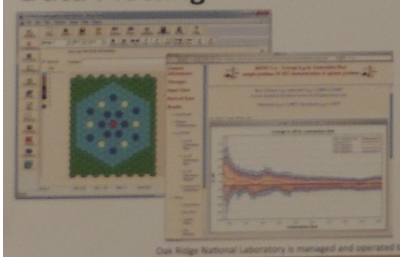
Verification

6300 Transmission Tests
5000 Infinite Medium Tests
2000 Unit/Regression Tests
70,000 Tests/Day Across All Platforms



User Interfaces

Input Generator
Interactive Output
Model Visualization
Data Plotting



Distribution

Quality Assurance

ISO 9001-2008, DOE 414.1D, ORNL SMBS

Availability

RSICC, NEA Data Bank, RIST

User Base

8000 Copies to 5500 Individuals

Technical Support

10 Weeks of Training Available Annually
Online User Forum
E-mail Helpline: scalehelp@ornl.gov

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MC21 v.6.0

A Continuous-Energy Monte Carlo Particle Transport Code with Integrated Reactor Feedback Capabilities

D.P. Griesheimer, D.F. Gill, B.R. Nease, T.M. Sutton, M.H. Stedry, P.S. Dobreff,
D.C. Carpenter, T.H. Trumbull, E. Caro, H. Joo, D.L. Millman

Bechtel Marine Propulsion Corporation

Feedback Sequence and Job Control

- MC21 provides integrated support for feedback effects relevant to reactor analysis applications.
  - Depletion (Constant Power)
  - T/H Feedback
  - Xenon Feedback
  - Photon Heating
  - Eigenvalue Search
- Accounts for non-linear reactivity effects at steady-state.
- Each feedback effect in MC21 is driven by a separate solver kernel, each of which is tightly integrated into the overall code system.
  - Communications between solver kernels and transport kernel is performed through application program interfaces (APIs).
  - Data is exchanged via local memory, avoiding inefficient file passing.
- MC21 simulations include one or more timesteps, which model the behavior of the problem over a fixed period of time.
  - Control input is divided into independent timestep sections, each containing a user defined sequence of control cards.
  - Control cards are used to define all aspects of the simulation, including running strategy, physics options, and feedback effects.
  - Within each timestep, execution cards are used to instruct MC21 to perform a given type of calculation.
  - Each execution card defines a single feedback iteration for the timestep.
- MC21 uses a predictor-corrector methodology to solve for the feedback behavior over the length of a timestep .
  - Methodology assumes that reaction rates throughout the problem vary linearly between beginning-of-timestep (BOT) and end-of-timestep (EOT).
  - Time is advanced from BOT to EOT immediately after the first depletion iteration in the timestep. Iterations prior to the first depletion calculation are at BOT; Additional feedback iterations are at EOT.
  - User is responsible for defining the feedback sequence.

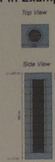
```
job_type                     k-eff
histories                    5000
batches                      100
discard                      10
seed                          587
num_timestep                 4
rated_power                  100.0 MW

<TIMESTEP> 1
case_title    'Source Convergence Step'
source_coordinates           point  0.0  0.0  0.0
source_energy                mono 2.0e6
(EXECUTE) spatial

<TIMESTEP> 2
case_title    'Depletion: 1000h @ 10MW'
source_definition            last
timestep_length              1000.0 hours
depletion_power_fraction     0.1
(EXECUTE) depletion

<TIMESTEP> 3
case_title    'Depletion: 1000h @ 100MW'
histories                      10000
depletion_power_fraction       1.0
(EXECUTE) depletion

<TIMESTEP> 4
case_title    'Shutdown Depletion: 3y'
depletion_power_fraction       0.0
timestep_length                3 years
(EXECUTE) depletion
```

Example MC21 control input file for a multiple timestep depletion calculation.

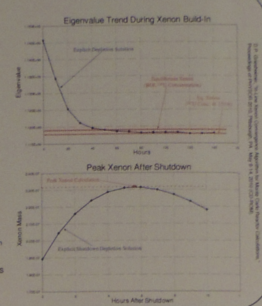
Xenon Feedback

- MC21 supports in-line convergence to equilibrium xenon during criticality calculations as well as calculation of post-shutdown peak xenon conditions.
  - Avoids the need for small timestep depletion after power change.
- Convergence to equilibrium xenon is achieved by periodically updating xenon and iodine densities between neutron generations.
  - MC21 tallies xenon and iodine production and xenon absorption rates in each region containing a depletable fissionable material.
  - Reaction rates are used to compute the equilibrium xenon and iodine number densities by region using a simple two nuclide depletion chain.
  - Process allows for convergence of the xenon and iodine number densities as well as the consistent convergence of the fission source distribution.
- An in-line algorithm for determining post-shutdown peak xenon condition in a reactor is also available in MC21.
  - Algorithm uses a simple bisection search technique to determine the elapsed time after shutdown at which the xenon mass in the reactor is maximized.
  - The xenon/iodine decay equations are solved in each fuel depletion region throughout the reactor in order to determine the distribution of iodine and xenon throughout the reactor at the calculated peak xenon time.

Simple PWR Fuel Pin Example



- Infinite PWR Pin Lattice
  - 12 axial segments of 20 cm
  - 0.020325 MW power
- 22 million neutron histories
  - 220 batches (20 discard)
  - 100,000 histories/batch



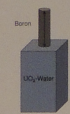
D.P. Griesheimer, "In-Line Xenon Convergence Algorithm for Monte Carlo Reactor Calculations," Proceedings of PHYSOR 2010, Pittsburgh, PA, May 9-14, 2010 (CD-ROM).

Eigenvalue Search

- MC21 includes the capability to search to a user-specified eigenvalue, within a specified confidence interval, by manipulation of the movable geometry.
- The criticality search algorithm is a *regula falsi* method with special considerations taken to deal with the stochastic nature of the Monte Carlo solution.
  - The convergence criteria is modified to include confidence interval information calculated from the Monte Carlo solution.
  - After each batch, method determines whether the Monte Carlo calculation should be continued, the search iteration should be rejected, or the search iteration has converged,
  - Modified criteria minimizes the amount of time spent per iteration while ensuring that the Monte Carlo solution (with uncertainty) falls within an interval defined by the target eigenvalue and a user-input width (ε) around the target.
- Eigenvalue searches can be performed in two different ways:
- Movable Search
  - Allows the user to define a single movable group to be moved during the search, along with the lower and upper bounds of the search space.
  - During a movable search MC21 will move (translate or rotate) the search group through the range specified until the desired eigenvalue is found with the desired confidence interval or it is determined that there is no solution within the interval specified.
- Search Sequence
  - a more complex search type which allows for a series of movable searches to be performed in a sequential manner until the desired eigenvalue is found with the desired confidence interval or the end of the sequence is reached without convergence.
  - Sequences can be defined in a manner such that the specific series of movable searches to execute is dependent on the elapsed time in the simulation.

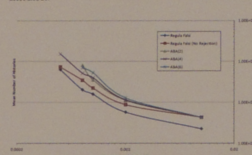
Boron Rod Search Example

- Problem composed of
  - Homogenized UO_2-Water parallelepiped (10×10×50) cm
  - Boron control rod (r=3, h=10)cm
  - Rod translates along z-axis
- Problem details
  - Target eigenvalue: 1.0000
  - 100 active batches, 25 discards, 5000 neutrons per batch.
  - Several values of ε considered.



ε	Falsi		Falsi (No Reject)		ABA(2)		ABA(4)		ABA(6)	
	Hist	2σ	Hist	2σ	Hist	2σ	Hist	2σ	Hist	2σ
0.01	2.3	0.2	4.3	0.1	4.3	0.1	4.3	0.1	4.3	0.1
0.002	5.8	1.4	6.8	1.7	11.3	3.5	11.5	5.0	12.8	4.9
0.001	16.0	3.3	22.5	4.4	35.9	12.1	40.5	30.9	53.2	28.8
0.0008	20.4	6.6	35.0	17.5	80.9	45.9	51.8	29.1	71.3	44.1
0.0005	63.7	19.7	74.3	27.9			154.2	162.4		

Number of histories (10^6) versus ε for several search algorithms along with the associated 2σ.

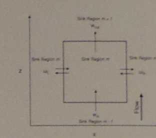


Mean number of histories versus ε for several search algorithms.

D.F. Gill, B.R. Nease, D.P. Griesheimer, "Movable Geometry and Eigenvalue Search Capability in the MC21 Monte Carlo Code," Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013), Sun Valley, Idaho, USA, May 5-9, 2013 (CD-ROM).

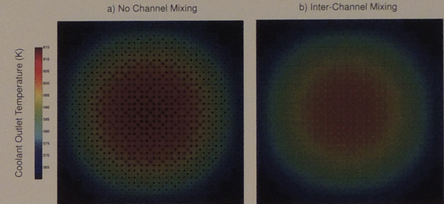
Thermal Hydraulic Feedback

- MC21 supports in-line steady-state thermal feedback calculations through the use of an integrated thermal model.
  - The thermal feedback model is based on a user-input description of heat transfer and coolant flow paths in the problem geometry.
  - Based on the assumption of steady-state conservation of energy and mass under constant pressure.
- In thermal feedback calculations each distinct spatial cell in the model is identified as a source, sink, or non-thermal region.
  - Sources are the heat-producing regions in the core.
  - Sink regions contain coolant that removes heat from the core.
  - Non-thermal regions are assumed to neither produce nor remove heat.
- Once each spatial cell is assigned a thermal region, the heat transfer mapping is applied.
  - Describes the flow of heat from source to sink and flow of coolant from sink to sink.
  - Code provides the flexibility to homogenize source and sink regions over arbitrary volumes of the core.
- The thermal feedback module produces estimates for the temperature distribution in the source and sink regions and sink density values.
  - The thermal feedback module tallies the power distribution by source region during the Monte Carlo transport simulation.
  - Empirical correlations are used to determine the heat transfer coefficient and void fraction in the supported flow regimes.
  - The conduction of heat through the fuel element is approximated by solving a one-dimensional conduction equation.



Example coolant heat transfer model showing a single coolant region (heat sink) surrounded by adjacent coolant regions.

Calvert Cliffs Coolant Temperature



Full-core coolant outlet temperature for the Calvert Cliffs commercial PWR (a) without and (b) with coolant mixing between adjacent channels. Both temperature distributions were calculated with the in-line thermal feedback capability in MC21. Simulation included 11 thermal feedback iterations, each with a simulation running strategy of 220 batches of 500,000 neutrons, with the first 20 batches discarded for source convergence. Temperature results were collected for each of the 39,396 coolant channels. Total simulation time was 19 hours on 64 Intel Xeon Nehalem 2.4GHz processors.

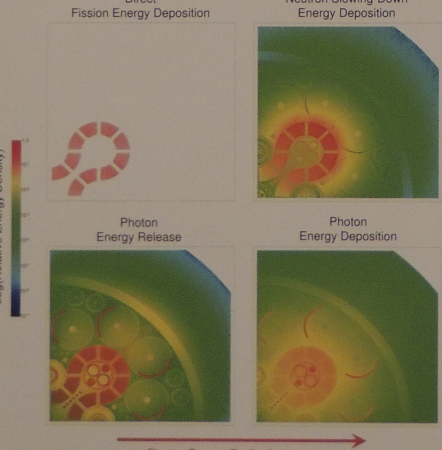
B.R. Hanna, D.F. Gill, D.P. Griesheimer, "Spatial Homogenization of Thermal Feedback Regions in Monte Carlo Reactor Calculations," Nuclear Technology, v. 183, pp. 367-378 (2013).

Source-Sink
Heat Flow Map

Sink-Sink
Coolant Flow Map

Photon Heating

ATR Quarter Core Energy Deposition
NE Quadrant 2D Slice (z = 85 – 90 cm)

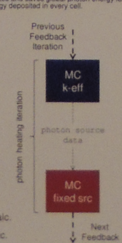


Quarter-core photon energy redistribution in the Advanced Test Reactor (ATR), showing relative spatial density of energy release and deposition. Results were generated with the in-line photon heating capability in MC21, with fully-coupled neutron/photon transport. Heating calculation included separate neutron and photon simulations, each with 5,000 active batches of 10,000 particles. Flux results were collected using track length estimators on a 1000×1000×1 mesh tally. Total simulation time was 3 hours on 64 Intel Xeon Nehalem 2.4GHz processors.

- MC21 includes a generalized energy deposition modeling framework allows control over the accuracy, and expense, of calculations.
  - Framework supports coupled transport along with three approximate energy deposition treatments.
  - Approximate treatments neglect transport of secondary radiation(s) while still preserving energy.
  - Flexibility allows users to tailor accuracy of energy deposition calculation to the needs of a particular application or to meet resource limitations.
- Framework gives flexibility to choose, at run-time, from among four self-consistent energy deposition treatments
  - Constant energy release per fission
  - Constant indirect energy release per fission
  - Local photon energy deposition treatment
  - Fully coupled neutron/photon transport energy deposition
- The most-detailed energy deposition mode includes explicit energy transport for both neutrons and photons.

Full Transport Heating

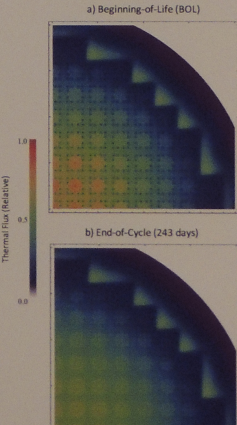
- Neutron Transport Simulation
  - Samples fission and capture photons created during neutron transport and saves source information to a photon source data file.
- Photon Transport Simulation
  - Photon source sites are read in from the photon source data file
  - MC code computes and saves global photon energy leakage and photon energy deposited in every cell.



D.P. Griesheimer, M.H. Stedry, "A generalized Framework for In-Line Energy Deposition during Steady-State Monte Carlo Radiation Transport," Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013), Sun Valley, Idaho, USA, May 5-9, 2013 (CD-ROM).

Depletion

HB Robinson PWR Depletion



Quarter-core thermal flux distributions at core mid-plane for the HB Robinson commercial PWR at (a) beginning-of-life and (b) at the end of the first cycle (5834 full-power hours). Constant-flux depletion analysis was performed with the in-line MC21 depletion solver, using 200,000 depletable compositions. Depletion sequence included 7 timesteps, with a simulation running strategy of 120 batches of 150,000 neutrons, with the first 20 batches discarded for source convergence for each timestep. Flux results were collected using track-length estimators on a 600×600×1 mesh tally. Depletion study ran in 1.93 hours on 192 cores (24 Intel Xeon Sandy Bridge 2.6GHz processors, 8 threads per processor).

- Depletion feedback capability in MC21 is handled by direct coupling with a dedicated depletion solver based on the Variable-coefficient Ordinary Differential Equation (VODE) solver package.
  - MC21 supports both constant-flux and constant-power modes of depletion.
  - Parallelism has been achieved by having multiple depletion code processes running simultaneously, one for each depletable composition.
- In constant-flux mode, MC21 solves the depletion equations assuming the reaction rates for each nuclide are held constant during the depletion step.
  - Nuclidic reaction rates are obtained from beginning-of-time step (BOT) transport calculations.
- In constant-power mode, a predictor-corrector methodology is used.
  - During the predictor phase, constant-flux depletion is performed, followed by an end-of-time step (EOT) transport calculation.
  - The changes between BOT and EOT nuclide reaction rates are approximated as linear in time.
  - These computed time derivatives for the reaction rate are then used in a corrector depletion where the coefficient matrix is incrementally changed during the multi-step solution of the VODE depletion solver.
  - The continual update of the coefficient matrix simulates the changing of the reaction rates that would actually occur during a timestep.
  - If desired, the corrector process may be repeated multiple times to improve convergence of the EOT number densities. However, experience to date has indicated that one corrector step is sufficient in most cases.

MCATK

Monte Carlo Application Toolkit

Los Alamos National Laboratory, Los Alamos, NM, USA

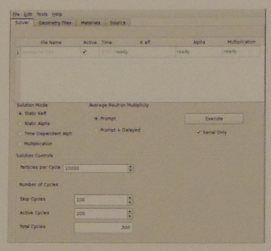
LA-UR-13-27925

Collaborators Wanted!

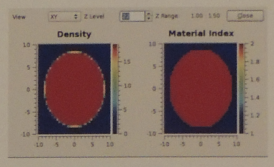
We are looking for students and University collaborators to extend MCATK.
Help us to grow this modern tool. E-mail: `mcatk@lanl.gov`

Automated Testing

QT Gui's



Stand-alone
MCATK driver GUI

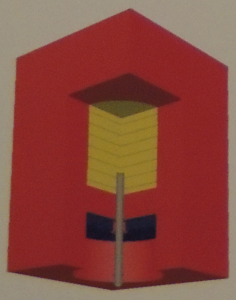


LNK3DNT mesh
geometry plotter

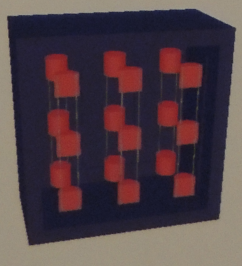
MCATK is easy to extend

C++ class inheritance makes it easy to extend MCATK for your own uses.

For example: one user extended MCATK to track through ROOT geometry for criticality calculations.

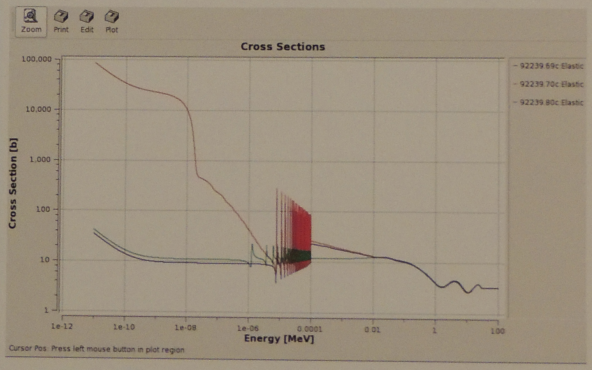


ZEUS2 Critical
Assembly



TinkerToy 2 Critical
Assembly

Cross-Section Viewer



Interactive viewer showing U-239 Elastic cross-section for T-16 2003, ENDF/B-VII and ENDF/B-VII.1.

MCATK Contributors

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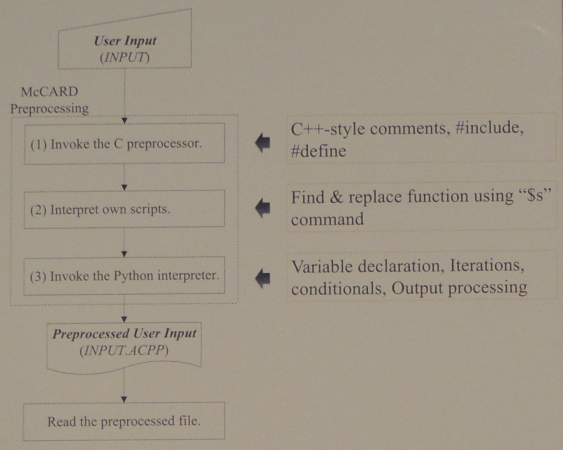
Los Alamos National Laboratory, Los Alamos, New Mexico, U.S.A.
*AWE Aldermaston, Berkshire RG7 4PR, U.K.

Monte Carlo Code for Advanced Reactor Design and Analysis

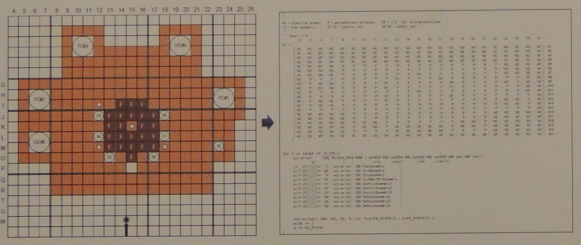
McCARD

Monte Carlo Lab., Nuclear Engineering Dept., Seoul National Univ.

Input Preprocessing System

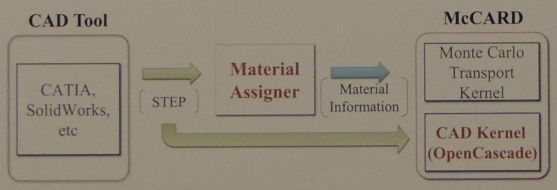


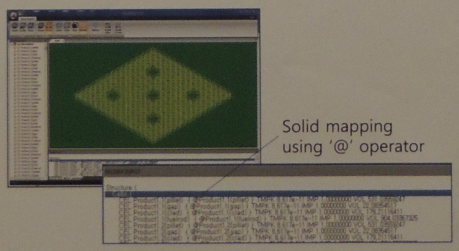
- **Modeling of Kyoto Univ. Critical Assembly**



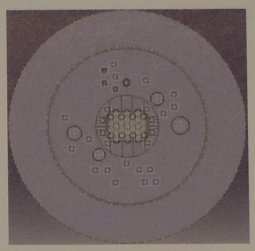
CAD-Based Geometry Processing Module

- **Development of McCARD/CAD**
  - Has the capability to directly utilize the CAD geometry data by converting the CAD model to the internal data structure of the constructive solid geometry to be used by the code with help of a CAD kernel, OpenCASCADE (OCC).

