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Title: MCNP Developments

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Recent Nuclear Criticality Safety Program Technical Accomplishments
ANS Winter Meeting 2011 - Washington, DC
LA-UR-11-06130

MCNP Developments

Recent Monte Carlo Progress in Support of the US DOE Nuclear Criticality Safety Program

Forrest Brown & Brian Kiedrowski
Monte Carlo Codes, XCP-3
Los Alamos National Laboratory

MCNP Developments

Forrest Brown & Brian Kiedrowski, XCP-3, LANL

This presentation covers recent progress in development and support of the MCNP Monte Carlo code during FY 2011 in support of the US DOE/NNSA Nuclear Criticality Safety Program.

Activities and accomplishments are summarized in six major areas:

- MCNP5-1.60 Release
- MCNP6 Status
- Verification / Validation
- User Support & Training
- R&D Work in Progress
- Future Release Plans

US DOE/NNSA Nuclear Criticality Safety Program –

What have we done for you lately ?

- MCNP5-1.60 Release
- MCNP6 Status
- Verification / Validation
- User Support & Training
- R&D Work in Progress
- Future Release Plans

MCNP5-1.60 Release (1)

- **Chronology**
  - Development: Fall 2009 – Spring 2010
  - Extensive testing & V&V: Summer 2010
  - Sent to RSICC: September 2010
  - RSICC release: October 2010, July 2011

- **Focus**
  - **Stability + reliability for criticality calculations**
  - **Support for latest computers – multicore, Windows/Mac/Linux, 32/64 bit**
  - **Rigorous, extensive code V&V**
  - **A few new features, many minor bug-fixes**
  - **Last version of MCNP5 – want strong base for going forward with MCNP6**

- **Notable**
  - **Most rigorous & extensive MCNP testing ever**
  - **Over 5,000 hr computer time for V&V, mostly on criticality problems**
  - **First release of adjoint-weighted tallies (kinetics parameters)**

MCNP5-1.60 Release (2)

Monte Carlo Codes
XCP-3, LANL

- **Adjoint-weighted Tallies for Point Kinetics Parameters**
  - **β_{eff}, Λ_{eff}, Rossi-α using continuous-energy Monte Carlo**
  - **Adjoint-weighted tallies from iterated fission probability**

- **Mesh Tallies for Isotopic Reaction Rates**
  - Previously, could only do flux, dose, material reaction rates
  - **Important extension to specific isotopes**

- **Increased Limits for Geometry, Tally, and Source Specifications**
  - **Allow up to 100M for cell, surface, material specs.** Previous 100K limit
  - Complex cell spec up to 9999 items, previous 999 limit

- **General**
  - Improved threading on multicore computers, Mac/Linux/Windows
  - 12 other minor enhancements to code
  - 30 minor bug-fixes (none affect results for criticality calculations)

MCNP5-1.60 Release (3)

- **Testing + V&V Suites**

`REGRESSION`	- 66 installation & regression test problems
`VALIDATION_CRITICALITY`	- 31 ICSBEP Handbook cases
`VERIFICATION_KEFF`	- 75 analytic problems, exact results
`VALIDATION_SHIELDING`	- 19 shielding/dose problems vs experiment
`KOBAYASHI [new]`	- void & duct streaming, point detectors
`POINT_KINETICS [new]`	- adjoint weighted Rossi-α, β_{eff}, Λ_{eff}

- **Computers**
  - Mac / Linux / Windows, 32 / 64 bit
  - Sequential, threads, MPI, threads+MPI
  - Over 5,000 hr computer time
  - 2 students full-time + 2.5 staff part-time for 3 months

- **Criticality calculations**
  - Tested with ENDF/B-VI & ENDF/B-VII.0
  - All results should match previous versions of MCNP5

MCNP5-1.60 Release (4)

MCNP Criticality Validation Suite, Results on Mac OS X for ENDF/B-VII.0

	Experiment	MCNP5-1.51	MCNP5-1.60
U233 Benchmarks			
JEZ233	1.0000 (10)	0.9989 (6)	0.9989 (6)
FLAT23	1.0000 (14)	0.9990 (7)	0.9990 (7)
UMF5C2	1.0000 (30)	0.9931 (6)	0.9931 (6)
FLSTF1	1.0000 (83)	0.9830 (11)	0.9830 (11)
SB25	1.0000 (24)	1.0053 (10)	1.0053 (10)
ORNL11	1.0006 (29)	1.0018 (4)	1.0018 (4)
HEU Benchmarks			
GODIVA	1.0000 (10)	0.9995 (6)	0.9995 (6)
TT2C11	1.0000 (38)	1.0018 (8)	1.0018 (8)
FLAT25	1.0000 (30)	1.0034 (7)	1.0034 (7)
GODIVR	0.9985 (11)	0.9990 (7)	0.9990 (7)
UH3C6	1.0000 (47)	0.9950 (8)	0.9950 (8)
ZEUS2	0.9997 (8)	0.9974 (7)	0.9974 (7)
SB5RN3	1.0015 (28)	0.9985 (13)	0.9985 (13)
ORNL10	1.0015 (26)	0.9993 (4)	0.9993 (4)