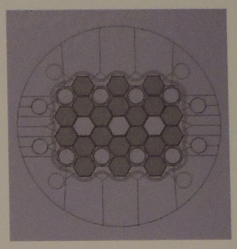




- **CAD Modeling of HANARO Research Reactor Core**



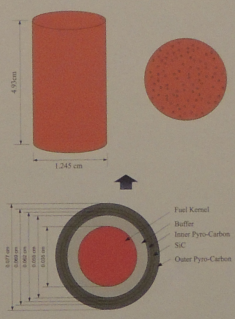
HANARO Reactor



HANARO Core

VHTR Analysis

- **Exact Modeling of Double Heterogeneity**
  - Models **the random distributions of pebbles as well as fuel particles in a fuel compact or a pebble.**
  - Samples TRISO particles of up to ~62% packing fraction by the Jodrey and Tory Algorithm.
- **FCEL Card**

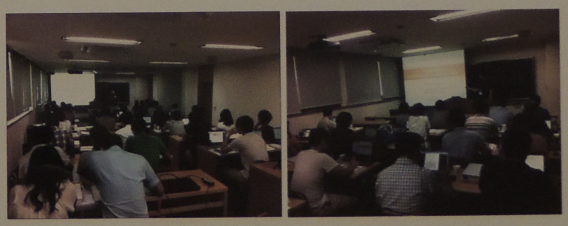



```
FCEL Compact Graphite
     { -cylinder AND +pzB AND -pzT }
     RUSE {  USE Particle
             PackRatio 0.28916
             Merge 1
             Shape CYL (0,0,0)
                   RAD (0,0.6225)
                   EXT (4.93)
          }
```

```
//Composition cell for fuel particle
CCell Particle (
Cells ( //Cell division
        CEL k1  *Fuel { -s1 }
        CEL k2  Buf   { +s1 AND -s2 }
        CEL k3  IPC   { +s2 AND -s3 }
        CEL k4  SiC   { +s3 AND -s4 }
        CEL k5  OPC   { +s4 AND -s5 }
      );
      Surfaces ( //Surface division
         SUR s1  SO 0.0175
         SUR s2  SO 0.0275
         SUR s3  SO 0.0310
         SUR s4  SO 0.0345
         SUR s5  SO 0.0385
      );
);
```

Domestic Release

- **Domestically released for research and noncommercial usage**



< User Training Course, Aug. 21-23, 2013, SNU >

- Hyung Jin Shim, Beom Seok Han, Jong Sung Jung, Ho Jin Park, Chang Hyo Kim, "McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis," *Nucl. Eng. Technol.*, 44[2], pp. 161~176 (2012).

SNA MC
Joint Int. Conf. on Supercomputing in Nuclear Applications + Monte Carlo
La Cité des Sciences et de l'Industrie, Paris, France, October 27-31, 2013

Seoul National University
Nuclear Engineering Department

LA-UR-13-28083

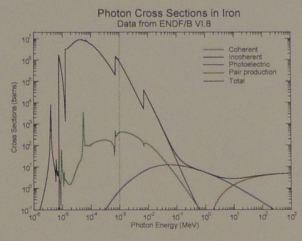
New Electron-Photon Capability in MCNP6

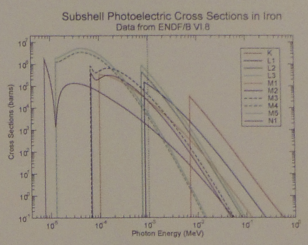
H. Grady Hughes
Los Alamos National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

Photon Enhancements

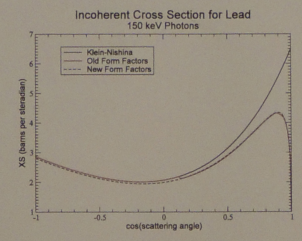
- Extension of existing data: from ≥ 1 keV down to ≥ 1 eV
  - Coherent scattering
  - Incoherent scattering
  - Photoelectric absorption
- New kinds of photoatomic data
  - Subshell-wise photoelectric cross sections
    - Detailed sampling of initial vacancy now possible
  - Complete information for electron subshells
    - Binding energies, electron populations, transitions, etc.
    - Accurate kinematics for photoelectron
- Extended scattering form factors
  - Coherent and incoherent scattering
  - Complete range of energy and angle
  - Accurate interpolation (especially for coherent scattering)

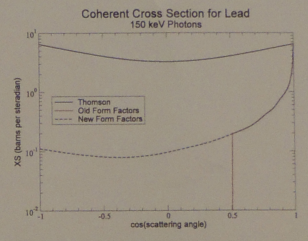




Photon Scattering Form Factors

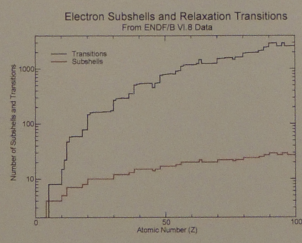
- Incoherent: $\sigma(Z,\alpha,\mu) \sim I(Z,\nu)\,(\alpha'/\alpha)^2\,(\alpha'/\alpha + \alpha/\alpha' + \mu^2 - 1)$
- Coherent: $\sigma(Z,\alpha,\mu) \sim C^2(Z,\nu)\,(1 + \mu^2)$
- ...where $\alpha = E/m_ec^2$; $\alpha' = E'/m_ec^2$
  $\mu = \cos(\theta)$; $\nu = K\,\alpha\,(1-\mu)^{½}$
  $K = 10^{-8}\,m_ec/(2^{½}\,h) \approx 29.1445$
- Old incoherent data: tabulated for $\nu = 0 \ldots 8$
  - Full tabular angular coverage for E ≤ ~99 keV
- Old coherent data: tabulated for $\nu = 0 \ldots 6$
  - Full angular coverage for E ≤ ~74 keV
    - e.g. at 250 keV, no coherent scattering beyond ~ 35°

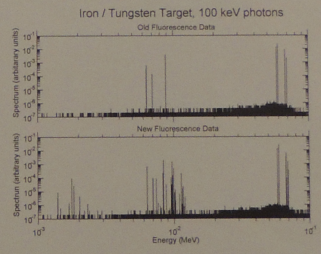




Atomic Relaxation

- Consistent data for electron subshells
  - Binding energies
  - Electron populations
  - Number of transitions
  - Photoelectric subshell cross sections down to 1 eV
- Consistent data for transitions
  - Transitions with photon fluorescence (radiative)
  - Auger and Coster-Kronig transitions (non-radiative)
- Full analog sampling of the relaxation cascade
- New process: Compton-induced atomic relaxation



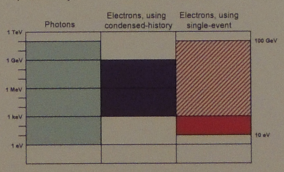


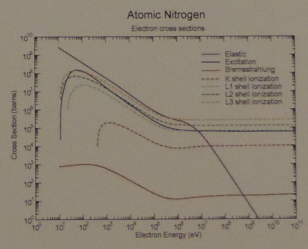
Electron Enhancements

- Microscopic electron cross sections down to 10 eV
- Electron elastic scattering
  - Electron angular distribution as function of electron energy
- Atomic excitation
  - Electron mean energy loss as function of electron energy
- Subshell-wise electroionization
  - Knock-on energy distribution as function of electron energy
  - Knock-on direction and primary energy loss from conservation
- Bremsstrahlung
  - Photon energy distribution as function of electron energy
  - Electron mean energy loss as function of electron energy
  - Photon angular distribution: analytic or from condensed-history

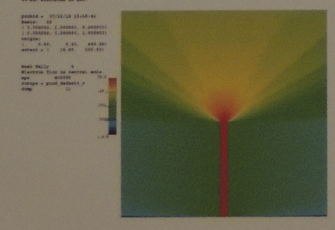
Energy Ranges for Transport

- Photons: 1 eV –100 GeV
- Condensed-history electrons: 1 keV – 1 GeV
- Single-event electrons: 10 eV – 1 keV or above,
  potentially: 10 eV – 100GeV

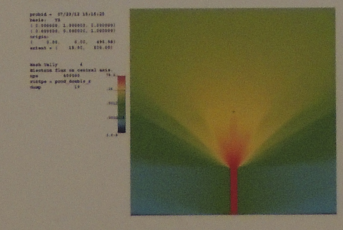




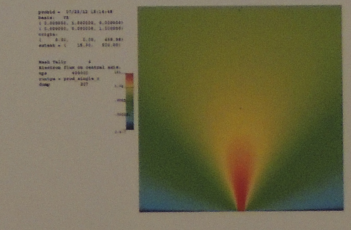
60-MeV electrons in air, default condensed history.



60-MeV electrons in air, more angular substeps.



60-MeV electrons in air, single-event transport.



LA-UR-13-27914

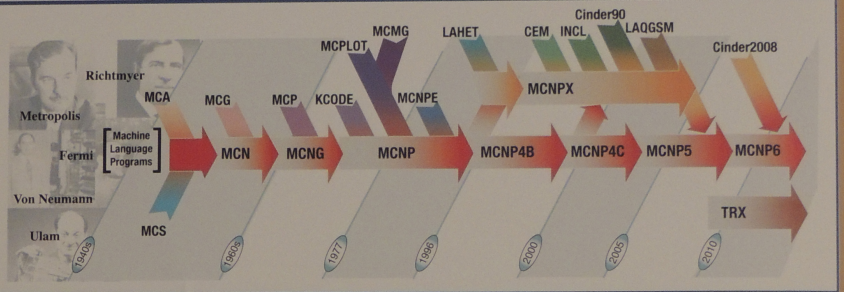
MCNP6 Development

T Goorley, M James, T Booth, F Brown, J Bull, L Cox, J Durkee, J Elson, M Fensin, A Forster, G Hughes, R Johns, B Kiedrowski, R Martz, S Mashnik, G McKinney, D Pelowitz, J Sweezy, L Waters, T Wilcox, T Zukaitis.
XCP-3 and NEN-5, Los Alamos National Laboratory.
R Prael, J Hendricks, contractors.

Production MCNP6 Released

The newest version of MCNP, the production release MCNP6.1, began distribution through RSICC in July, 2013 (http://rsicc.ornl.gov). This release marks the culmination of 5 years of effort to combine MCNP5 and MCNPX into a single code. Both MCNP5 and MCNPX are now frozen and all future development will occur in MCNP6.

MCNP has a long and distinguished history, dating from the early days of Los Alamos. To the right is an overview of decades of MCNP development, from the first computers to the present day, and looking forward to the future.



What is MCNP?

MCNP is a general purpose Monte Carlo N-Particle radiation transport code. It tracks 36 different kinds of particles (neutrons, photons, electrons, protons, pions, etc.) and heavy ions. Important standard features that make MCNP versatile and easy to use include a powerful general source, criticality source, and surface source; geometry, cross section, and output tally plotters; many variance reduction techniques; a flexible tally structure; and an extensive collection of cross-section data.

MCNP is rich in physics.

The chart to the right shows the particles and energy ranges that MCNP can utilize. Recently added physics includes:

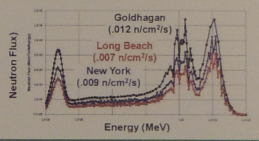
- Photon-induced fission N multiplicity
- Characteristic muon-induced gamma rays
- Exact delayed gamma emissions
- Visible light
- Improved photon-electron transport and atomic relaxation
- Upgrades to CEM & LAQGSM
- GEF Photofission yield

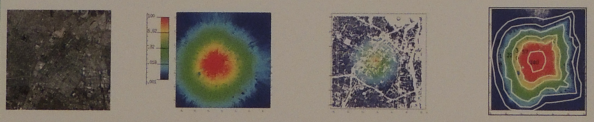
MCNP has many uses.

- Stockpile Stewardship
- Threat Reduction
- Non-Proliferation
- Safeguards
- Criticality Safety
- Medical and Health Physics
- Radiation Measurement
- Urban Consequences
- Astrophysics
- Space Applications
- CAE / CAD Interface

Reactor Design: MCNP can perform detailed depletion at the assembly level for nuclear reactor life-cycle analysis.

Radiation Measurement: MCNP now includes natural background radiation sources, important for signal to noise comparisons for homeland security applications.





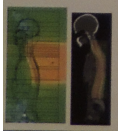
Urban Consequences: MCNP is being used to model US cities and simulate the radiation effects of improvised nuclear devices (INDs). The above images show a 6km x 6km model of Los Angeles and the effects from a 20 kT "FatMan" nuclear weapon. When combined with US Census Bureau, estimates of affected populations are created. FEMA is using these results to make policy decisions.

Asteroid Itokawa energy deposition results for near earth orbit asteroid deflection studies.

Space Applications & CAE Interface: MCNP can now track particles in and plot unstructured meshes and directly read Abaqus geometries. Abaqus, a finite element engineering code, can also read AutoCAD and ProE files, allowing MCNP to access many complex geometry models.

Neutron beam for brain tumor therapy, CT-based geometry (left) and dose (right)

Medical & Health Physics: MCNP is used to calculate human dose resulting from many different kinds of radiation, optimizing possible treatment, and frequently the sources of radiation themselves.



Simulation of proton therapy (left) and dose overlay on CT (right). Thanks to MD Anderson Cancer Center

Future MCNP Efforts:

The LANL MCNP6 team has more than 12 full time and 5 part time staff working on the following:

- Improved physics (incorporate new INCL, add delta rays, improve condensed-history methods, consider charge pickup at low energies, enable data table transport for light ions).
- Improved single-event electron transport and advanced photon-electron transport.
- Improved software parallelism (utilize >10K processors w/ mpi, R&D into co-array Fortran 2008).
- Improved delayed particle emissions (better energy and angle correlations, beta and alpha emissions).
- Efforts for EMP (adding electric fields, improved magnetic fields, specialized tallies).
- Integration of unstructured mesh (work with weight windows mesh, charged particle tracking).
- Visible light (refraction, reflection, Cherenkov radiation, molecular transport libraries).
- Moving objects (realistic simulation of moving vehicles, in vivo organ motion)
- Sensitivity and uncertainty.
- Automatic weight windows generation from SN calculations – LANL's PARTISN.

MCNP has received funding from DOE, DoD (especially DTRA), DHS/DNDO, NASA and others, supporting a wide variety of missions.

We appreciate your past and future support.

Overview of the MCU Monte Carlo Software Package

M.A. Kalugin, D.S. Oleynik, D.A. Shkarovsky
National Research Centre "Kurchatov institute"

General information

MCU (Monte Carlo Universal) is a project on development and practical use of a universal computer code for simulation of particle transport (neutrons, photons, electrons, positrons) in 3D systems by means of the Monte Carlo method.

The project started in 1982 at Kurchatov Institute.

Current stable version of the software package is MCU-5 (hereinafter – MCU)

MCU-6 software package is under development within the framework of the MCU project now.

The modules of MCU for particle transport simulation are written in Fortran 90/95.

MCU is parallelized using MPI.

Approved operating systems are Windows and Unix/ Linux.

Verification reports of the MCU software package have been issued for nuclear reactors with thermal, intermediate and fast neutron spectrum including power and research reactors, special types of reactors, high-temperature gas-cooled reactors, burners of minor actinides as well as fuel storages and shipping casks.

Particle physics treatment

The MCU package allows simulating neutron, photon, electron and positron trajectories.

Neutron physics treatment

It is possible to build physical model from pure multigroup to pure point-wise approximation using different combinations of physical submodules and corresponding data libraries.

Photon physics treatment

The interaction of photons with matter can be simulated using both multigroup and point-wise representations of the cross-sections. The following processes are simulated: coherent and incoherent scattering, photoelectric effect and production of electron-positron pairs with the possibility of generation of photoneutrons and secondary photons, electrons and positrons.

Electron and positron physics treatment

The following processes of electron-positron interaction with matter are simulated by MCU: elastic interaction with the Coulomb field of nuclei of the medium, inelastic scattering on bound atomic electrons with ionization and excitation of atoms, inelastic interaction with the Coulomb field of nuclei and atomic electrons accompanied by bremsstrahlung, and annihilation of positrons on electrons.

It is possible to use the scheme of individual collisions or condensed collision model.

Particle transport

By means of the MCU package one can solve

- Criticality problem using generations with a fixed total weight of the neutron sources in one generation
- Fixed source problem
  - with modeling of secondary particles
  - without modeling of secondary particles

Traditional variance reduction techniques such as a weight window, energy cutoff, energy and geometry splitting with Russian roulette, ring and point detectors are implemented in MCU.

Nuclear data

Two data banks have been developed for the MCU package using different evaluated nuclear data files and data libraries

- The main data bank MCUDB50 contains data for 375 isotopes.
- The additional MCUDB50RF data bank is based on the RUSFOND library and contains data for 460 isotopes.

Main sources for the data bank development are as follows: ENDF/B, RUSFOND, JENDL, JEFF, LIPAR, BNAB, VITAMIN, IRDF, RRDF, etc.

The libraries of constants forming the data banks are processed using different widely-used codes: NJOY, PREPRO, GRUCON and our own processing codes.

MCU modules

Geometry module

The geometry module allows modeling of 3D systems with arbitrary geometry using combinatorial approach. The code provides about 20 simple bodies (spheres, parallelepipeds, cylinders and etc.) that may be combined using intersection, union, and complement operations.

There are means to simplify the description of the geometries with repeating elements. Such elements can be defined by means of lattices and nets.

The special algorithm allows considering effects of double heterogeneity when the fuel elements contain tens of thousands of the fuel kerns.

The Woodcock method gives an opportunity to carry out calculations of complex geometrical objects, which surfaces are not described by planes or surfaces of the second order.

MCU modules

Source module

Source module provides an opportunity to perform calculation with 3D particle distributions of almost any complexity.

Surface source is implemented. It allows particles crossing a surface in one problem using to be used as the source for a subsequent problem.

Tally module

Tally module calculates the following global tallies for the system as a whole: K_{eff}, β_{eff}, neutron lifetime, average lethargy causing fission, leakage and etc.

The following tallies are available for arbitrary energy ranges and isotopes in tally areas: fluxes over the volume or surface, surface current, various reaction rates and their macroscopic cross-sections, dosimetry reactions rate, nuclear heating, flux at a point, neutrons and photons dose characteristics, few-group constants of fuel pins and fuel assemblies, scattering and fission matrixes, diffusion coefficient, and etc.

For photons, electrons and positrons it is possible to estimate the fluxes, reaction rates, the charge, and the energy absorbed by the material.

MCU has no restrictions on the number of materials and tallies.

Depletion module

The MCU package contains its own depletion module that allows calculating changes in nuclide compositions of reactor materials in the process of reactor operation and estimating radiation characteristics of irradiated nuclear fuel.

The library for depletion contains data for more than 1000 nuclides.

T/H feedback module

The MCU package contains the module to provide feedback on coolant temperature and density, fuel temperature and equilibrium xenon concentration. At present it supports only VVER calculations and allows receiving data on coolant, fuel and xenon for the hot state of the reactor on the defined power level without any use of additional codes in full scale model calculation.

Module of uncertainty analysis

The module of uncertainty analysis allows calculating the influence of input data uncertainties (fuel densities, fuel enrichment, geometry parameters and etc.) on the final result.

Control module

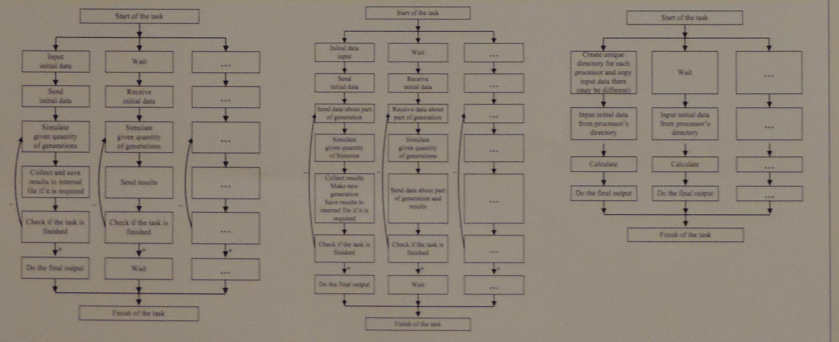
The control module has the possibility to change parameters of the system during its operation between depletion steps (control rods movement, boric acid concentration change, geometry change and etc.)

Parallel calculation

MCU package is parallelized using MPI. It may be used at a single computer, several computers connected through a local area network, and at supercomputers. The use of graphics processing units is not supported.

Three different modes are realized for multiprocessor calculations in which the unique random number sequence is used for each processor.

In case of depletion calculation each processor deals with part of burnable materials.



Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013)
La Cité des Sciences at de l'Industrie, Paris, France, October 27—31, 2013

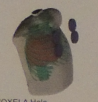
amec

MONK 10 and MCBEND 11

A summary of recent developments

Geometry Modelling

The PIPES Hole


The VOXELA Hole

An example CAD import

MONK® and **MCBEND** use a common package for geometry modelling comprising two complementary components: Fractal Geometry; and Hole Geometry.

Improvements to the **Fractal Geometry** package include:

- a new TRI body, providing a simpler alternative to the existing PRISM body for triangular prisms;
- a new TETMESH zone to support ray tracing through a zone containing materials in a tetrahedral mesh;
- a new IGES body for importing CAD geometry models in IGES format;
- a new POLY body formed from a closed surface defined by a set of triangular facets;
- support for multiple successive rotations about different points; and
- improved checking of models to ensure that:
  - each body in a nest is enveloped by the next body;
  - all inner bodies of a simple cluster are enveloped by the container;
  - all inner bodies of a simple cluster are non-intersecting; and
  - bodies in a cluster are declared with overlaps which intersect as stated.

The PBMR Hole with a subsidiary PEBBLE Hole. A pebble-bed reactor may contain 500,000 pebbles, each containing 15,000 multilayer coated fuel particles. Each grain in each pebble can be modelled explicitly using these Holes.

Improvements to the **Hole Geometry** package include:

- a new PIPES Hole for modelling arrangements of pipes, defining: locations; radii and materials of annuli; connections; and interstitial material;
- a new BENTPINS Hole for modelling damaged fuel pins which have undergone bending or buckling;
- a new VOXELA Hole used for the approximate representation of an object as an array of cubic voxels;
- a new TETMESH Hole for importing CAD models as Hole Geometries;
- a new RANDROD Hole for modelling random distributions of rods (e.g. cut fuel pins in dissolvers);
- improvements to the QUADRIC Hole for modelling pipes with elliptical cross sections and an elliptical axis; and
- new PBMR and PEBBLE Holes for modelling pebble bed reactors in great detail — each multilayer coated fuel grain in each fuel pebble is modelled explicitly.

Parts, Materials and Holes can all be given user-defined names so that they can be referenced by name in other parts of the model. This makes construction and maintenance of models more user-friendly and aids quality assurance.

Physics Features

Collision processing and nuclear data

MONK and **MCBEND** feature both the established DICE point energy and the more recent BINGO continuous energy nuclear data and collision processing packages. Improvements in BINGO include:

- the use of cross-sections tabulated at energy points optimised for each nuclide;
- improved variable temperature treatment with run-time Doppler broadening;
- enhanced thermal scattering modelling including the use of bound carbon data for graphite;
- better representation of correlated energy/angle laws;
- a more detailed representation of the tails of the fission spectrum;
- point energy burnup;
- explicit modelling of Bremsstrahlung; and
- new nuclear data libraries, including: JEFF-3.1, ENDF-B/VII and CENDL3.2.

Run-time Doppler broadening

The BINGO collision processor includes a run-time Doppler broadening capability:

- The effect of temperature on resonances is evaluated at each collision event to derive appropriate cross-section data and event outcomes.
- Run-time Doppler broadening provides the ability to follow temperature variation throughout a reactor core and throughout its lifetime, providing a route for thermal hydraulic feedback.
- The nuclear data library contains data at relatively few specific base temperatures; the code broadens from the nearest lower temperature data to the temperature of interest.
- Any material temperature can be modelled within the range covered by the library (currently 293.6 K to 80,000 K).

Graphics Features

Visual Workshop

Visual Workshop is an integrated development environment for preparing, running, checking, modifying and analysing results from the ANSWERS® suite of codes including **MONK** and **MCBEND**. Its **key features** include:

- an interactive 2D and 3D ray trace of the model using the same routines as the physics codes;
- a wireframe display of the model; and
- built-in editing, running and diagnostic capabilities.

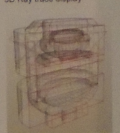
Recent developments include:

- results visualisation — the following results can be plotted as 3D contours or iso-surfaces, 2D contour plots or 2D cell plots:
  - importance map values and particle inflows (**MCBEND**);
  - fluxes in Unified Tally meshes (**MONK** and **MCBEND**);
  - responses and doses in Unified Tally meshes (**MCBEND**); and
  - action tallies in Unified Tally meshes (**MONK**);
- event localisation and track visualisation, including:
  - history log and collision log data;
  - source log, forced flight log and leakage log data; and
  - birth store data.
- 3D stereo viewing—the 3D wireframe view can be displayed in stereo using a compatible combination of graphics card, monitor and stereo glasses.

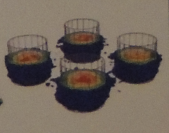
3D Ray trace display

3D Response contours

History log wire frame display


3D Wireframe display

History log ray trace display


3D Neutron flux contours

Scoring Features

Unified Tally Module

MONK and **MCBEND** feature a new **Unified Tally** scoring module with the following features:

- Scoring bodies may be overlaid on, and are independent of, the underlying model geometry;
- Scoring bodies may be subdivided to form 1D, 2D or 3D meshes of any required size;
- Any number of bodies may be defined and may overlap freely;
- Each scoring body may optionally score in a different energy group scheme;
- The following types of scoring are supported:
  - Track length and collision density estimates of scalar flux and currents (**MONK** and **MCBEND**); and
  - all other scores except for sensitivities and energy deposition (**MCBEND** only).
- Scoring body geometries include:
  - a cuboidal BOX, optionally subdivided to form a Cartesian mesh;
  - a cylindrical ROD, optionally subdivided to form an *R*θ*Z* mesh;
  - a SEC body forming a sector of a cylindrical annulus, optionally subdivided in *R*, θ and *Z*;
  - a rectanglular PLANE surface, optionally subdivided in either or both directions;
  - a circular DISC surface, optionally subdivided radially and/or azimuthally;
  - an ARC surface forming a sector of a cylindrical surface subdivided azimuthally and/or axially; and
  - a SPHERE surface, optionally subdivided in azimuthal and/or polar directions.
- The Unified Tally module includes the capability to score by material. This divides the scores recorded in a given mesh between the events in individual materials.

Action Tallies in Unified Tally

In **MONK** the following action tallies can be scored in any solid Unified Tally body, which can optionally be subdivided to form a mesh and can use any energy group scheme:

- Capture;
- Fission and number of fission children;
- Elastic and inelastic scatter; and
- (n,2n) and (n,3n) reactions.

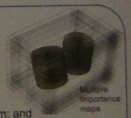
These events can optionally be scored by material and/or nuclide.

Code-specific Features

New features specific to MONK 10A

- New Action Tallies:
  - Region Fission — tallies by energy and region of the samples that cause fission and samples that emerge from fission events; and
  - Neutron Balance — tallies of various events by energy group.
- Shannon Entropy of the scalar flux in a 2D or 3D Unified Tally mesh
- Sensitivity to nuclear data:
  - Extended to BINGO continuous energy data;
  - Includes sensitivity to material density; one or more reaction cross-sections in a specific nuclide; all reactions excluding specific reactions; and mean number of secondary neutrons per fission, $\bar{\nu}$.
  - Estimates of uncertainties by combining sensitivity results with covariance data;
  - An option to adjust nuclear cross-sections and $\bar{\nu}$ for sensitivity analysis and data assimilation.
- Fixed source option for modelling systems with an external, fixed source (e.g. accelerator-driven systems);
- Parallel processing — a 64-bit version of MONK which uses OpenMPI to run in parallel on high performance computing architectures;
- A novel method for spatially-dependent depletion calculations using an overlaid mesh;
- Coupling to a thermal hydraulics model to account for the inherent coupling between core neutronics and thermal hydraulics;
- Coupling to **MCBEND** to account for gamma heating in non-fissile regions;
- An updated validation database, comprising analyses of over 800 experimental configurations.

New features specific to MCBEND 11A


Multiple importance maps

- Improvements to coupled calculations, including:
  - processing of up to nine collisions files;
  - coupled neutron-gamma calculations in a single step; and
  - combining of neutron and gamma responses to give a single dose.
- Improvements to variance reduction methods, including:
  - the ability to use different importance maps in different parts of the problem; and
  - forced flight enhancements to allow a sequence of forced flight surfaces to be defined.
- New response libraries including:
  - IRDF-2002 detector cross-section library (13,230 energy groups) and covariances (25 groups);
  - ICRP-74 neutron and gamma dose rate conversion factors; and
  - dose rates due to beta radiation.
- Support for GRID calculations — combining results from parallel, independent calculations.

MONK and **MCBEND** and **Visual Workshop** are developed, maintained and supported by the ANSWERS® Software Service.

The current version of **MCBEND** is MCBEND11A, released in 2013.

The current version of **MONK** is MONK9A. MONK10A, is due to be released in late 2013 or early 2014.

The current version of **Visual Workshop** is version 2A. Version 3A will be released with MONK10A.

Contact the ANSWERS Software Service

Telephone +44 (0) 1305 851240
Fax +44 (0) 1305 851105
Email answers@amec.com
Web www.answerssoftwareservice.com

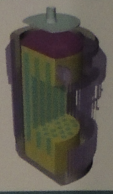
MONK and MCBEND

Advanced Monte Carlo codes for the analysis of: nuclear criticality; reactor physics; radiation shielding; and dosimetry.

The ANSWERS® Software Service has for over 30 years provided clients in the nuclear industry with high quality software and consultancy services in nuclear criticality, reactor physics, radiation shielding, dosimetry, and nuclear data.

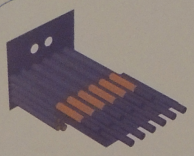
ANSWERS® codes are widely used in over 30 countries around the world and on a range of reactor types including: AGR, BWR, CANDU, MAGNOX, RBMK, PBMR, PWR, VVER and experimental reactors and materials testing reactors.

ANSWERS® software is validated for a wide range of applications, and is supplied with full nuclear data libraries and test cases. Its ready-to-run packages are available for a range of platforms. The comprehensive and easy-to-use documentation and software interfaces ensure immediate usability. Regular upgrades are available as each software product is fully maintained and actively developed to meet the needs of our world-wide customer base. Quality is assured in a quality management system certified to BS EN IS0 9001 Series.



MONK

Nuclear Criticality Safety and Reactor Physics



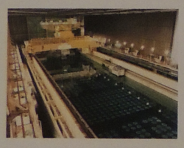
MONK® is a powerful Monte Carlo software tool for nuclear criticality safety and reactor physics analysis.

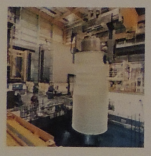
MONK's advanced geometry modelling and detailed continuous energy collision treatment provides realistic 3D models for an accurate simulation of neutronic behaviour. MONK's superhistory algorithm provides robust and reliable estimates of the neutron multiplication factor, *k*-effective and other parameters of interest.

Nuclear data libraries exist for MONK from a variety of sources including JEFF, ENDF, JENDL and UKNDL. These exist in continuous energy and hyperfine group form for definitive criticality analyses and, for JEFF and UKNDL, in multigroup form for reactor analysis. A microscopic depletion capability is available with the multigroup data option.

Validation is of prime importance for a criticality code and the MONK package contains a large set of validation data, drawing heavily on experiments in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook. Support in the use of the code and its application is available from our dedicated help-desk, providing direct access to our criticality, reactor physics and shielding expertise.

Applications



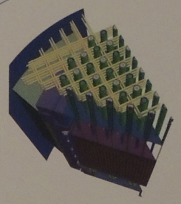


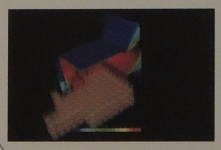
MONK has been successfully used in support of the design and operation of a wide range of nuclear facilities covering the complete fuel cycle including:

- uranium enrichment covering diffusion and centrifuge plant;
- fuel fabrication for thermal, fast and experimental reactors;
- new and spent fuel transportation both within countries and between countries;
- design studies for fissile material transport containers;
- spent fuel handling and long term pool storage;
- spent fuel dry storage;
- fuel consolidation and dry cell handling;
- fuel dissolution;
- chemical separation involving mixer-settlers and pulsed columns;
- reactor core loading assessment;
- product finishing and storage;
- waste treatment and handling;
- waste storage including evaporation, vitrification, encapsulation and consolidation;
- plutonium metal production and handling;
- reactor analysis for all thermal reactor types; and
- burnup credit analyses.

MCBEND

Radiation Shielding and Dosimetry





MCBEND is a powerful Monte Carlo software tool for general radiation transport analysis for shielding and dosimetry applications.

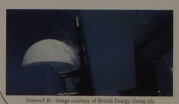
MCBEND is a general purpose radiation transport code that can calculate neutron, gamma-ray and charged particle transport in sub-critical systems; coupling of the different radiation types is also possible. MCBEND models the transport of individual particles accurately by using a very fine energy group representation of nuclear data and a flexible geometry modelling package.

In addition to its powerful geometry modelling package MCBEND has versatile source description options and powerful automatic acceleration options for maximum productivity. Nuclear data libraries exist for MCBEND from a variety of sources including UKNDL, JEFF, ENDF and JENDL.

MCBEND is validated for an extensive range of applications. The validation database covers many of the materials and geometries that are encountered in the nuclear industry and is subject to ongoing review and enhancement.

Support in the use of the code and its application is available from our dedicated help-desk, providing direct access to our shielding and dosimetry expertise.

Applications



Sizewell B – Image courtesy of British Energy Group plc

MCBEND has been successfully applied to such problems as:

- shield design and optimisation for reactor plant;
- interpretation and analysis of measurements on operating plant and in experimental facilities;
- new and spent fuel transportation both within countries and between countries;
- neutron damage in reactor pressure vessels and other reactor components;
- design studies for fissile material transport containers;
- decommissioning preparation and planning;
- shield design for waste storage facilities;
- reprocessing facilities;
- fusion devices;
- fuel storage facilities support;
- prediction and calibration of nuclear instruments;
- geophysical logging tool analysis and operations support;
- prediction of personnel dose levels;
- calculation of radiation-induced material changes;
- shield design for irradiation plant;
- sterilisation of products by irradiation; and
- medical physics treatment planning.

Benefits of MONK and MCBEND

- The codes offer an unrivalled geometry modelling capability and acceleration options (MCBEND) for optimum accuracy and efficiency of analysis.
- They are recognised as effective and reliable analysis tools in safety case submissions to regulators.
- They are continually maintained and developed to meet our customers' operational needs.
- Nuclear data libraries are available to support international needs and to provide valuable cross-checking capabilities.
- Visual Workshop integrated development environment with powerful interactive 2D and 3D ray trace graphics for model development and verification; and results display.

What our customers say…

'I struggled to find a way of representing the system with anything like the required degree of accuracy - moving to MONK® solved that problem immediately'.

ANSWERS customers include the following:

AF-Consult Switzerland Ltd, Areva NP, Argonne National Laboratory, Aripps, AWE Aldermaston, Babcock International Group, BAE Systems, Battelle Pacific Northwest Laboratory, Cambridge University, China Institute for Atomic Energy, China Nuclear Power Engineering, Dounreay Site Restoration Ltd, DSO National Laboratories, EDF Energy, Enrichment

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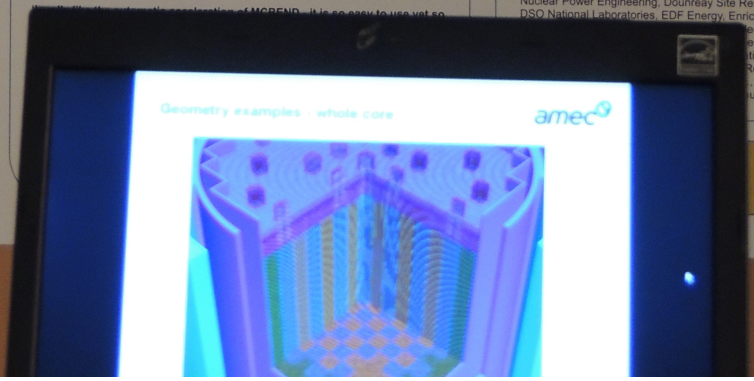
Regulation, Rolls
, Springfields
urst, Xi'an



Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013) - La Cité des Sciences et de l'Industrie, Paris, France, October 27-31, 2013

IRSN
INSTITUT DE RADIOPROTECTION ET DE SÛRETÉ NUCLÉAIRE
Enhancing nuclear safety

Capabilities Overview of the MORET 5 Monte Carlo Code

SNA + MC

B. Cochet[1*], A. Jinaphanh[1], L. Heulers[1], O. Jacquet[2]

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[2] *External consultant, Saligna, 33240, France*
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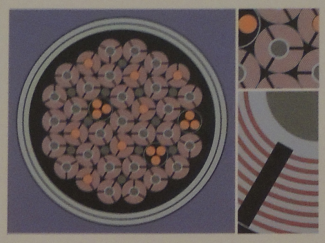
The MORET code is a simulation tool that solves the transport equation for neutrons using the Monte Carlo method. From its inception, the code has been constructed with the aim of providing a great flexibility to implement new components or methods without any difficulties. The result is a code that allows users to model complex three-dimensional geometrical configurations, use various evaluations and treatments for nuclear data to describe the materials, select the best adapted simulation method (from all methods available) related to their problem, define their own tallies and analyze the results. Initially designed to perform calculations for criticality safety assessments, the code includes new features to expand its use for reactor applications.

Geometry modelling



The modular geometry allows to model complex geometries by using basic building blocks, called modules. The geometry of each subsystem is described in a combinatory way using volumes.

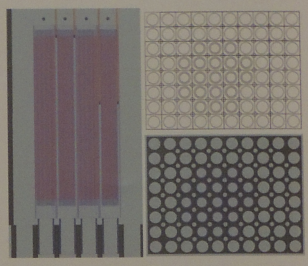
The volume is characterised by its properties: the mother volume, its shape, its position and the material it contains. Available basic shapes are spheres, ellipsoids, boxes, cylinders, hexagons, cones and planes.

Geometrical operators may be added to describe the combinatorial properties of the volumes, such as how they intersect one another, or how they may be positioned one another:

- Overwrite, union, truncation, intersection.

New geometrical operators have been added in this version:

- Revolution and rotation.



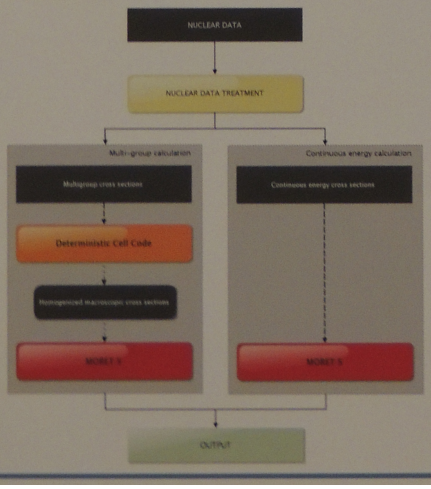
The lattices make possible to describe only once the volumes of any structure that appears more than once in a geometry. Two types are available using rectangular or triangular pitch and can be included in volumes of any shape. The definition of secondary mesh volumes allow users to describe alternative contents in the mesh volumes.

A geometry-plotting function helps the users to check their geometry modeling (in complement of several internal code checking to find input errors).

Material: two calculation routes

The MORET 5 Monte Carlo code is a neutron simulation tool which calculates different physical quantities such as the multiplication factor k_{eff}. It includes two calculation routes:

- a multi-group route based on macroscopic homogenized cross-sections calculated previously from various deterministic cell codes such as APOLLO2, DRAGON4 or SCALE 5.1. The code allows loading cross sections made with different cell codes into a unique input data. This can be useful in R&D to estimate the sensitivity of the results to the used nuclear data.
- a continuous energy calculation based on home-made nuclear data libraries with ACE format (these libraries are performed using the common processing tool NJOY). The development of this new feature required significant work for the modeling of unresolved resonance range, the temperature treatment and the neutron thermal scattering.



Initial distribution of neutrons

The calculation is an iterative process, following the neutrons from their birth until death (whatever the cause). For each cycle, the distribution of the neutron is defined on the basis of fissions generated in the previous cycle. Nevertheless the user must provide the distribution for the first cycle to initialize the iterative process. Two ways are available:

- in a volumic manner: neutrons are uniformly distributed in a volume;
- in a point wise manner: coordinates of starting neutrons are given.

Neutron tracking

When tracking a particle, the MORET code calculates the distance to the limit of the current volume, the distance to next collision, check if the neutron encounters a volume contained in the current one and takes the minimum as the distance traveled by the neutron. If the distance to the next collision is the lowest, then the neutron undergoes an interaction; else the neutron leaves the current volume, enters a new volume and undergoes a new transport calculation.

Woodcock method

The MORET code can also perform the tracking with the Woodcock Method. This tracking can be done on the whole geometry or in some parts of the geometry.
This alternative tracking method may be used to treat complex geometries with a large number of volumes in order to reduce the computational time.
It is particularly useful when volumes are significantly smaller than the mean free path or have complex shapes such as the pebble-bed reactor HTR-PROTEUS.

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SNA + MC

Simulation methods for source convergence

The source convergence is an important issue in Monte Carlo particle simulations. Beyond the natural method, other sampling methods were designed to address two concerns:

- force neutrons to visit all fissile volumes to reduce the risk of weak coupling;
- accelerate the convergence to achieve more quickly a neutron distribution close to the reality and get the value of the reactivity of the system.

The MORET code embeds several techniques for sampling source neutrons among potential fission sites.

➢ Stratified sampling, Fission matrix method, Importance sampling, Oversampling, Super-history, Wielandt method.

Set & Analyse the outputs

The code allows estimating various physical quantities for neutrons. Designed for criticality safety assessments, it can calculate k_{eff} but also the fluxes and the reaction rates in the volumes, the neutron leakage of the whole geometry or the neutron source number for each volume.

The MORET 5 code improves the output capabilities, allowing user to obtain any physical values using customized tallies described by:

➢ the type of the response function to be calculated;
➢ their characteristics such as the selected volumes, the materials or isotopes, the energy group structure, etc.

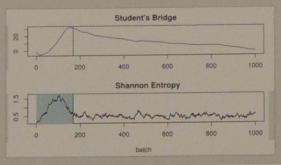
Kinetic parameters

The MORET 5 code provides an one-run estimation of the effective kinetic parameters for the continuous energy route:

➢ the effective neutron generation lifetime Λ_{eff};
➢ the effective delayed neutron fraction β_{eff}.

Delayed neutron data, production and fission spectrum per precursor group are fully handled by the code.

Tests for the calculation convergence



In the MORET 5 code, two main tools are available to help the user detect convergence issues:

➢ statistical tests to determine normality of samples;
➢ automated transient detection based on an indicator (k_{eff} or Shannon entropy), a statistical test and a truncation method using a bridge constructed from the Student Statistic.

The normality of k_{eff} sample is checked with two statistical tests:

➢ Chi-square test which is often used for its ease of implementation;
➢ Lilliefors method which is an adaptation of the Kolmogorov-Smirnov test for Gaussian samples.

Verification & Validation

Verification process

Many capabilities result from the interaction of code components. New features could change the overall operation of the software. A large set of verification tests is launched to ensure that the code still meets previous specifications (this is also known as non-regression tests). In the development phase, the verification procedure involves performing specific tests to model the new capability introduced in the code and then proceed to an analysis of the results.

Validation process

The validation is done through the comparison of the calculated k_{eff} with the benchmark k_{eff}. If the discrepancy between these two k_{eff} is higher than the combined standard deviation $\sigma_{combined}$ of the benchmark uncertainty and the Monte Carlo standard deviation, a bias can be identified.

$$\sigma_{combined}=\sqrt{\sigma_{MC}^2+\Delta k_{eff_{benchmark}}^2}$$

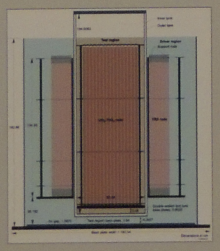
The k_{eff} results for both calculation routes (using the same libraries) are then compared together. It allows enhancing biases due to the multi-group treatment and physical models implemented in the codes.

Validation database

Currently, the experimental validation database is essentially dedicated to the validation of the MORET code for nuclear criticality safety applications. This database covers a broad variety of configurations in terms of fissile medium, moderator, reflector and neutron spectrum (to validate different materials and cover a wide moderation ratio range). It is made up of 2200 critical experiments (included in 244 series of experiments) divided into 8 categories.

Some efforts are made to continue and expand the validation of the code for reactor applications. For example, recent work has been done using the Epithermal Test Assembly (ETA) experiments. This work is still in progress.

Some results for reactor applications



The table below gives some k_{eff} results.