	Experiment	MCNP5-1.51	MCNP5-1.60
IEU Benchmarks			
IMF03	1.0000 (17)	1.0029 (6)	1.0029 (6)
BIGTEN	0.9948 (13)	0.9945 (5)	0.9945 (5)
IMF04	1.0000 (30)	1.0067 (6)	1.0067 (6)
ZEBR8H	1.0300 (25)	1.0195 (6)	1.0195 (6)
ICT2C3	1.0017 (44)	1.0037 (7)	1.0037 (7)
STACY36	0.9988 (13)	0.9994 (6)	0.9994 (6)
LEU Benchmarks			
BAWXI2	1.0007 (12)	1.0013 (7)	1.0013 (7)
LST2C2	1.0024 (37)	0.9940 (6)	0.9940 (6)
Pu Benchmarks			
JEZPU	1.0000 (20)	1.0002 (6)	1.0002 (6)
JEZ240	1.0000 (20)	1.0002 (6)	1.0002 (6)
PUBTNS	1.0000 (30)	0.9996 (6)	0.9996 (6)
FLATPU	1.0000 (30)	1.0005 (7)	1.0005 (7)
THOR	1.0000 (6)	0.9980 (7)	0.9980 (7)
PUSH2O	1.0000 (10)	1.0012 (7)	1.0012 (7)
HISHPG	1.0000 (110)	1 0122 (5)	1.0122 (5)
PNL2	1.0000 (65)	1.0046 (9)	1.0046 (9)
PNL33	1.0024 (21)	1.0065 (7)	1.0065 (7)

MCNP5-1.60 Release (5)