	JEFF-3.1	ENDFB/-VII.0
CONTINUOUS ENERGY	0.99141 (30)	0.99659 (30)
MULTI-GROUP	0.99488 (30)	-

Preliminary analyses show that there is a negative bias for both calculation routes compared to the benchmark k_{eff} (0.9995 ± 0.00200).
The multi-group treatment has also a small impact on the results.

Some results for criticality safety applications

The average C-E (in pcm) per 4 categories are given below. Preliminary analyses show that the results for continuous energy route (using the JEFF-3.1 library) are in good agreement with the benchmark k_{eff} for the majority of cases. Regarding the multi-group route (using the APOLLO2 code and the JEFF-3.1 library), some improvements are still needed.

	AVERAGE	LATTICES		METAL		DISSOLVERS	SOLUTIONS
MULTIGROUP	k_{eff} discrepancy	211 (1)	903 (2)	-183 (1)	1051 (2)	337	348
	Dispersion	315 (1)	342 (2)	483 (1)	1475 (2)	499	649
CONTINUOUS ENERGY	k_{eff} discrepancy	-166 (1)	121 (2)	182 (1)	271 (2)	280	203
	Dispersion	147 (1)	257 (2)	353 (1)	859 (2)	505	588

(1) No reflector, reflector CH2 or H2O ; (2) Metallic reflector (steel, aluminium, etc.)

The MORET code is a simulation tool that solves the transport equation for neutrons using the Monte Carlo method. It allows modelling complex three-dimensional geometrical configurations, describe the materials, define the tallies in order to analyze the results. The MORET 5 release introduces new capabilities that have been tested continuously during their development and, in particular, before and during the V&V process. Initially designed to perform calculations for criticality safety assessments, the

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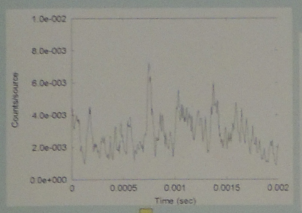
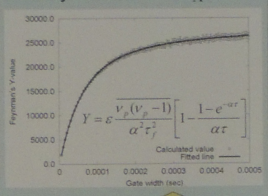
Recent Developments of JAEA's Monte Carlo Code MVP

Simulation of Feynman-α experiment

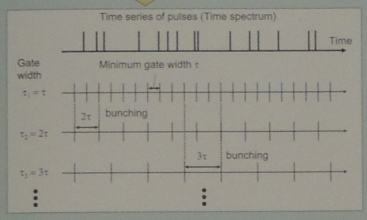
- MVP can simulate the Feynman-α to calculate the prompt neutron decay constant.

prompt neutron decay constant $\alpha = \frac{\beta_{eff} - \rho}{\Lambda}$





$$Y = \varepsilon \frac{\overline{\nu_p(\nu_p - 1)}}{\alpha^2 \tau_f^2}\left[1 - \frac{1 - e^{-\alpha\tau}}{\alpha\tau}\right]$$



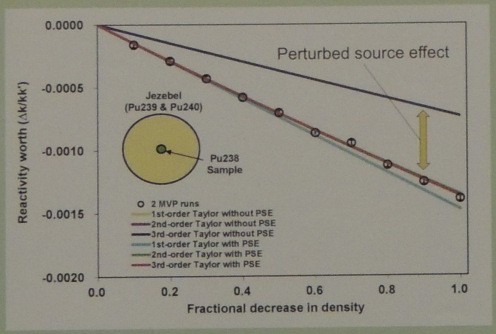
Feynman's Y value

$$1 + Y \equiv \frac{\overline{C^2(\tau)} - \overline{C(\tau)}^2}{\overline{C(\tau)}}$$

Mean and mean squared counts for each gate width

Perturbation calculation for k_{eff}

- MVP can calculate Δk_{eff} with the differential operator sampling and correlated sampling techniques.[1,2]
- The perturbed source effect can be estimated with the techniques.

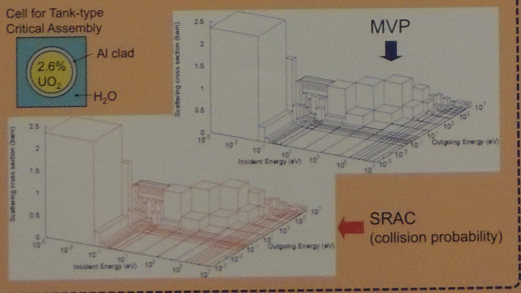


1) Y. Nagaya, T. Mori, *J. Nucl. Sci. Technol.*, **42**, 428-441 (2005).
2) Y. Nagaya, T. Mori, *Prog. Nucl. Sci. Technol.*, **2**, 842-850 (2011).

Group Constant Generation

- MVP can generate a set of group constants via the scattering matrix and matrix moment tallies.

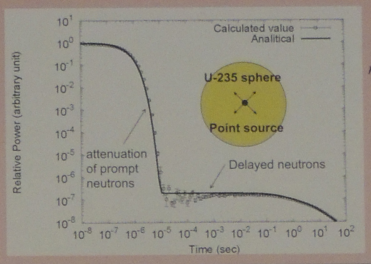
Seventeen-group macroscopic scattering matrices for TCA cell



- The scattering matrix moment tally generates
  - diffusion coefficient D for diffusion calculations,
  - Legendre (P_L) cross sections for transport calculations.

Simulation of Delayed Neutrons

- Delayed neutrons can be treated explicitly.



Analytical solution

$$n(t) = \ell \sum_{j=1}^{m+1} \frac{e^{\omega_j t}}{\ell + \sum_i \frac{\beta_i \lambda_i}{(\omega_j + \lambda_i)^2}}$$

ℓ : Generation time
β_i : Delayed neutron fraction
λ_i : Decay constant
ω_j : Root of inhour equation

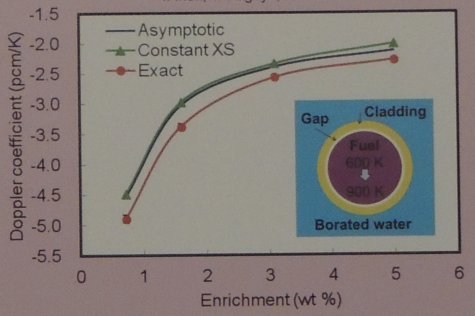
New Resonance Elastic Scattering Model

- The resonance elastic scattering model has a great impact on the Doppler reactivity calculation for thermal systems.
- MVP implements following 3 models:
  - Asymptotic Slowing-Down Scattering Model (Asymptotic model),
  - Free-Monatomic-Gas Model with Constant Cross Section (Constant cross section model, Free-gas model),

$$\sigma_s^{eff}(v) = \frac{1}{v}\iint \sigma_s(v_{rel}) v_{rel} M(V,\mu) dV d\mu \approx \frac{\sigma_{s0}}{v}\iint v_{rel} M(V,\mu) dV d\mu$$

  - Free-Monatomic-Gas Model with Resonance Cross Section (Exact Model, newly implemented).
- Results for Mosteller Doppler defect benchmark.

T. Mori, Y. Nagaya, *J. Nucl. Sci. Technol.*, **46**, 793 (2009).



Reactor Kinetics Parameters

Y. Nagaya et al., *Ann. Nucl. Energy*, **38**, 254 (2011).

- Effective elayed neutron fraction β_{eff} and neutron generation time Λ can be calculated with a new approach: eigenvalue method + differential operator sampling.
- Consider a system where the number of delayed neutrons can be changed. (a is the fractional change in the number of delayed neutrons.)

$$\beta_{eff} = \lim_{a \to 0} \frac{1}{k(0)} \frac{k(a) - k(0)}{a} = \frac{1}{k(0)} \left.\frac{\partial k(a)}{\partial a}\right|_{a=0}$$

Estimate differential coefficient

- Comparison with the deterministic results for simple geometries.

Fast systems

Category	Core	β_{eff} (pcm) Det.* (Ref)	MC(MVP) (1σ)
Fast, Bare	Godiva	632.6	630.8(3.5)
	Jezebel	182.9	180.3(2.1)
	Jezebel-23	291.9	293.1(2.6)
Fast, Reflected (Normal U)	Flattop-25	678.5	679.8(3.4)
	Flattop-Pu	281.0	280.0(2.3)
	Flattop-23	376.7	375.2(2.7)

Thermal systems

Category	Core	β_{eff} (pcm) Det.* (Ref)	MC(MVP) (1σ)
Thermal, Unreflected	Sphere-U	716.1	721.1(5.4)
	Sphere-Pu	225.4	228.8(2.8)
	Sphere-23	298.9	300.8(3.4)
Thermal, Reflected (Water)	Sphere-U	842.4	849.9(7.5)
	Sphere-Pu	275.2	270.7(4.1)
	Sphere-23	350.4	352.0(4.8)

* Deterministic calculations with an inhouse code CBG, JENDL-3.3.

- Calculation of Λ will be presented in the oral session of this conference.

Concluding Remarks

- The current development status of MVP has been overviewed.
- Capabilities have been enhanced for reactor physics applications.
- MVP Version 3 will be released in near future.

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013)
La Cité des Sciences et de l'Industrie, Paris, France, October 27-31, 2013

Recent Developments of JAEA's Monte Carlo Code MVP for Reactor Physics Applications

Yasunobu NAGAYA, Keisuke OKUMURA, Takamasa MORI

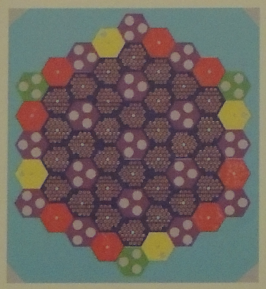
Japan Atomic Energy Agency, Nuclear Science and Engineering Directorate,
Tokai-mura, Naka-gun, Ibaraki 319-1195, Japan

Introduction

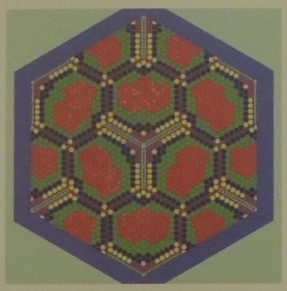
- MVP : a general-purpose continuous-energy Monte Carlo code for neutron and photon transport.
- Developed since the late 1980s at JAEA (formerly JAERI).
- Main field : nuclear reactor analysis (critical experiment analysis, core design), criticality safety, reactor shielding, etc.
- The first version was released for domestic use in Japan in 1994.
- MVP Version 2 was released for worldwide use in 2005.

General Description of MVP

- Problems to be solved: Eigenvalue and fixed-source problems for neutron, photon and neutron/photon coupled transport. Time-dependent problems (ex. pulsed neutron simulation).
- Geometry representation:
  - Combinatorial geometry.
  - multiple lattice capability (repeated geometry).
  - Statistical geometry model (stochastic geometry).



MVP calculation model for High Temperature Engineering Test Reactor (HTTR)



MVP calculation model for Reduced-Moderation Water Reactor (a Y-shaped control rod is located at the center.)

- Particle sources:
  - Sampling functions: `TABLE`, `UNIFORM`, `SPHERE`, `GAUSS`, etc.
  - Data transformation functions: `SWAP`, `LOTATE2D`, etc.
- Cross sections:
  - Cross section data generated with the LICEM code.
  - Unresolved resonance ⇨ probability table method.
  - Cross sections at arbitrary temperature are available.
  - JENDL-4.0, ENDF/B-VII.0, JEFF-3.1, etc.
- Variance reduction techniques: Russian roulette kill, splitting, importance, weight window, path stretching, etc.
- Estimators:
  - Track length, collision, point, surface-crossing.
  - k_{eff}: combined estimator with track length, collision, analog for neutron production and balance.
- Symbolic parameters: User-defined variables.

Example of MVP material input

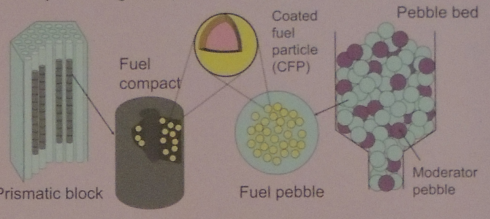
```
& IDMAT(1) /* material ID                    symbolic parameters
  TEMPMT(900.0) /* Kelvin                    ↙
% CR50=4.345, CR52=83.789, CR53=9.501, CR54=2.365
% CRN=1.399E-2 ←——— atomic density for natural element
  CR0500J40(<CRN*CR50/100>)
  CR0520J40(<CRN*CR52/100>)  atomic density for each isotope
  CR0530J40(<CRN*CR53/100>)
  CR0540J40(<CRN*CR54/100>)
```

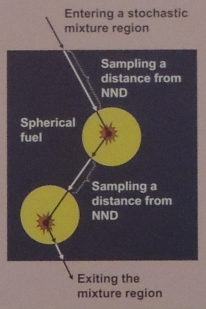
- Vectorized algorithm : Stack-driven zone-selection method. (a variant of the standard event-based stack-driven algorithm)
- Code validation : ICSBEP, IRPhEP, critical experiments at JAEA.

Statistical Geometry Model

I. Murata et al., *NSE.*, **123**, 96 (1996).

- Developed for high-temperature reactors (HTRs).





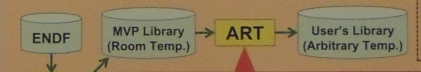
- Not locate all spherical fuels explicitly but locate each spherical fuel stochastically.
- The position of each sphere is sampled from a probability density function (Nearest Neighbor Distribution: NND).
- How to obtain NND
  - MCRDF code
  - Theoretical approximation based on statistically uniform distribution

$$\frac{dNND(r)}{dr} = \frac{3}{2}\cdot\frac{f_p}{1-f_p}\cdot\exp\left(-\frac{3}{2}\cdot\frac{f_p}{1-f_p}\cdot r\right)$$

f_p : packing fraction

Calculations at arbitrary temperatures

- MVP generates cross section data at specified temperatures internally before MC calculations.



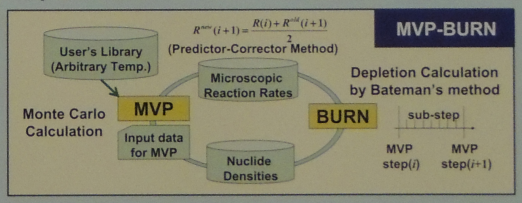
Example of MVP input

```
$CROSS SECTION
& IDMAT(1)
  TEMPMT(600.0)
  U02350J40(5.070E-5)
  U02380J40(1.685E-2)
$END CROSS SECTION
```

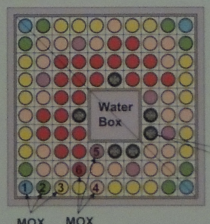
- Doppler broaden resolved resonance cross sections.
- Interpolate data for thermal scattering and unresolved resonance.

Burnup Calculations

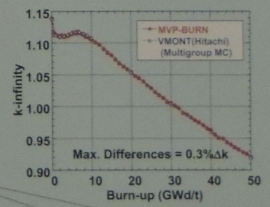
K. Okumra et al., *J. Nucl. Sci. Technol.*, **37**, 128 (2000).



OECD/NEA/NSC Benchmark for MOX-BWR



Number of Depletion Zones = 142



UO_2-Gd_2O_3 Rod
32 zones in a poisoned fuel
(8 annuluses * 4 sectors)

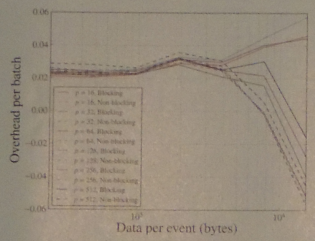
Research and Development with OpenMC

Paul K. Romano[1], Nicholas Horelik[1], Bryan Herman[1], Andrew Siegel[2], Kyle Felker[2], Adam Nelson[3], Timothy Burke[1], Benoit Forget[1]

[1]Massachusetts Institute of Technology [2]Argonne National Laboratory [3]University of Michigan

Data Decomposition

MIT and ANL have been studying algorithms for overcoming per-node memory limits in Monte Carlo simulations with the goal of being able to perform full-core LWR simulations. One such algorithm is based on *tally servers* [1, 2], processes that are dedicated solely to receiving and storing tally data rather than tracking particles. Research has shown that this algorithm can successfully circumvent memory constraints with minimal overhead on contemporary supercomputers, such as Titan at ORNL and Mira at ANL. The figure below shows the results of a sensitivity study looking at the overhead due to using tally servers on a simulation of the BEAVRS reactor benchmark.

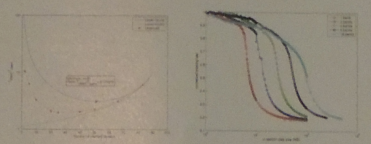


Recent work has confirmed that it is possible to perform simulations with over 100 GB of tallies with very little overhead using tally servers.

Energy Band Memory Server

An algorithm designed to reduce the on-node footprint of cross section memory is also being developed [4, 5]. The classic method of per-node replication of cross section data is replaced by a memory server model, in which the read-only lookup tables reside on a remote set of disjoint processors. The main particle tracking algorithm is then modified in such a way as to enable efficient use of the remotely stored data in the particle tracking algorithm.

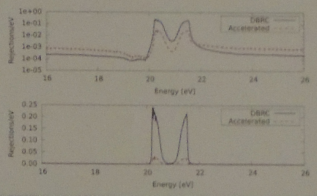
The figure below on the left shows the performance of a prototype code on a BG/Q machine implementing the energy band memory server algorithm as a function of the number of memory clusters. On the right, the figure shows that if the cross section memory can be reduced to fit in cache, the tracking performance can improve significantly.



Resonance Scattering Treatments

OpenMC is being used to investigate various methods for the accurate treatment of resonance elastic scattering. These methods reproduce the exact scattering kernel by correctly accounting for the energy dependence of cross sections in the sampling of target nuclei velocities. The methods have been verified against deterministic and Monte Carlo literature results through comparisons of differential scattering kernel energy distributions, mean scattered energies, and upscatter probabilities.

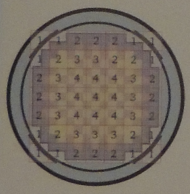
The Doppler broadening rejection correction (DBRC), an established method for treating elastic scattering from resonant nuclei, has been implemented and tested in OpenMC. Additionally, an accelerated target velocity rejection sampling technique has been introduced. The figure below shows the distribution of rejected samples observed with both the DBRC and the new accelerated method.

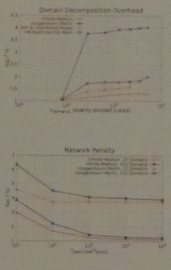


Domain Decomposition

Spatial domain decomposition algorithms are also being explored to address per-node memory limitations that preclude high-fidelity LWR simulations. Successful decomposition of both material and tally data has been demonstrated on Bluegene/Q.

- Low network overhead
- Load balancing:
  - Restricted domain mesh
  - Matching resources to load

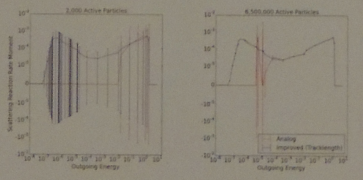




Convergence of Scattering Moments

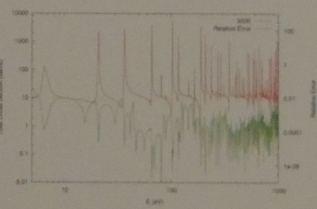
Monte Carlo tallies of scattering moment matrices are prohibitively slow to converge since the tallies must resolve the outgoing energy and change in angle. OpenMC is being modified [6] to significantly improve the figure-of-merit of such tallies. This improvement is achieved by taking advantage of the complete scattering probability distribution function described in the ACE data library.

The figures below show the tallied P_1 moment and its associated 95% CI for ^{1}H within a group at 2.3 MeV to the outgoing energy groups using both the current and improved methods at 2,000 and 6.5 million active histories. These figures show that the mean value of the improved method converges quite rapidly while maintaining accuracy of the final product.



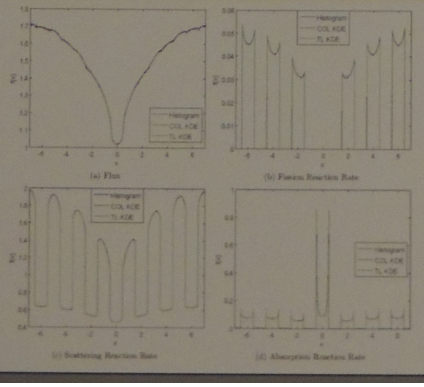
Multipole Representation

An innovative approach for direct Doppler broadening of cross sections using the multipole representation is being investigated using OpenMC [7]. By transforming resonance parameters into a set of poles and residues, it's possible to express the dependence on temperature analytically similar to the $\psi - \chi$ formalism. This enables simulations to be performed at any temperature with cross section memory requirements 1–2 orders of magnitude smaller than conventional techniques. Preliminary investigations have demonstrated that the use of the multipole representation would only introduce a small loss in particle simulation rates. The figure below shows the accuracy of the ^{238}U cross section using the multipole representation compared to pointwise data produced by NJOY.



Kernel Density Estimators

Researchers at the University of Michigan are currently looking at kernel density estimators (KDEs) as an alternative to the traditional histogram estimator. KDEs offer the promise of fine-resolution tallies that do not suffer from high variance due to low collision density. A new method for obtaining an optimal physics-based bandwidth for KDE tallies of fluxes and reaction rates has been developed and implemented in OpenMC [3]. The figure to the right demonstrates excellent agreement between KDE and histogram tallies in a 1D problem in OpenMC. Ongoing research is focused on achieving 2D and 3D KDE tallies for curvilinear geometries.



References

[1] P. K. ROMANO, A. R. SIEGEL, B. FORGET, and K. SMITH, "Data decomposition of Monte Carlo particle transport simulations via tally servers," *J. Comput. Phys.*, **252**, 20 (2013).

[2] P. K. ROMANO, B. FORGET, K. SMITH, and A. SIEGEL, "On the use of tally servers in Monte Carlo simulations of light-water reactors," *Proc. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo*, Paris, France, 2013.

[3] T. P. BURKE, B. C. KIEDROWSKI, and W. R. MARTIN, "Flux and Reaction Rate Estimators in OpenMC," LA-UR-13-20477, Los Alamos National Laboratory (2013).

[4] A. SIEGEL et al., "Improved cache performance in Monte Carlo transport calculations using energy banding," *Comput. Phys. Commun.* (2013). Submitted.

[5] K. G. FELKER, A. R. SIEGEL, K. S. SMITH, P. K. ROMANO, and B. FORGET, "The energy band memory server algorithm for parallel Monte Carlo calculations," *Proc. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo*, Paris, France, 2013.

[6] A. G. NELSON and W. R. MARTIN, "Improved Convergence of Monte Carlo Generated Multi-Group Scattering moments," *Proc. Int. Conf. Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Sun Valley, Idaho, 2013.

[7] B. FORGET, S. XU, and K. SMITH, "Direct Doppler broadening in Monte Carlo simulations using the multipole representation," *Ann. Nucl. Energy* (2013). Submitted.

PENELOPE: Monte Carlo electron-photon transport

Francesc Salvat

Introduction

- PENELOPE is an acronym for "Penetration and ENErgy LOss of Positrons and Electrons"
- A general-purpose Monte Carlo simulation code system with
  - Realistic, well defined interaction models
  - Fast and accurate random sampling algorithms
  - Efficient tools for tracking particles through complex geometries (constructive quadric geometry)
  - Complementary tools: variance reduction, transport in electro-magnetic fields, tabulation of macroscopic interaction parameters, ...
- Distributed by the OECD/Nuclear Energy Agency Data Bank (Paris) and the RSICC (Oak Ridge).
  More than 1,000 copies distributed
  List server: http://www.oecd-nea.org/lists/penelope.html
- Main applications:
  - Radiotherapy and Nuclear Medicine
  - Dosimetry and radiation metrology
  - Electron microscopy (SEM, electron-probe microanalysis)
  - Detector response, x-ray generators, ...

Introduction

- Main reference: very detailed manual, free hard copies available

F. Salvat, J.M. Fernández-Varea and J. Sempau
PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon Transport
OECD NEA Data Bank/NSC DOC(2011)/5
(OECD Nuclear Energy Agency, Issy-les-Moulineaux, 2011)
http://www.oecd-nea.org/dbprog/courses/penelope-2011.pdf

- Other references:

J. Baró, J. Sempau, J.M. Fernández-Varea and F. Salvat
"PENELOPE: an algorithm for Monte Carlo simulation of the penetration and energy loss of electrons and positrons in matter"
Nucl. Instrum. Meth. B 100 (1995) 31-46

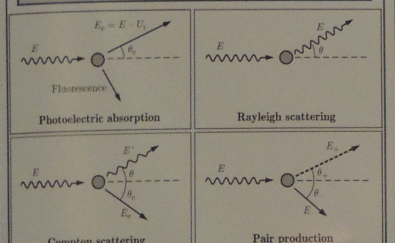
J. Sempau, J.M. Fernández-Varea, E. Acosta and F. Salvat
"Experimental benchmarks of the Monte Carlo code PENELOPE"
Nucl. Instrum. Meth. B 207 (2003) 107-123

F. Salvat and J. M. Fernández-Varea
"Overview of physical interaction models for photon and electron transport used in Monte Carlo codes"
Metrologia 46 (2009) S112-S138

Main features

- All kinds of interactions (except nuclear reactions) in the energy range from 50 eV to 10^9 eV
- Implements the most accurate physical models available, limited only by the required generality
- Uses an elaborate mixed scheme to simulate the transport of high-energy electrons and positrons
- Simulates fluorescent radiation from the K-shell, and L-, M-, and N-subshells
- Subroutine package pengeom for tracking particles in quadric geometries (i.e., material systems consisting of homogeneous bodies limited by quadric surfaces)
- Electron and positron transport in electric and magnetic fields (in matter)
- Scattering of polarized photon beams (synchrotron)

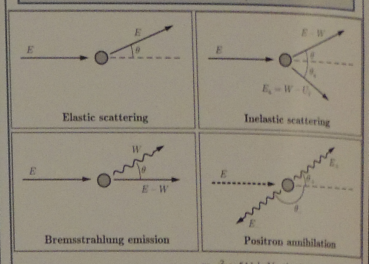
Interactions of photons



$m_e c^2 \simeq 511$ keV, electron rest energy

- Photoelectric effect:
  - Total cross sections calculated from the DHFS atomic potential (equivalent to Scofield's LLNL database; Cullen *et al.*, 1997)
  - Angular distribution of photoelectrons from Sauter's (1931) formula (plane-wave Born approximation for K-shell hydrogenic ions)
  - Atomic relaxation from the EADL (Perkins *et al.*, 1991)
- Coherent (Rayleigh) scattering:
  - Total cross sections from the EPDL (Cullen *et al.*, 1997), includes anomalous atomic scattering factors
  - Angular distribution from atomic form factors
- Incoherent (Compton) scattering:
  - Double-differential cross sections (DDCS) calculated from the relativistic impulse approximation (Ribberfors, 1983) using analytical Compton profiles (Brusa *et al.*, 1996)
  - Total cross sections obtained as integrals of the DDCS
  - Subsequent atomic relaxation from the EADL (Perkins *etal.*, 1991)
- Electron-positron pair production:
  - Total cross sections from the EPDL (Cullen *et al.*, 1997), includes triplet production
  - Energies and directions of the pair particles from the Bethe-Heitler theory

Interactions of electrons and positrons



$m_e c^2 \simeq 511$ keV, electron rest energy

- Elastic collisions:
  - Atomic differential cross sections (DCS) calculated using the Dirac partial-wave expansion method (ICRU 77, 2007)
  - High-energy modified Wentzel model with correct first and second moments (ICRU 77, 2007) for energies above 100 MeV
- Inelastic collisions:
  - DDCS from the Born approximation, using the Sternheimer-Liljequist GOS model, with resonance energies fitted to reproduce the mean excitation energies from ICRU 37 (1984)
  - Secondary electrons emitted in the direction of momentum transfer
- Bremsstrahlung emission:
  - Photon-energy scaled DCSs of Seltzer and Berger (1985, 1986)
  - Photon angular distribution fitted to partial-wave data of Kissel *et al.* (1983)
- Impact ionization of inner shells
  - Total cross sections for K, L and M shells calculated from the distorted-wave Born approximation (Bote *et al.*, 2009)
  - Subsequent atomic relaxation from the EADL (Perkins *et al.*, 1991)

Electron/positron transport mechanics

- Mixed simulation algorithm:
  PENELOPE uses a pure class II (mixed) algorithm for electrons/positrons. Allows verifying the stability under variations of simulation parameters

  Hard interactions (with angular deflection larger than a cutoff angle θ_c or energy loss larger than selected cutoffs) are simulated individually

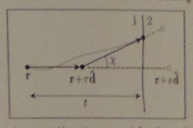
- Hard elastic interactions:
  The cutoff angle is determined by two user parameters, C_1 and C_2, according to the formula (Eq. 4.85 of the manual)

$$\lambda_{\rm el}^{\rm (h)}(E) = \max\left\{\lambda_{\rm el}(E), \min\left[C_1\lambda_{\rm el,1}(E), C_2\frac{E}{S(E)}\right]\right\}$$

- Hard energy loss events:
  The user defines the cutoff energies $W_{\rm cc}$ (col) and $W_{\rm cr}$ (brems), in accordance with the required energy resolution
- Maximum allowed step length between hard interactions:
  An additional parameter, $s_{\rm max}$, sets a limit to the step length (needed to account for the variation of energy along the step, and for consistency of the simulation of soft events)

Electron/positron transport mechanics

- Simulation of soft interactions: Random hinge method
  - The global effect all the soft interactions in a step s between a pair of hard interactions is simulated as a single event, a hinge
  - The angular deflection and the energy loss at the hinge are sampled from approximate distributions having the correct first and second moments
  - The position of the hinge, τ, is sampled uniformly in $(0,s)$
  ⇒ simple and accurate scheme for interface crossing



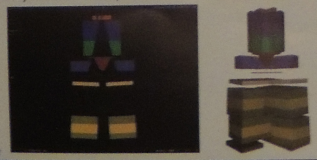
- Includes elaborate corrections to account for the variation of energy along the step

Role/effect of the simulation parameters

- Step-length control (for each material):
  C_1 limits the average angular deflection per step, $1-\langle\cos\theta\rangle \lesssim C_1$
  Influences the simulation speed only at intermediate energies
  C_2 limits the average fractional energy loss per step, $\langle E_0 - E\rangle \lesssim C_2 E_0$
  Affects simulation speed only at high energies
- Energy-straggling control (for each material):
  $W_{\rm cc}$ energy-loss threshold (in eV) for hard inelastic collisions
  $W_{\rm cr}$ energy-loss threshold (in eV) for hard bremsstrahlung events
  These cutoffs govern energy resolution. Mild effect on speed
- Geometrical constraints (local):
  $s_{\rm max}$ maximum step length for "critical" geometries (needed for thin bodies, backscattering, ...)
- Reasonable "blind" choices:
  C_1 and C_2 : 0.05 to 0.1; $W_{\rm cc}$ and $W_{\rm cr}$: ~ 1,000 eV
  $s_{\rm max}$: one tenth of the minimal thickness

Transport in complex geometries

- The subroutine package PENGEOM
  - Tracks particles within material systems consisting of homogeneous bodies limited by (fuzzy) quadric surfaces
  - Highly accurate (effective nm resolution near the origin)
  - Tailored to minimize numerical work
  - Generally applicable to detailed and mixed simulations
- Geometry viewers: 2- and 3-dimensional viewers are provided
  - Images of the geometry are rendered by using the tracking routines
  ⇒ what you see is what is passed to the simulation program



Variance-reduction techniques

- Statistical uncertainties
  The quantity of interest, Q, is evaluated from the contributions q_j of N simulated showers. The sample average and variance are

$$\overline{Q} = \frac{1}{N}\sum_{j=1}^{N} q_j \quad \text{and} \quad \text{var}_Q = \frac{1}{N}\sum_{j=1}^{N} q_j^2 - \left[\frac{1}{N}\sum_{j=1}^{N} q_j\right]^2$$

  The Monte Carlo estimator is $\overline{Q} \pm n\sigma_{\overline{Q}}$, where $\sigma_{\overline{Q}} = \sqrt{\text{var}_Q}$ is the standard deviation. Typically, $n = 3$ (3σ rule, probability = 0.997)

- Simulation efficiency

$$\epsilon_Q = \left(\frac{\overline{Q}}{\sigma_Q}\right)^2 \frac{1}{T}$$

  T: computing time

  The time needed to get a given relative uncertainty $(\sigma_{\overline{Q}}/\overline{Q})$ is

$$T = \frac{1}{(\sigma_{\overline{Q}}/\overline{Q})^2 \epsilon_Q}$$

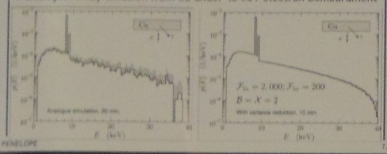
Universitat de Barcelona

PENELOPE: Monte Carlo electron-photon transport

Francesc Salvat

Variance-reduction techniques

- Techniques implemented in PENELOPE, and VR parameters
  - Particle splitting. Splitting number, N
  - Russian roulette. Killing probability, λ
  - Interaction forcing. Forcing factors, $\mathcal{F}$
  - Bremsstrahlung splitting. Splitting number, $\mathcal{B}$
  - X-ray splitting. Splitting number, $\mathcal{X}$
  - Woodcock delta scattering for photons. yes/no
- Example. X ray emission from Cu under 40-keV electron bombardment



PENELOPE 13

Structure of the code system

- The PENELOPE code system consists of
  - The subroutine package penelope.f, which defines the interaction properties of materials and performs the simulation of interactions
  - The geometry package pengeom.f, and the 2D and 3D viewers (gview2d.exe and gview3d.exe)
  - The variance-reduction routines penvared.f (include particle splitting, Russian roulette, interaction forcing, and delta scattering of photons)
  - The database: 995 ascii files with interaction cross sections and other properties of the elements Z=1–99 (hydrogen to einstenium)
  - Steering main programs for cylindrical and quadric geometries, pencyl.f and penmain.f. They can simulate a variety of radiation sources, allowing scoring of different transport properties
  - Routines penfield.f for tracking charged particles in static electro-magnetic fields

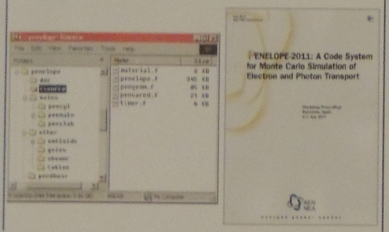
PENELOPE 14

- ...
  - Program tables.f for displaying plots of energy-dependent interaction properties. Macroscopic quantities are made available numerically and graphically
  - A program for displaying electron-photon showers in material slabs, shower.exe
  - Documentation: Manual and tutorial
- All source programs are written in Fortran, *i.e.*, they can be run on any operating system with a Fortran compiler
- The geometry viewers gview2d and gview3d, and the program shower work only on MS Windows (for the time being)
- The output of the simulation programs and of tables.f is formatted for visualization with the plotting program gnuplot, available for Windows and Linux (http://www.gnuplot.info)

PENELOPE 15

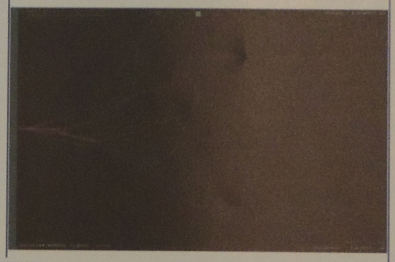
Distribution package

- A single zip compressed file, penelope.zip (~74 Mb)



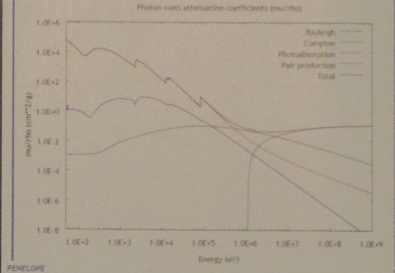
PENELOPE 16

Screenshot of "shower": 10 MeV electrons in water



PENELOPE 17

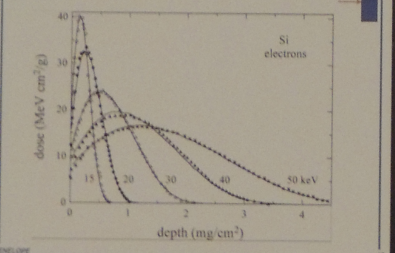
Screenshot of "tables": photons in gold



PENELOPE 18

Example: depth-dose distribution, electrons in Al

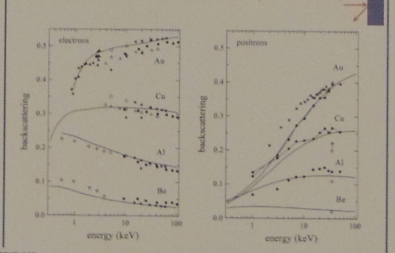
- Experiment of Werner *et al.*, *JPD* (1988)



PENELOPE 19

Example: backscattered fractions of electrons and positrons

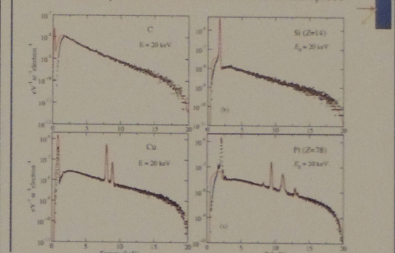
- Experimental data from different authors (Sempau *et al.*, 2003)



PENELOPE 20

Example: x-ray spectra from electron beams

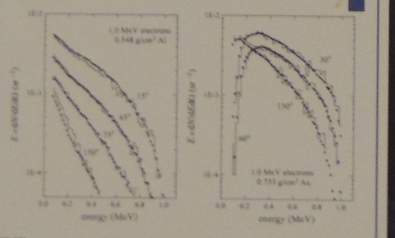
- Measurements by Llovet and Merlet on an electron microprobe



PENELOPE 21

Example: bremsstrahlung energy spectra

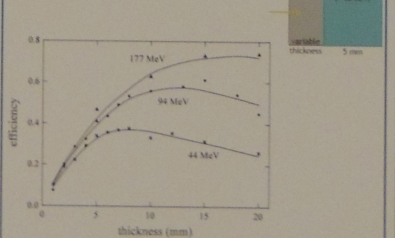
- Experiment of Rester *et al.*, *J. Appl. Phys.* (1970)



PENELOPE 22

Example: efficiency of a radiation converter

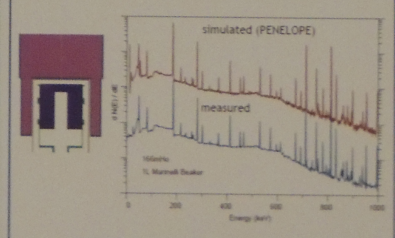
- Experiment of Darriulat *et al.*, *NIM* (1975)



PENELOPE 23

Example: gamma-ray spectrometry

- p-type HP Ge detector, Marinelli beaker (Garcia-Toraño, *NIMA*, 2005)



PENELOPE 24

PHITS

Particle and Heavy Ion Transport code System

Presenter: T. Ogawa (JAEA)

P1. General Features of PHITS

Q. What is PHITS?
A general purpose Monte Carlo particle transport code written in FORTRAN90

Q. How to obtain?
Full PHITS package is available from OECD/NEA databank, RSICC, and RIST (see P2)

Q. Is the source code available?
Yes. All contents of PHITS are included in one package (see P3)

Q. Who are developing?
5 institutes in Japan and 2 institutes in Europe (see P4)

Q. How to use?
Make an input file written in free-format text (see P5)

Q. What particles can be transported in PHITS?
Nearly all particles up to 100 GeV/u (see P6)

Q. What are the specialties of PHITS?
Event generator mode, microdosimetric function, beam transport function (see P8)

Q. What are the application fields of PHITS?
Accelerator design, radiation therapy and protection, cosmic-ray dosimetry etc. (see P9-P11)

P2. How to obtain PHITS?

It depends on the country where you work in

If you work in Japan
Send a request to RIST (cost 12,810 JPY), or
Join in PHITS tutorial in Japan
If you work in USA or Canada
Send a request to RSICC (800 USD except for student)
If you work in OECD/NEA databank member countries*
Send a request to your liaison officer
If you work in other countries
Contact to non-NEA Databank nominated establishment**

P3. Contents of PHITS package

- Source files
- Binary (executable) files for Windows & Mac
- Installers for Windows and Mac (just double click!)
- Nuclear and atomic data libraries
- Graphic utility ANGEL
- Lecture notes & manual

All contents of PHITS are included in one package!

*Austria, Belgium, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Italy, Japan, Korea, Mexico, Netherlands, Norway, Portugal, Russia, Slovak Republic, Slovenia Space Sweden Switzerland, Turkey, United Kingdom
** see http://www.oecd-nea.org/dbprog/pretlo.cgi?iaea

P4. PHITS Development Team

Kyushu Univ.
Improvement and verification of nuclear reaction model

KEK
Incorporating EGS5

Chalmers (Sweden)
- Application to space science and biology
- Tutorial in Europe

JAEA
- Managing the entire project
- Tutorial
- Distribution

RIST
- Programing
- Improvement of the nuclear reaction model

RIKEN
Application to biology using super computer "K"

JAXA
Application to space science

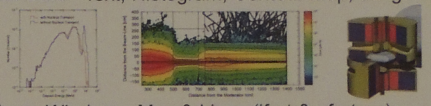
CEA (France)
Implementation and improvement of the INCL model

P5. User Interfaces of PHITS

Input file: Free-format text

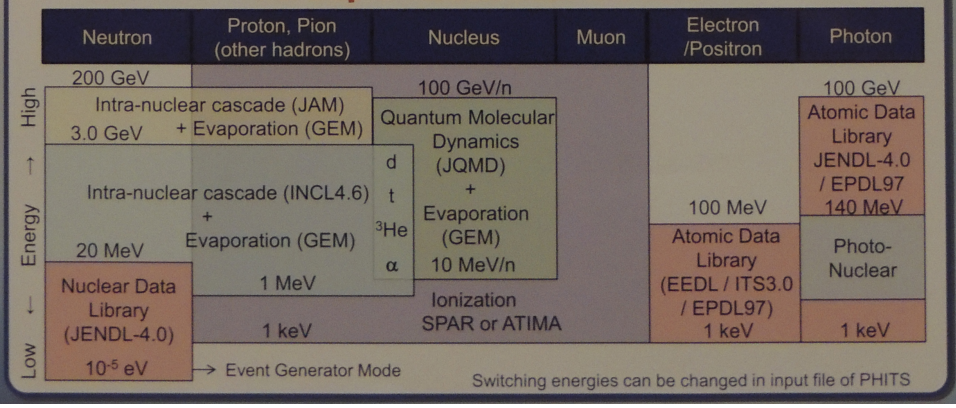
You do not have to write Fortran program at all!

Geometry: General Geometry (MCNP style)
SimpleGEO (GUI software originally for FLUKA)
Tally functions: Fluence, Dose, Yield, LET distribution etc.
Output Data: Text, Histogram, Contour map, 3D-geometry



Platform: Windows, Mac & Linux (ifort & gfortran)
Parallelization: MPI, OpenMP, and their hybrid

P6. Map of Models used in PHITS



PRIZMA STATUS

Y.Z. Kandiev, E.A. Kashaeva, K.E. Khatuntsev, E.S. Kuropatenko, L.V. Lobanova, G.N. Lukin, A.A. Malakhov, G.N. Malyshkin*, D.G. Modestov, R.F. Mukhamadiev, V.G. Orlov, S.I. Samarin, E.V. Serova, S.G. Spirina, T.V. Vakhonina, N.A. Voronina, O.V. Zatsepin
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Snezhinsk, Russia 456770
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History

- 1956 : started development of Monte Carlo techniques and codes for radiation transport at RFNC-VNIITF. The first code solved neutron transport in axially symmetric systems and ran the STRELA computer
- 1969: PRIZMA development started
- 1979: PRIZMA v.1 (BESM-6 computer, ALGOL-60)
  - neutrons, gammas, electrons, positrons, protons, alpha-particles
  - variance reduction
  - tagged particles
- 1988: ELBRUS-2 computer, EL-76
- 1998: PCs and clusters, C++

Current status

- Separate and coupled transport of neutrons, gammas, electrons, positrons and ions
- Linear transport from a source
- Conditional criticality
- State-of-the-art interaction data libraries
- Rich capabilities for geometry definition
- Sources with analytical and tabulated distributions
- Diversified tallies
- Correlated calculations
- Variance reduction
- Data exchange with nuclear kinetics and heat&hydraulics
- C++, Windows and Linux, parallelism

Particle interaction with matter

Neutrons

Libraries:
BAS, ENDF/B-V, -VI, -VII, ROSFOND, CENDL, JENDL, JEFF, TENDL
Energy range: 10^{-5} eV – 150 MeV
Cross-section temperature dependence: free gas, majorized cross-section.
Chemical bond under thermodynamic equilibrium with coherent elastic, incoherent elastic and incoherent inelastic scattering.