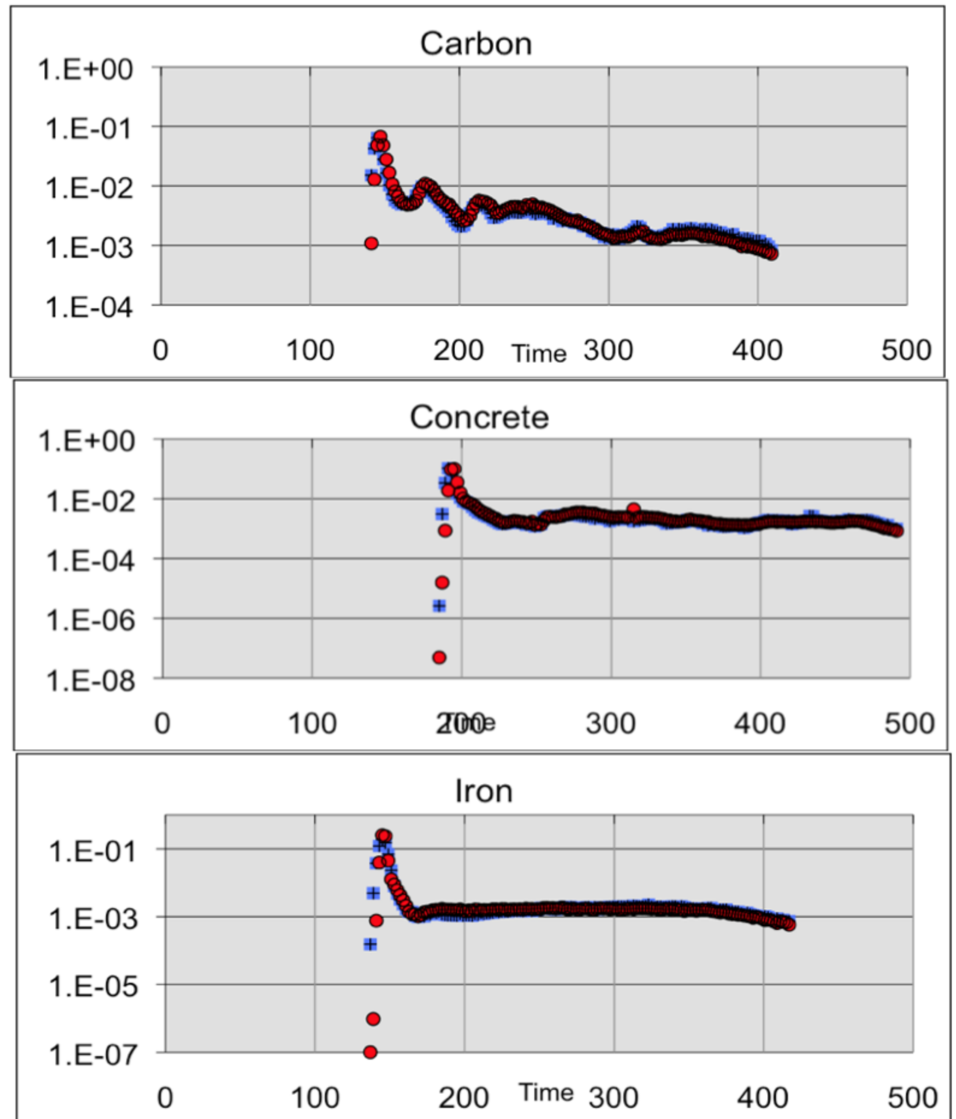
Monte Carlo Codes
XCP-3, LANL

MCNP Kinetics Parameter Validation Suite Results on Linux

	Benchmark		MCNP5	
Rossi-Alpha vs Experiments				
GODIVA	-0.0011	2e-05	-0.001131	7e-6
JEZPU	-0.00064	1e-05	-0.000649	8e-6
BIGTEN	-0.000117	1e-06	-0.0001156	7e-7
FLAT23	-0.000267	5e-06	-0.0002931	3e-6
STACY29	-0.000122	4e-06	-0.0001222	9e-7
WINCO5	-0.001109	3e-06	-0.001124	1e-5
Generation Time vs Exact Analytic Solutions				
ONEINF	10		9.999	0.00085
TWOINF	14.17		14.16	0.00275
Generation Time vs PARTISN Solutions				
BARESLAB	9.793		9.792	0.00594
REFLSLAB	135.2		135.1	0.1068
THRESLAB	49.17		49.28	0.1018
INTRSLAB	112.1		112.7	0.4397
BARESPHR	1.721		1.722	0.00102
REFLSPHR	10.19		10.19	0.00737
SUBCSLAB	10.17		10.17	0.0073
SUPCSLAB	9.673		9.674	0.00526

Pulsed Sphere Problems (3 of 8)