Photons

Libraries: EPDL-92, EPDL-97
Energy range: 100 eV – 100 MeV
Form-factors

Electrons and positrons

Libraries: EADL and analytics
Energy range: 1 keV – 100 MeV

Ions

Libraries: TNRDAT and analytics
Energy range: 100 eV – 300 MeV

Catastrophic collisions

Geometry

Blocks
One-dimensional: plane, sphere, cylinder,
Two-dimensional: axially symmetric, cylindrical
Three-dimensional:
- combinatorial approach
- pieces of surfaces

2D and 3D lattices (possibly nested)
Stochastic geometry

Sources

Uniform over the volume of arbitrary geometrical regions or the area of geometrical surfaces; a wide set of primitives for independent sources
1D analytical, and 1-, 2- and 3-D tabulated distributions for energy, angle and time dependences of source particles

Importance Sampling

The developed importance sampling techniques allows tracking algorithms to adapt to the specific features of each particular problem.

The technique includes the tentative approximation of the particle importance function to calculate the appropriate weight function and parameters for biased distributions.

The technique is used for the following problems (and their combinations) :
- penetration through optically thick regions
- low-probability interactions
- radiation transport to detectors in vacuum or pure absorber
- radiation transport to detectors in emitting and scattering media

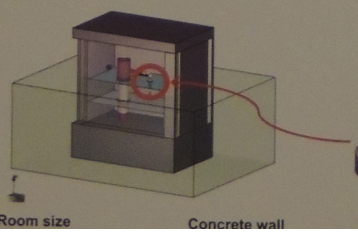
Tallies

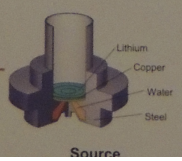
- Conditional results
- Multi-variant correlated calculations to estimate the effect of perturbations in :
  - position
  - size
  - composition
  - density

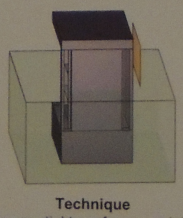
Parallelization

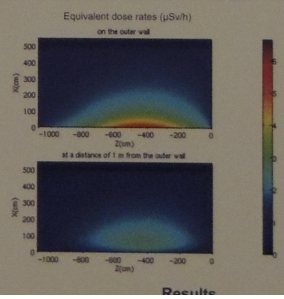
Maximum separation between batch calculation and calculated data collection at minimal wastage. Calculated results are collected with a two-level algorithm: intra-node summation through common memory with current random numbers saved; and inter-node summation on a separate thread with MPI functions which does not require main calculations to stop.

Neutron therapy









RMC - A Monte Carlo Code for Reactor Core Analysis

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Tsinghua University, Beijing 100084, P.R. China

INTRODUCTION

A new Monte Carlo transport code named RMC has been developed by Reactor Engineering Analysis Laboratory (REAL) in Department of Engineering Physics, Tsinghua University, Beijing, CHINA.
RMC now has the following functions and special techniques:

- Criticality calculation;
- Point depletion and MC burnup calculation;
- CPU/GPU parallelization for criticality and burnup calculation;
- Fixed source calculation and kinetics simulation;
- Temperature-dependent cross-sections processing;
- High efficiency searching methods;
- Source convergence acceleration;
- Hybrid calculation methods (RMMC method);
- Data and domain decomposition techniques;
- Continuously varying medium simulation;
- Perturbation calculation and S/U analysis;
- Criticality search capability;
- N-TH coupling, and so on.

CAPABILITIES

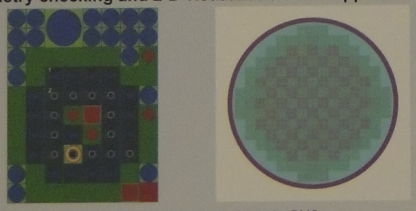
1. Criticality calculation

a. Basic physics

- Ray-tracking method for neutron transport simulation.
- Currently using the ACE format cross-section.
  - Generated by RXSP from ENDF/B data;
  - 1-STEP searching method acceleration.
- Thermal treatments are used for the thermal motion of collision
  - Free gas approximation;
  - S(α,β) treatment;
  - Temperature interpolation techniques.
- The probability tables are used to account for self-shielding effects in the unresolved resonance energy range.

b. Geometry treatment

- The constructive solid geometry (CSG) representation.
- 2 or 3-D quadrilaterals or hexagons repeated geometry.
- Geometry checking and 2-D visualization are supported.



2-D reactor geometry drawn by RMC

c. Source convergence acceleration

- Asymptotic Wielandt Method (AWM) and Asymptotic Super-history Method (ASM) are developed and implemented in RMC
  - Acceleration of source convergence without large fluctuation;
  - No restriction on geometry and cross-sections.

d. Tallies in RMC

- Basic tally capabilities available in RMC.
  - The effective multiplication factor;
  - Flux, reaction rates, power distribution for regions;
  - Multi-group xs for regions or homogenized assemblies;
  - Shannon entropy, and so on.
- Efficient massive tally capability for millions or billions of regions.
  - The cell map method to efficiently handle massive tallies;
  - Bin map method to improve the efficiency of binary search;
  - Level flags to avoid unnecessary search of tally cells.

e. Perturbation and related calculations

- Differential operator method with perturbed source effects;
- Up to 6th order can be calculated for perturbation problems;
- Basis of S/U analysis and criticality search in RMC.

f. Criticality search capability

- New perturbation based criticality search method;
  - Only one criticality run with perturbation tally;
  - More accurate and stable criticality search results.

2. Burnup calculation

- The RMC burnup calculation couples internally a series of MC criticality calculations and point-burnup calculations.
- A new depletion module named DEPTH is developed, which is able to handle detailed depletion chains containing thousands of isotopes at extremely fast speed with accuracy.
- Such techniques as parallel burnup, material-expanding, xenon oscillation control and data decomposition are implemented in RMC to improve efficiency and accuracy, and to reduce memory requirement for burnup calculations.

3. Parallel calculation

- Parallel criticality calculation
  - Peer-peer parallel mode;
  - MPI and OpenMP hybrid parallel techniques;
  - Batch tally techniques in collecting results;
  - GPU 3-D multigroup criticality parallel acceleration.
- Parallel burnup calculation

RELEASE AND DOCUMENTATIONS

- Release Flash Disk : RMC executable code with libraries processed by RXSP (2013SR092123, not included), User Manual, Examples.
- Computer Platforms
  - Windows OS, Win XP and later, Win 7 suggested;
  - Linux OS, Red Hat 5.0 suggested.
- RMC has Chinese computer software copyright No. 2013SR056821

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RMC Code Verification and Validation

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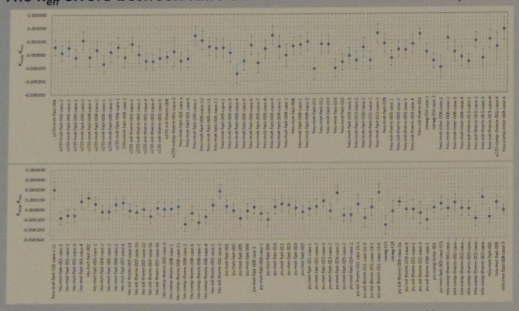
CRITICALITY CALCULATION

1. Criticality Benchmark Calculation Results

- Combine benchmark suite with 133 benchmark problems;
- Automatic running test scripts coded in Python;
- The k_{eff} errors between RMC and MCNP5 are less than 20 pcm.



k_{eff} errors between RMC and MCNP5 for all criticality benchmark problems

2. Nuclides Problem Results

- All 393 nuclides, including thermal, resonance and fast spectrums;
- 800 cycles (100 inactive) of 200,000 neutrons each cycle;
- The k_{eff} errors between RMC and MCNP5 are less than 100 pcm.

keff errors between RMC and MCNP5 for all nuclide problems (partial data)

3. Geometry Treatment Results

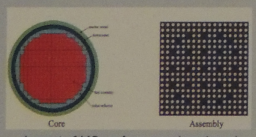
- 21,181 random tests generated by automatic CSG modeling code.

The number of geometry treatment tests

Test type	Number	Test type	Number
Boolean operation tests	12112	Assembly problem tests	190
Repeated structure tests	322	Single surface tests	8000
NOT logical operation tests	501	Complex geometry system tests	28

4. Full Core Benchmark Results

- MC Performance benchmark

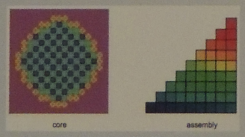


Layout of MC performance benchmark

Comparisons between RMC and MCNP5 without tallies

Codes	k_{eff}	Calculation time (min per 100 cycles) Inactive cycle	Active cycle
RMC	1.00023±0.00019	3.80	3.82
MCNP5	1.00040±0.00020	6.73	6.77

- EDF multigroup benchmark



Geometry layout of EDF benchmark

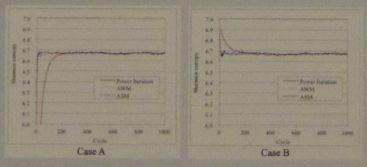
Average keff results of EDF benchmark compared with RMC and MCNP

Results(10 runs average)	k_{eff}	std	[g=1,g=2]
RMC	1.009205	0.5pcm	[0.21%, 0.15%]
MCNP5	1.009203	0.9pcm	[0.19%, 0.17%]

5. Source Convergence Acceleration

- A 2-D PWR core with 121 homogenized assemblies problem
  - Case A, the initial sources in the central assembly
  - Case B, the initial sources in the center of all assemblies

PWR core with homogenized assemblies



Shannon entropy evolution of two cases

6. Massive Tally Performances

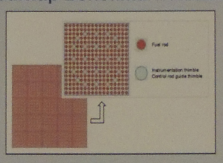
- MC performance benchmark is calculated and flux are tallied for all 6,362,400 fuel cells.

Comparison of different tally methods

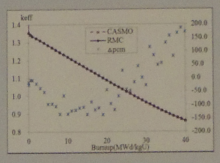
Method used			Calculation time (min per 100 cycles)		
Cell map	Bin map	Level flag	Inactive cycle	active cycle	Time increment
×			3.91	4.82	23.28%
×	×		3.96	4.65	17.54%
×	×	×	3.93	4.26	8.45%

BURNUP CALCULATION

1. Burnup Benchmark Results



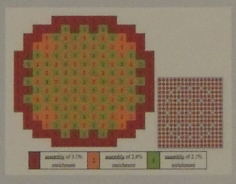
Geometry of the 5x5 assembly-group case



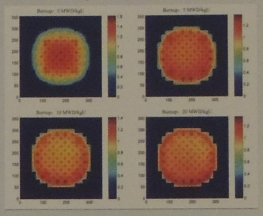
Assembly group burnup results

2. Massive-Region Burnup Results

- Full core burnup with 50,952 burnup regions
- 720 CPU cores, memory is below 2.0 Gbytes per processor



Configuration of 2D PWR core and assembly model

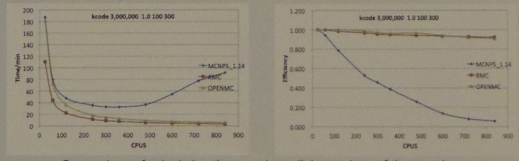


Power distribution of 2D PWR core with burnup

PARALLEL CALCULATION PERFORMANCES

1. Criticality Parallel Calculation Performances

- MC Performance Benchmark
  - More than 6M regions in the problem
  - 3,000,000 particles, 300 total cycles (100 inactive)



Comparison of calculation times and parallel speedups of three codes

- EDF Benchmark
  - 10,000,000 particles, 500 total cycles (with 200 inactive)
  - The parallel efficiency is more than 90% even with 2,400 processors.

Parallel performance of RMC code for EDF problem

CPUs	12	120	360	600	1,200	2,400
Time / min	516.4	51.67	17.34	10.39	5.25	2.76
Speedup	12.0	119.9	357.3	596.4	1179.5	2247.3
Efficiency	1.0000	0.9994	0.9925	0.9940	0.9829	0.9364

2. Burnup Parallel Calculation Performances

- 64 processors parallel calculation for 5*5 assembly problem

Results of two cases of 5x5 assembly group

Calculation condition	Calculation time (min) Criticality	Burnup	Total
Parallel criticality+serial burnup	93.4	302.3	395.7
Parallel criticality+parallel burnup	94.9	7.3	102.2

ork supported by the fund of National Science and Technology

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The Serpent Monte Carlo Code: Status, Development and Applications in 2013

Jaakko Leppänen, Maria Pusa, Tuomas Viitanen, Ville Valtavirta, and Toni Kaltiaisenaho
VTT Technical Research Centre of Finland

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013)
La Cité des Sciences et de l'Industrie, Paris, France, October 27–31, 2013

Background

The development of Serpent started at VTT in 2004, for the purpose of creating a simplified Monte Carlo neutron transport code dedicated to homogenization and other reactor physics applications. The code has been in public distribution since 2009, with applications ranging from group constant generation and fuel cycle studies to research reactor modeling and coupled multi-physics calculations. The code is currently developed by a five-member team at VTT, supported by feedback and contributions from active users around the world. The work is funded from three public research programs: the KÄÄRME project in the Finnish National Research Program on Nuclear Power Plant Safety (SAFIR-2014), the Academy of Finland Numerical Multi-Physics project (NUMPS), and the High Performance Monte Carlo Reactor Core Analysis (HPMC) Project within the 7th EU Framework Program.

Methods and Capabilities

Based on its methods and capabilities, Serpent is best characterized as a continuous-energy Monte Carlo reactor physics burnup calculation code. The neutron transport simulation can be run in external and *k*-eigenvalue criticality source modes, and a dynamic simulation mode for the modeling of short reactivity transients is under development. Work on gamma and coupled neutron-gamma transport simulation modes has been started, and is to be completed in 2014. Transport and burnup cycles can be run in parallel, using OpenMP and MPI techniques.

Calculation routines in Serpent are designed and optimized for reactor physics calculations:

Geometry Routine: Three-dimensional universe-based constructive solid geometry (CSG) model, neutron tracking based on combination of conventional surface-tracking and the Woodcock delta-tracking method. Explicit stochastic geometry model for randomly distributed HTGR particle fuels.

Interaction Physics: Continuous-energy ACE format cross-section libraries, including thermal scattering data for important moderator materials and probability table sampling in the unresolved resonance region. Option to reconstruct all reaction cross-sections on a single unionized energy grid. Built-in Doppler-broadening preprocessor and on-the-fly temperature treatment routine based on target motion sampling (TMS).

Burnup Calculation: Self-contained burnup calculation capability with a built-in depletion solver based on the Chebyshev rational approximation method (CRAM). Advanced depletion algorithms, including higher-order interpolation and extrapolation and sub-step methods.

Multi-Physics Coupling Scheme: Coupling to thermal hydraulics and fuel behaviour at two levels – standardized multi-physics interface for external coupling complemented with built-in light-weight solvers. All state-point information passed to tracking routine without modifications in the geometry input.

Output: Automated generation of homogenized group-constants needed for nodal diffusion calculations. Nuclide, radioactivity and decay heat data in burnup calculation. User-defined flux, reaction rate and current tallies.

http://montecarlo.vtt.fi

http://ttuki.vtt.fi/serpent/

On-going and Future Work

Serpent development work is currently focused on two specific areas: **1) homogenization**, and **2) multi-physics**, with topics including:

- Automated fuel cycle simulations
- Uncertainty propagation
- Gamma and coupled neutron-gamma transport mode
- Time-dependent simulation
- Internal and external multi-physics coupling

User Community

Serpent was released at the OECD / NEA Data Bank in May 2009, and the user community has grown from 35 registered users at the end of 2009 to about 260 in October 2013. The code is currently used in 100 organizations, 58 of which are universities, in 28 countries around the world. The typical code user is an M.Sc. or Ph.D. student, using Serpent for academic research and thesis work.

International meetings for Serpent users are organized annually:

2011 1st International Serpent User Group Meeting in Dresden, Germany, September 15-16 2011

2012 2nd International Serpent User Group Meeting in Madrid, Spain, September 19-21 2012

2013 3rd International Serpent User Group Meeting in Berkeley, California, USA, November 6-8 2013

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Homogenization

Homogenization has been one of the main applications of Serpent since the beginning of the project in 2004. The code is capable of automatically generating all group constants needed for full-core nodal diffusion calculations. The code has a special optimization mode for transport and burnup calculations at the fuel assembly level.

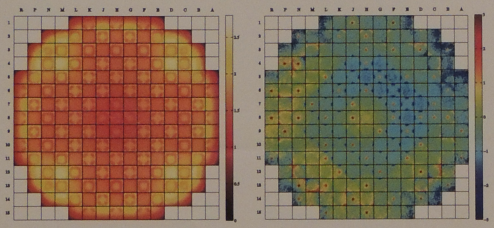

***Fig 1**. Radial pin-power distribution calculated using Serpent-ARES code sequence and comparison to 3D Monte Carlo reference solution.*

Serpent has been used to generate group constants for various LWR, SFR and other reactor configurations modeled using DYN3D and PARCS codes. At VTT, the code is currently being coupled to the ARES core simulator developed at the Finnish Radiation and Nuclear Safety Authority (STUK).

Multi-Physics

The multi-physics calculation scheme in Serpent 2 is based on the combination of internal solvers and external coupling via a universal multi-physics interface. The internal modules are:

1) The FINIX light-weight thermomechanical solver for steady-state and transient heat transfer at the fuel pin level.
2) The COSY light-weight three-dimensional system / component scale thermal hydraulics solver.

The multi-physics interface is designed to pass state variables and power distributions between Serpent and externally coupled CFD and system-scale thermal hydraulics codes and fuel performance codes. The interface has several formats for passing the data, including an unstructured 3D mesh based on the CGNS notation used by CFD codes. The implementation relies heavily on a built-in on-the-fly temperature treatment ("Doppler-broadening") routine and the capability to model continuously-varying temperature and density distributions without any modifications in the geometry input.

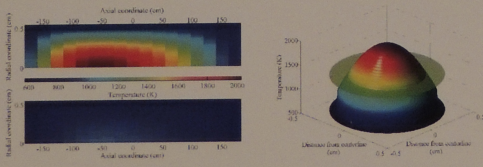

***Fig 2**. Left: The temperature distributions solved by FINIX for the hot pin and the absorber pin in an internally-coupled 3D assembly calculation. Right: Continuously modeled radial temperature profile in an internally-coupled pin-cell calculation.*

Burnup Calculation

The internal burnup calculation routine in Serpent enables tracking the evolution of nuclide compositions in irradiated materials. Typical applications include fuel cycle studies and assembly burnup calculations performed as a part of generating homogenized few-group constants.

Reactor Modelling

In addition to homogenization and assembly-level burnup calculations, Serpent has been used for various research reactor applications. The universe-based geometry routine allows the modeling of complicated three-dimensional systems. The code features a special geometry type for double-heterogeneous stochastic geometries. This includes particle distributions in HTGR fuels and pebble distributions in pebble-bed reactor cores, which enables the efficient modeling of these geometries practically without approximations.

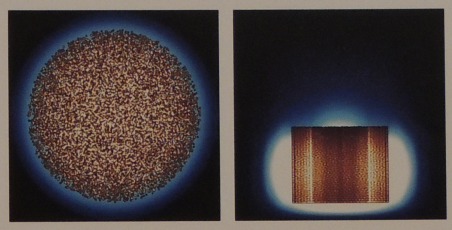

***Fig 3**. Left: Power and thermal flux distribution in a single PBMR fuel pebble. Right: Full-core power and thermal flux distribution in the ASTRA pebble-bed experiment. Both calculations were based on the explicit stochastic geometry model.*

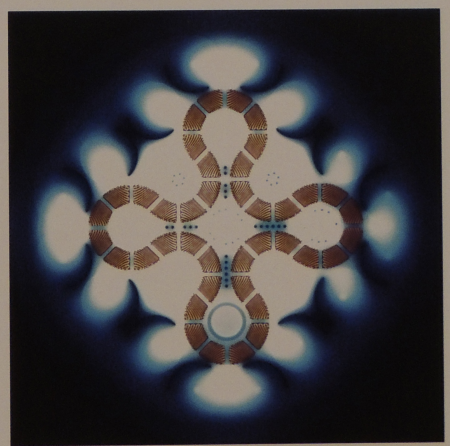

***Fig 4.** Power and thermal flux distribution in the Advanced Test Reactor (ATR) operated at Idaho National Laboratory.*

Institute of Nuclear Energy Safety Technology
Chinese Academy of Sciences · FDS Team

SNA&MC

SuperMC: Super Monte Carlo Calculation Program for Nuclear and Radiation Process

Jing SONG, Guangyao SUN, Huaqing ZHENG, Zhenping CHEN, Lijuan HAO, Cheng CHEN, Kuan ZHANG, Yongfeng WANG, Yawen YAN, Tao HE, Shengpeng YU, Chong CHEN, Qin ZENG, Pengcheng LONG, Liqin HU, Yican WU, FDS Team
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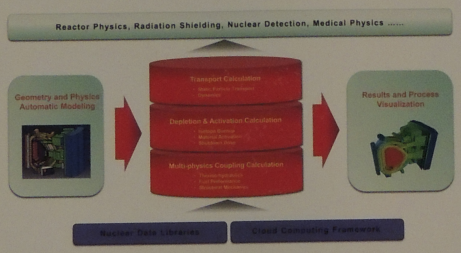
ABSTRACT : SuperMC is designed to perform transport calculation, depletion calculation (including isotope burnup, material activation, shutdown dose), multi-physics coupling calculation (including thermo-hydraulics, fuel performance, structural mechanics) with high efficiency and fidelity mainly based on Monte Carlo method and advanced computer technology. Systematically simulation from automatic modeling to calculation and visualized analysis can be performed by SuperMC.

1. Introduction

Radiation transport simulation is the foundation of reactor physics design and radiation shielding analysis. Monte Carlo (MC) method has notable advantages in dealing with complex geometries and multi-dimensional physics problem. It is becoming more and more systematic, multi-functional and intelligent for MC codes in the world over the past years.

SuperMC is designed to perform transport calculation of various particles type based on Monte Carlo (MC) and MC-deterministic method coupled transport approach, depletion calculation including isotope burn-up, material activation and shutdown dose, multi-physics coupling calculation including thermo-hydraulics, fuel performance, structural mechanics, etc. The bi-directional automatic conversion between general CAD models and full-formed calculation models and mixed visualization of dynamical 3D dataset and geometry model can be well user oriented performed. Continuous-energy cross section data from nuclear data library HENDL is adopted. Comprehensive design and analysis can be performed on cloud computing service platform.



2. Main Functions

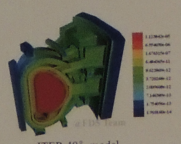
- **Radiation Transport Calculations**
  - Neutron, photon, proton, electron,etc.
  - Fixed source and criticality problem calculation
  - MC / SN / MOC and coupled methods
  - Uncertainty and sensitivity analysis
  - Time-dependent transport calculation
  - Cross section and parameters generation for deterministic codes
- **Depletion Calculations**
  - Isotopes burnup calculation
  - Material activation calculation
  - Shut-down dose calculation
- **Multi-Physics Coupling**
  - Thermal-hydraulics calculation
  - Fuel performance analysis
  - Structural mechanics analysis
- **Automatic Modeling and Treatment of Complex 3D Geometry**
  - CAD / Image-based automatic modeling
  - Arbitrary 3D combination of solids and surfaces
  - Unstructured geometry and stochastic geometry
- **Visualization of Process and Results**
  - Visualized analysis of results coupled with geometries
  - Real-time particles tracking visualization
- **Multi-Functional Nuclear Data Library**
  - Support multi-functional library for transport, burnup, activation, material damage etc. calculation)
  - Support multi-format work library (ACE, MATXS, AMPX, ANISNB, CARD, etc.)
  - Temperature effect treatment (OTF)
- **Acceleration Method**
  - Rich variance reduction techniques
  - MPI and OpenMP hybrid parallel computing technology
  - Efficient parallel algorithm on particles, domain and data field decomposition
  - Comprehensive service architecture based on cloud computing

3. Key Features

- **Reliable**
  - Standard validation and verification; V & V through amount of international benchmarks
- **High efficiency**
  - Parallel based on particles, domain/data decomposition, rich variance reduction techniques and acceleration algorithms
- **Easy to use**
  - Systematically modeling, calculation, visualization; cloud computing architecture, resource sharing, high performance calculation service
- **Multi-physics and high fidelity simulation**
  - Neutron/photon/electron/proton/etc.; ransport calculation, depletion calculation, multi-physics tight coupling; accurate and mature physical model, broad energy range

4. Benchmarking

- **International Criticality Safety Benchmark Experimental Problem**
- **Neutronics Calculation and Analysis of ITER**
- **Analysis of China LEAd-based Reactor (CLEAR)**



ITER 40° model

CLEAR

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[1] Yican Wu, Jing Song. Development of Super Monte Carlo Calculation Program SuperMC 2.0, ANS Winter Meeting, 2013, Washington DC, USA.

[2] Jing Song, Guangyao Sun, Huaqing Zheng, et al, Benchmarking of Super Monte Carlo Calculation Program for Nuclear and Radiation Process-SuperMC 2.0, ISFNT-11, 2013, Barcelona, Spain.

TRIPOLI-4® CEA, EdF and AREVA Reference Monte-Carlo Code

SNA + MC 2013, 27th-31st October, 2013, Paris, France

TRIPOLI-4® Project Team (by alphabetical order) : E. Brun, F. Damian, C. Diop, E. Dumonteil, F.-X. Hugot, C. Jouanne, Y.-K. Lee, F. Malvagi, A. Mazzolo, O. Petit, J.-C. Trama, T. Visonneau, A. Zoia
CEA Saclay - DEN/DANS/DM2S/SERMA 91191 Gif-sur-Yvette, France

TRIPOLI-4® is the reference industrial code for CEA (labs and reactors), EDF (58 PWRs), and branches of AREVA.
TRIPOLI-4® is the reference code of the CRISTAL Criticality Safety package developed with IRSN and AREVA
TRIPOLI-4® is developed at CEA/DEN in Saclay in a 75 permanent staff R&D unit (SERMA)

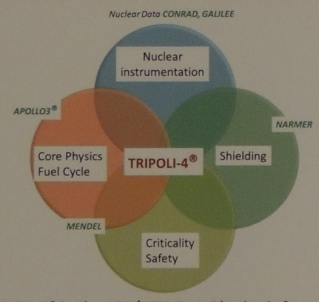
Highlights

TRIPOLI® is the corner stone of the CEA/DEN Neutronic Software Suite:

- deterministic code APOLLO3® (lattice and core)
- depletion code MENDEL (shared by APOLLO3 & TRIPOLI-4)
- nuclear data evaluation and processing (CONRAD and GALILEE)

Since the 60's, TRIPOLI® is the CEA/DEN Monte-Carlo radiation transport code dedicated to:

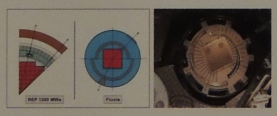
- radiation protection and shielding,
- core physics with depletion,
- criticality safety,
- nuclear instrumentation analyses.



TRIPOLI-4® in the CEA/DEN Core Physics Software Suite

Extensive V&V

The V&V Test base comprises several ICSBEP and SINBAD benchmarks, as well as proprietary benchmarks on CEA experimental facilities from various CEA centers.



FLUOLE experiment in the EOLE mockup reactor (validation of the RPV modelization)

Generic Features

- **Nuclear data librairies** available : JEFF (reference evaluation), ENDF-B , FENDL, JENDL.
- **Probability tables** from CALENDF in the UNRR.
- **Neutrons** tracked from 20 MeV down to 10^{-5}eV, **photons**, **electrons** and **positrons** from 100 MeV to 1 keV.
- 3D general **geometry**, own native geometry package (surface based & combinatorial), **ROOT** format compatible, linkable to **any third party geometry package**.
- Two main simulation modes : **fixed sources** & **criticality**.
- **Sources** : variety available within the code plus user-provided capability.
- **Depletion** capacity.
- **Tallies** : volume/surface/point fluxes, reaction rates, deposited energy, dpa, gamma spectroscopy, mesh tallies, Equivalent Dose Rate tallies, built-in kerma response, kinetic parameters for criticality...
- Extensively **validated**.
- Mainly developed from the 90's in **C++**, available 32 & 64 bits, linux distributions, unix.
- Proprietary **parallel mode** => multi-core single machines, heterogeneous workstations networks, massively parallel machines capability.

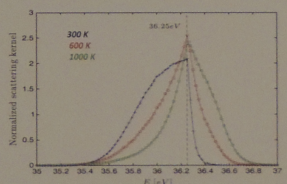
Variance Reduction

- Common variance reduction techniques: implicit capture, point estimator, splitting and Russian roulette.
- built-in functionality, ININPOND, based on the **Exponential Transform** and an **automatic pre-calculation of the importance map**.
- *Details: the biased cross-sections*
  $\Sigma_t^*(\mathbf{r},E,\Omega) = \Sigma_t(\mathbf{r},E,\Omega) - [K\,\Omega.\Omega_0](\mathbf{r},E,\Omega)$
  are derived from $\phi^* = I\,\phi$ *and used in the displacement operator kernel ;* I *is the importance.*
  K *(Placzek factors) and* Ω_0 *(direction of interest:* $K\,\Omega_0 = \nabla I/I$*) are computed by the code.*
  The source is also biased, based on I*.*
  A spatial and energy grid for the biasing initialization must be defined.
  "Fictive" detectors (just one or a few) must be set in the geometry, which act as "attractors" for simulated particles. The strength of the attraction is determined by a single parameter β*.*

Variance reduction : an example of neutron flux calculation in a Reactor Pressure Vessel (RPV) using ININPOND.
From top to bottom, 3 values of β *have been used : 0 (no attraction towards the RPV), 0.1 and 1. The respective Figures of Merit are 0.05, 0.15 and 5.33.*

Doppler Broadening of the Elastic Scattering Kernel

The treatment of **elastic scattering kernels in heavy nuclei close to cross section resonances** has a substantial impact on the calculation of reactor physics parameters.
In order to properly take into account these effects, the Doppler Broadening Rejection Correction (DBRC) and the Weight Correction Method (WCM) have been recently implemented in TRIPOLI-4®.



Distribution of outgoing neutron energy for a 36.25 eV incident neutron on ^{238}U*, using the DBRC model*

References: TRIPOLI-4® Project Team, "TRIPOLI-4® User Guide", CEA-R-6316, CEA Saclay, 2012
Contact: frederic.damian@cea.fr

Distribution & Licensing
TRIPOLI-4® is available from the NEA DataBank and RSICC, with a license covering code evaluation, teaching and R&D (ITER/DEMO activities included).
TRIPOLI-4® is also directly available from CEA for countries outside NEA DB and RSICC or companies requesting a business license, in both cases following an agreement with CEA.

TRIPOLI-4® and TRIPOLI® are registered trademarks of CEA. *We gratefully acknowledge EdF longtime partnership with TRIPOLI® as well as AREVA support.*

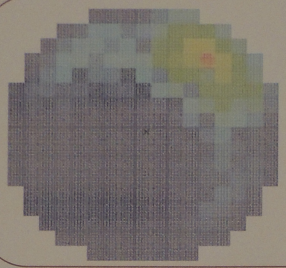
Examples of Nuclear Analysis with TRIPOLI-4® at CEA Saclay SERMA

SNA + MC 2013, 27th-31st October, 2013, Paris, France

SERMA Nuclear Analysis Team (alain.aggery@cea.fr),
SERMA Criticality -Safety Team (emmanuel.gagnier@cea.fr),
SERMA TRIPOLI-4® Project Team (frederic.damian@cea.fr),
CEA Saclay - DEN/DANS/DM2S/SERMA 91191 Gif-sur-Yvette, France

Highlights

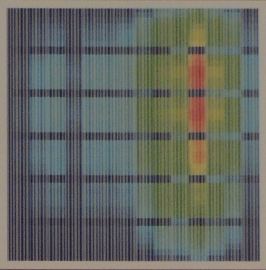
- TRIPOLI-4® is the reference Monte Carlo code of CEA, EDF and branches of AREVA.
- As such it is the central tool of the nuclear analysis conducted at CEA Saclay SERMA, in the domain of core physics, radiation protection and shielding, nuclear instrumentation and criticality safety.



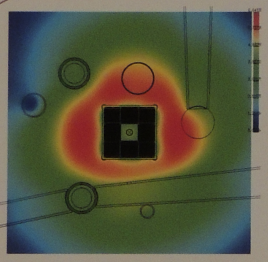
Innovative LWR core physics analyses (EPR core type) calculation of the fuel pin nuclear enthalpy elevation factor in static rod ejected configuration
J.C. Jaboulay, S. Douce *et al.*

Radial pin by pin power distribution

Axial pin by pin power distribution

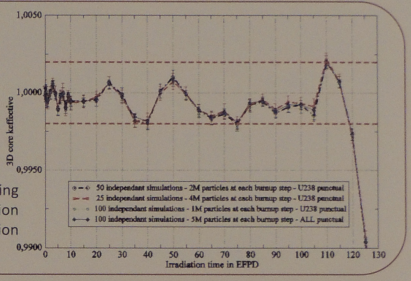


	TRIPOLI-4®
Ejected control rod worth in pcm	282 ± 5 pcm
3D Fuel assembly power peaking factor F_{xyz}	9,41 ± 0,04

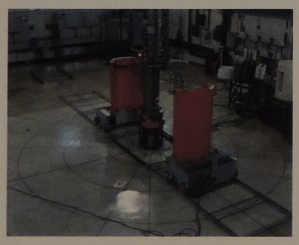


CEA Saclay ORPHEE Research Reactor 3D Core Depletion Study
F. Damian, E. Brun

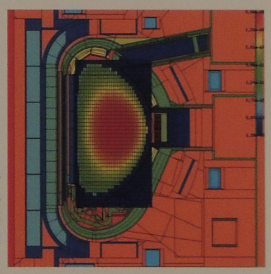
Radial Thermal Flux Distribution



Variation of the core k-effective during irradiation, time in EFPD , control rods insertion adjusted during irradiation

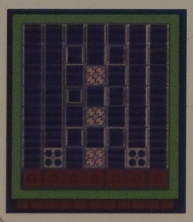


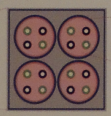
Criticality Accident Alarm System Benchmark Experiment at the CEA Valduc SILENE Facility (left). SILENE Reactor with Lead Shield
T. Miller, N. Authier, Y.K. Lee, E. Gagnier *et al.*

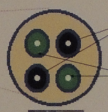


Neutron source density distribution (neutron.cm^{-3}.fusion^{-1}) in a logarithmic color scale (right). ITER Alite (from ITER IO) model converted from MCNP (LANL, USA) with MCAM 5 (FDS Team, INEST, China), then viewed with the TRIPOLI-4® 2D tool J.C. Jaboulay *et al.*

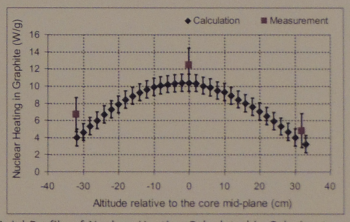
Nuclear Heating Evaluation in the CEA Saclay OSIRIS Material Testing Reactor - F. Malouch







Horizontal Cross-Section of the OSIRIS CEA Saclay MTR, with a zoom on a Central Water Box (middle) loaded with Differential Calorimeters (right)



Axial Profile of Nuclear Heating Calculated in Calorimeter and Compared with Experimental Points

References

- "A very heterogeneous 3D PWR core benchmark: deterministic and Monte Carlo method comparison", J.C. Jaboulay et al., *SNA&MC 2013*, October 2013, Paris, France
- "ORPHEE Research Reactor : 3D Core Depletion Calculation using Monte Carlo Code TRIPOLI-4®", F. Damian, E. Brun, *SNA&MC 2013*, October 2013, Paris, France
- "TRIPOLI-4® Monte Carlo Code ITER A-lite Neutronic Model Validation", J.C. Jaboulay *et al.*, *ISFNT-11*, September 2013, Barcelona, Spain
- "2010 Criticality Accident Alarm System Benchmark Experiments at the CEA Valduc Silene Facility", T. Miller, N. Authier, Y.K. Lee, E. Gagnier *et al.*, *ICNC 2011*, September 2011, Edinburgh
- "Development and Experimental Validation of a Calculation Scheme for Nuclear Heating Evaluation in the Core of OSIRIS Material Testing Reactor", F. Malouch, *Journal of ASTM International (JAI), Volume 9, Issue 4 (April 2012)*

Contacts at SERMA

Nuclear Analysis : alain.aggery@cea.fr - Criticality-Safety : emmanuel.gagnier@cea.fr - TRIPOLI-4 ® : frederic.damian@cea.fr

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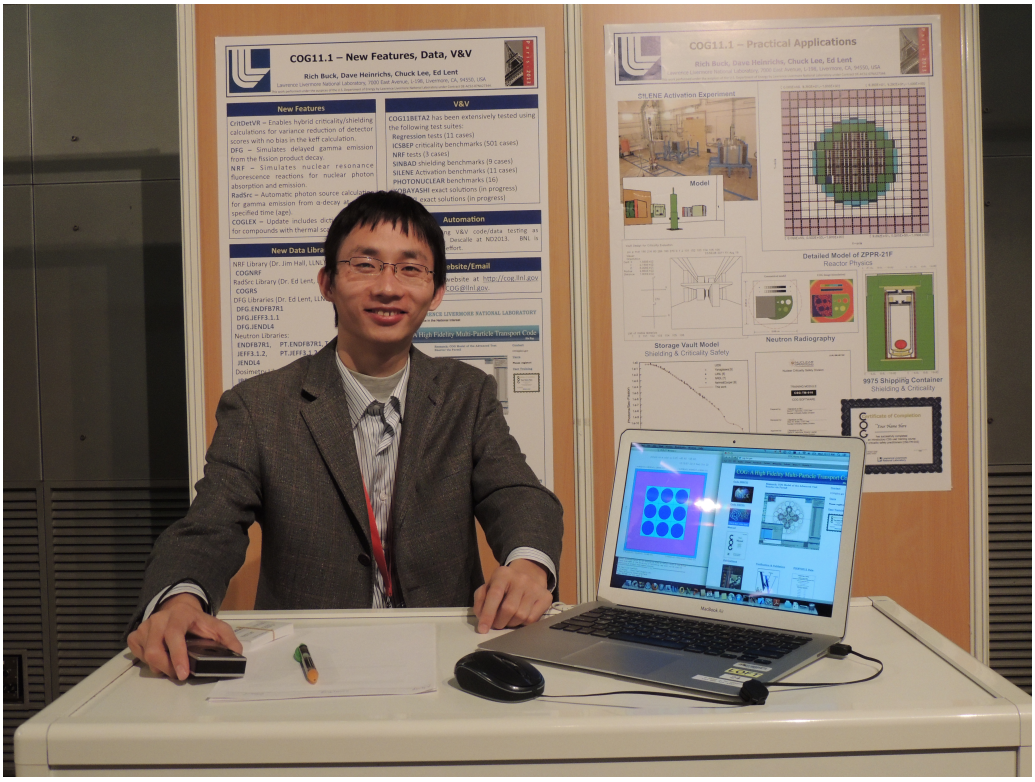
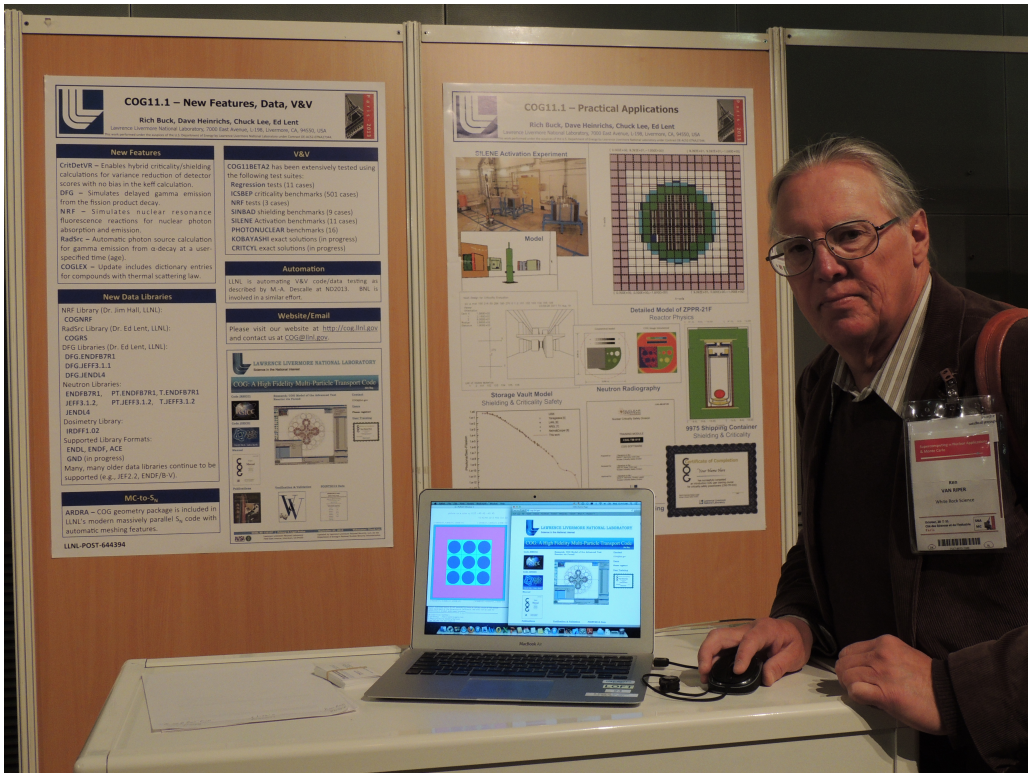
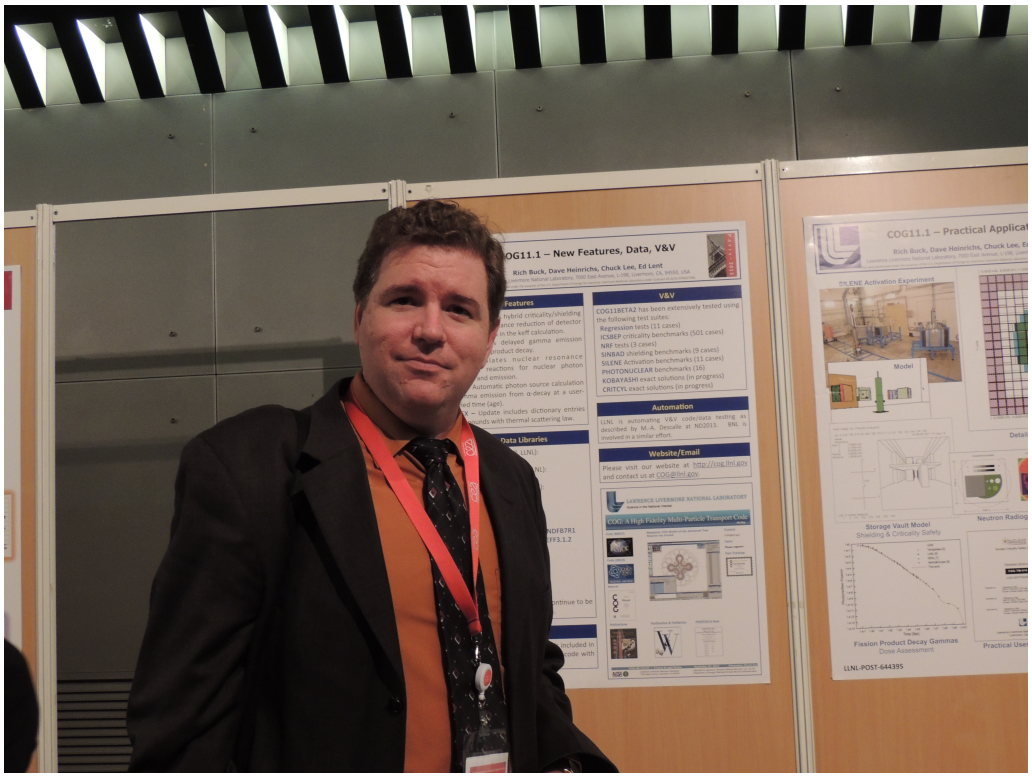
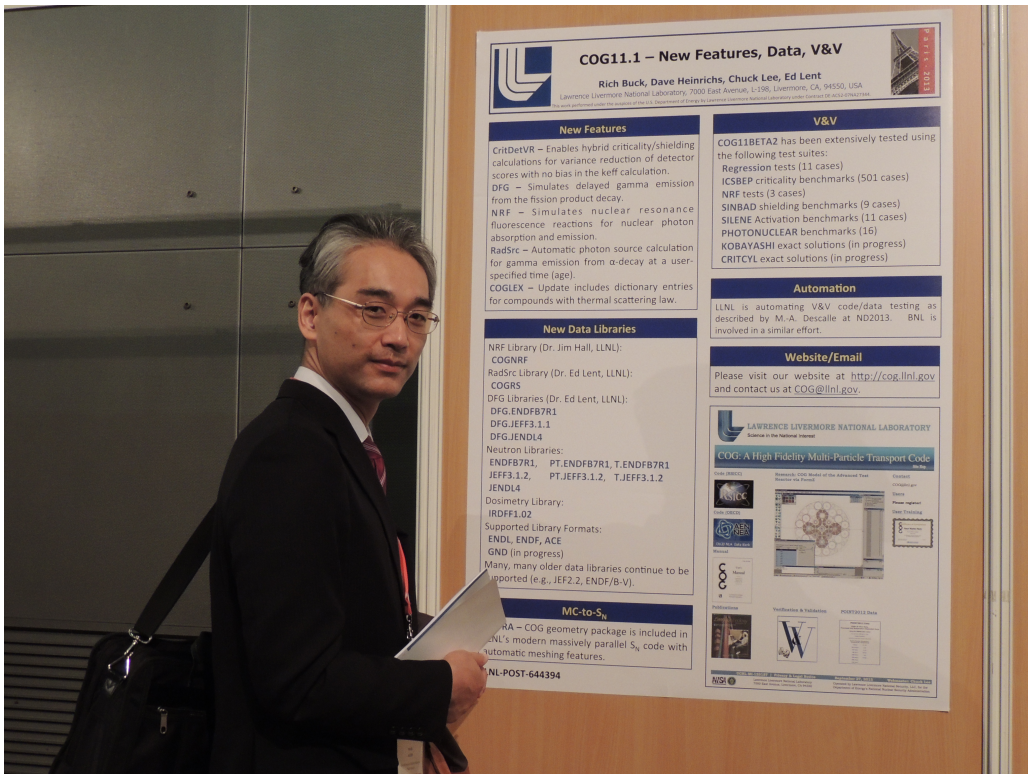
Pictures from the COG Exhibit

The following photos illustrate some of the interactions with visitors to the COG exhibit area during the Monte Carlo Codes Invited Session.






COG11.1 – New Features, Data, V&V
Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
V&V
Automation
Website/Email
COG11.1 – Practical Applica
Storage Vault Model
Shielding & Criticality Safety
Fission Product Decay Gammas
Dose Assessment
LLNL-POST-644395


COG11.1 – New Features, Data, V&V
Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
Lawrence Livermore National Laboratory, 7000 East Avenue, L-198, Livermore, CA, 94550, USA
New Features
CritDetVR – Enables hybrid criticality/shielding calculations for variance reduction of detector scores with no bias in the keff calculation.
DFG – Simulates delayed gamma emission from the fission product decay.
NRF – Simulates nuclear resonance fluorescence reactions for nuclear photon absorption and emission.
RadSrc – Automatic photon source calculation for gamma emission from α-decay at a user-specified time (age).
COGLEX – Update includes dictionary entries for compounds with thermal scattering law.
New Data Libraries
NRF Library (Dr. Jim Hall, LLNL):
COGNRF
RadSrc Library (Dr. Ed Lent, LLNL):
COGRS
DFG Libraries (Dr. Ed Lent, LLNL):
DFG.ENDFB7R1
DFG.JEFF3.1.1
DFG.JENDL4
Neutron Libraries:
ENDFB7R1, PT.ENDFB7R1, T.ENDFB7R1
JEFF3.1.2, PT.JEFF3.1.2, T.JEFF3.1.2
JENDL4
Dosimetry Library:
IRDFF1.02
Supported Library Formats:
ENDL, ENDF, ACE
GND (in progress)
Many, many older data libraries continue to be supported (e.g., JEF2.2, ENDF/B-V).
MC-to-S$_N$
RA – COG geometry package is included in NL's modern massively parallel S$_N$ code with utomatic meshing features.
NL-POST-644394
V&V
COG11BETA2 has been extensively tested using the following test suites:
Regression tests (11 cases)
ICSBEP criticality benchmarks (501 cases)
NRF tests (3 cases)
SINBAD shielding benchmarks (9 cases)
SILENE Activation benchmarks (11 cases)
PHOTONUCLEAR benchmarks (16)
KOBAYASHI exact solutions (in progress)
CRITCYL exact solutions (in progress)
Automation
LLNL is automating V&V code/data testing as described by M.-A. Descalle at ND2013. BNL is involved in a similar effort.
Website/Email
Please visit our website at http://cog.llnl.gov and contact us at COG@llnl.gov.
LAWRENCE LIVERMORE NATIONAL LABORATORY
Science in the National Interest
COG: A High Fidelity Multi-Particle Transport Code

COG11.1 – New Features, Data, V&V
Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
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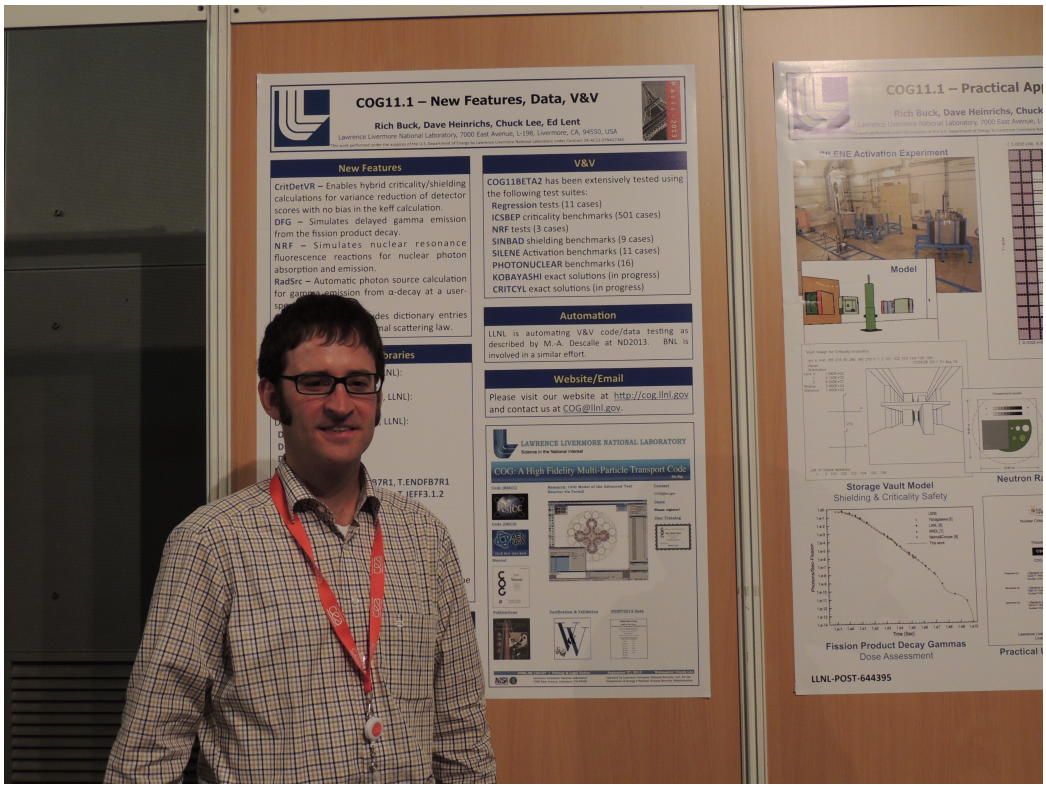
LAWRENCE LIVERMORE NATIONAL LABORATORY
COG: A High Fidelity Multi-Particle Transport Code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Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
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LAWRENCE LIVERMORE NATIONAL LABORATORY
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SILENE Activation Experiment
Model
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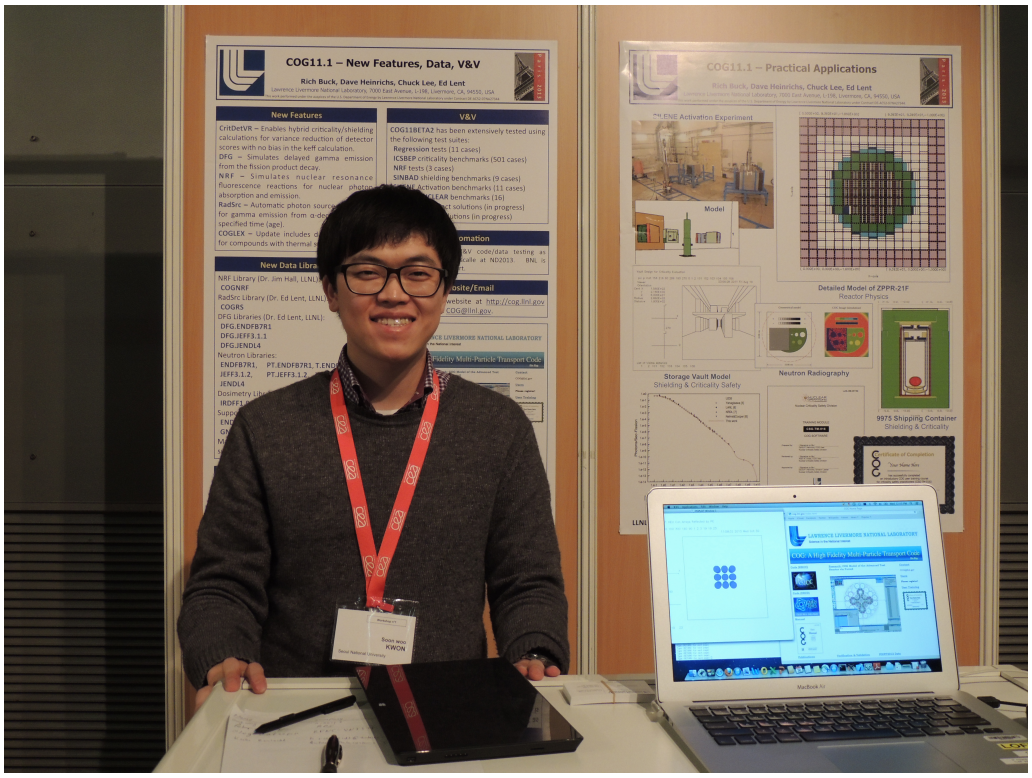
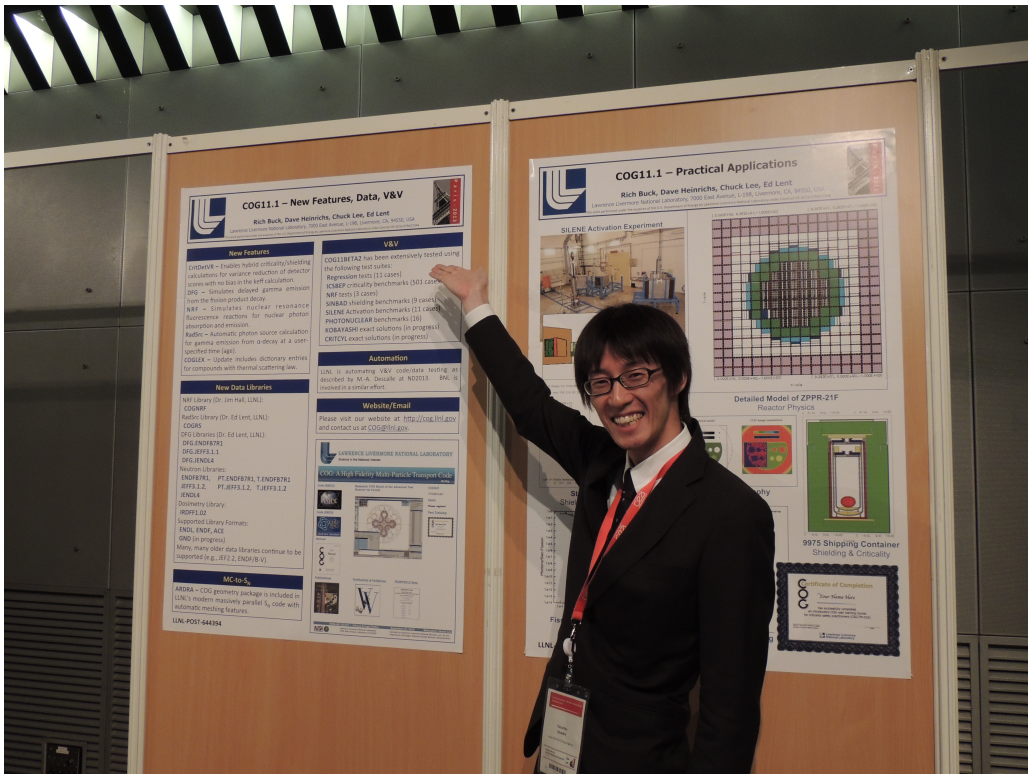
LLNL-POST-644395


COG11.1 – New Features, Data, V&V
Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
New Features
V&V
COG11.1 – Practical Applications
Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent
SILENE Activation Experiment
Model
Detailed Model of ZPPR-21F
Reactor Physics
Storage Vault Model
Shielding & Criticality Safety
Neutron Radiography
9975 Shipping Container
Shielding & Criticality
Certificate of Completion
Your Name Here
Boom Woo KWON
Nuclear Engineering
Oregon State University
LAWRENCE LIVERMORE NATIONAL LABORATORY
COG: A High Fidelity Multi-Particle Transport Code
MacBook Air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9975 Shipping Container
Shielding & Criticality
Certificate of Completion
Your Name Here
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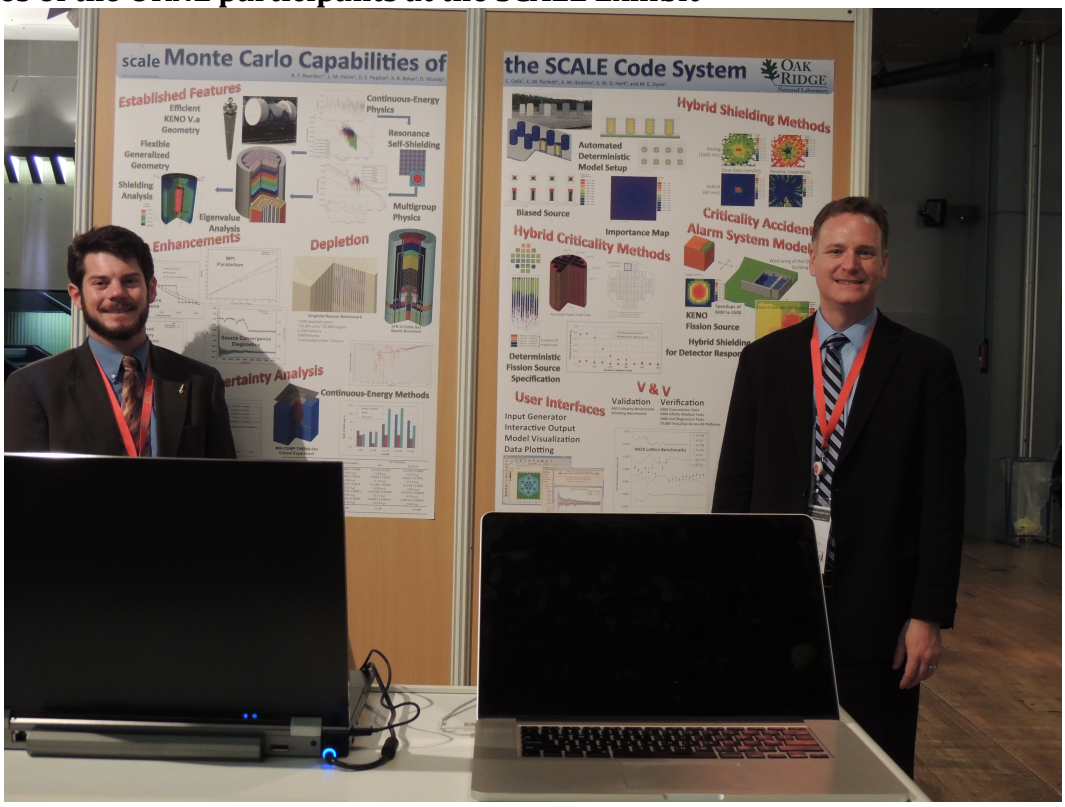
COG: A High Fidelity Multi-Particle Transport Code

Pictures of the ORNL participants at the SCALE Exhibit



A Picture of Forrest Brown Speaking in the Conference Area

Visitors to the COG Exhibit Requesting Additional Information

Name	company	email
Dong. wang	INEST	dong.wang@fds.org.cn
Peter Caracappa	RPI	caracp3@rpi.edu
Oleg Zatsepin	RFNC-VNIITF	o.v.zatsepin@vniitf.ru
Heiko Reinhardt	Antares Datasysteme GmbH	h.reinhardt@antares-gco.de
Soonwoo Kwon	Seoul National University	goldoe27@snu.ac.kr

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Clinical Assistant Professor, Nuclear Engineering

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Cellular: 505 660 1107
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kvr@whiterockscience.com
http://www.whiterockscience.com

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Chinese Academy of Sciences · FDS Team

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Tel:+86 15395003881 Fax:+86 551 65593681

JAEA

Tatsuhiko OGAWA, Ph.D.

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Research Group for Radiation Protection,
Division of Environment and Radiation Sciences,
Nuclear Science and Engineering Directorate

Japan Atomic Energy Agency (JAEA)

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Research Scientist
Sector, Nuclear Fuel & Reactor Core
Nuclear Technology Research Laboratory

Yasushi Nauchi, Dr .Eng.

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E-mail: nauchi@criepi.denken.or.jp
http://criepi.denken.or.jp/

Summary

In general, the Monte Carlo Codes Invited Session was very well received and the posters and demonstrations well presented. The participating Monte Carlo codes that can perform nuclear criticality safety analysis are:

COG11 – LLNL
MCNP6 – LANL
MONK – AMEC (formerly, SERCO)
MORET5 – IRSN
RMC – Tsinghua University, Peoples Republic of China
SCALE – ORNL
SUPERMONTECARLO – China Academy of Sciences, Peoples Republic of China
TRIPOLI-4 – CEA

Some of the other Monte Carlo codes can only perform electron-photon transport and are tailored to medical applications. These include:

ARCHER – RPI
PENELOPE – Spain

Interactions with users and researchers confirm that the most widely used Monte Carlo code for nuclear criticality safety is LANL's MCNP6. It is also widely used for general physics applications throughout the USA and internationally. It is the favor Monte Carlo code for nuclear criticality safety professionals.

One of session participant, Professor Peter Caracappa from RPI, visited the LLNL COG11 poster booth and asked if he can get a copy of COG11 for his student to start using it to benchmark and calibrate their detectors in support of NCSP sponsored nuclear data measurements. He was very interested in learning how to use COG11 with the various available nuclear data libraries such as JEFF, JENDL, ENDF-B, and ENDL for benchmarking and inter-comparison particularly in thermal energy regions without changing the analytical method. LLNL Ed Lent addressed this capability in the report entitled, "A Comparative Study of the COG Thermal Libraries", LLNL-TR-645096, Edward M. Lent, October 21, 2013. This report is publicly available on the COG web site at:

http://cog.llnl.gov/pdf/LLNL-TR-645096.pdf.

LLNL will follow-up and provide assistance to RPI for COG11 installation when time permits in the near future.

There were several Chinese participants that visited the LLNL COG11 poster booth and inquired how they can get a copy of COG11 software. I directed them to visit the OECD NEA Data Bank web site for this information. LLNL distributes COG software through the Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory (ORNL). Through reciprocal agreements, RSICC provides COG to the NEA Data Bank for countries that are members of the Data Bank.

Another session participant, Mr. Soon Woo Kwon from Soul National University, South Korea, visited the LLNL COG11 poster booth and also inquired on how to use COG11 for performing benchmark and detector calibration using different nuclear data libraries such as JEFF, JENDL, ENDF-B, and ENDL without changing analytical method.

As a final thought, I learned after interacting with many session participants who visited the LLNL booth, that they were not familiar with COG and were very impressed by COG's unique capability of supporting multiple nuclear data libraries of various origin in different formats. They were very interested in using COG11's multi-library capabilities in their future research and were interested in future collaborations. Consequently, in my opinion, this kind of forum for presentation, demonstration and informal interactions is an excellent way to showcase NCSP nuclear criticality safety codes (COG11, MCNP6, and SCALE6) and educate new users and users from related fields. A similar workshop should be held in conjunction with future ICNC and SNA-MC conferences.