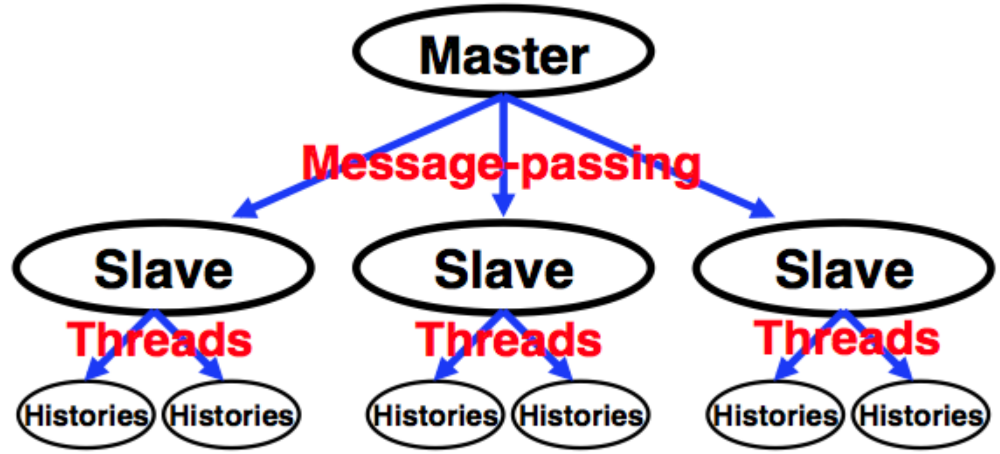
Experiment, MCNP5-1.60



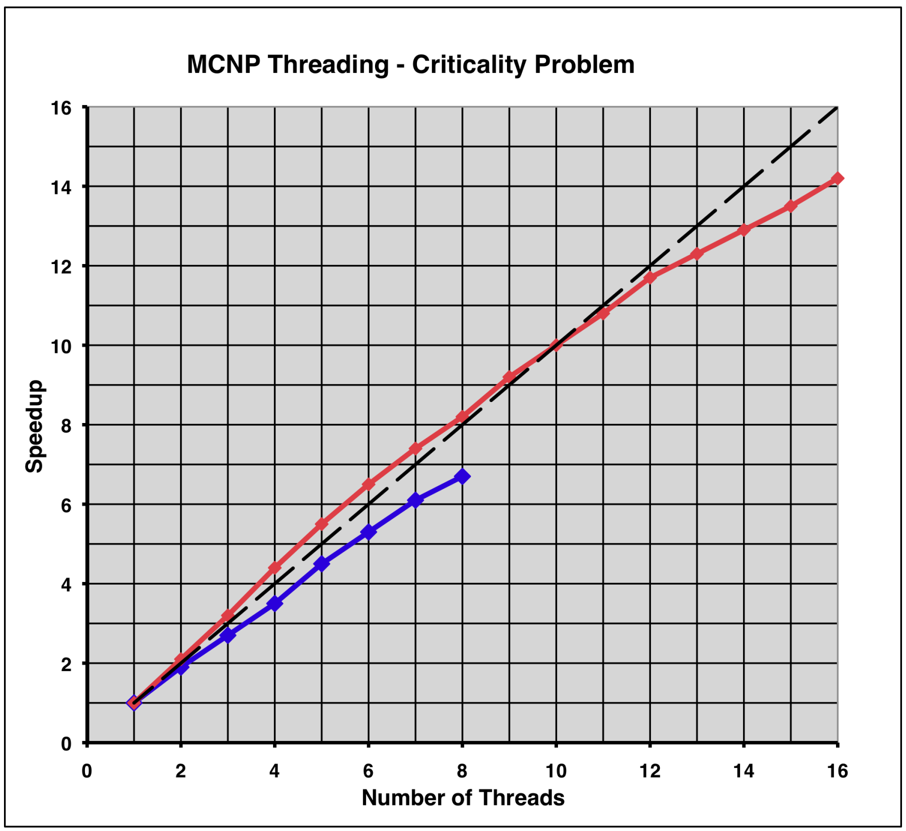
MCNP5-1.60 Release (6)

Monte Carlo Codes
XCP-3, LANL

- **Parallel performance**
  - MCNP5 has always used hierarchical parallelism with MPI + threading



Multicore threading speedups:



Hardware

– Lobo – 16 threads/node
   4 x Quad-core AMD Opteron, 2.2 GHz, 32 GB memory

– Mac Pro – 8 threads
   2 x Quad-core Intel Xeon, 3GHz, 8 GB memory

Software

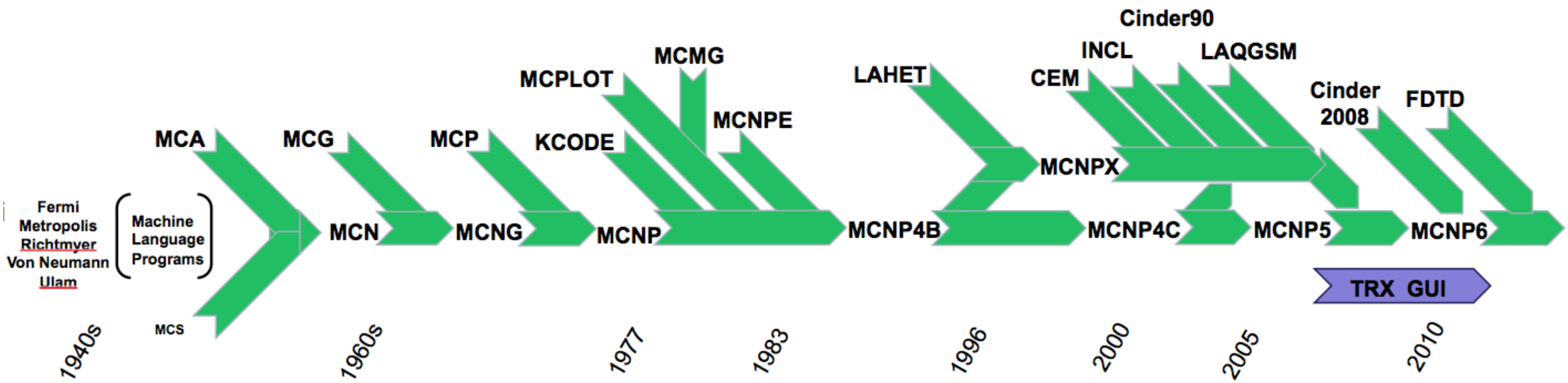
MCNP5, Intel-10 F90, "-O1 -openmp"

MCNP Criticality Calculation

BAWXI2 benchmark, kcode 25000 1 10 204

MCNP6 Status (1)

Monte Carlo Codes
XCP-3, LANL



- **MCNP6 – beta release sent to RSICC for a limited set of beta testers**
- **MCNP6 – full release by RSICC expected in 2012**
- **Culminates 5 years of effort combining features of MCNPX into MCNP5**
- **MCNP5 & MCNPX are now frozen – future development will occur in MCNP6**

Support from DOE/NNSA, DOE, DoD, DRTA, DHS/DNDO, NASA, & others

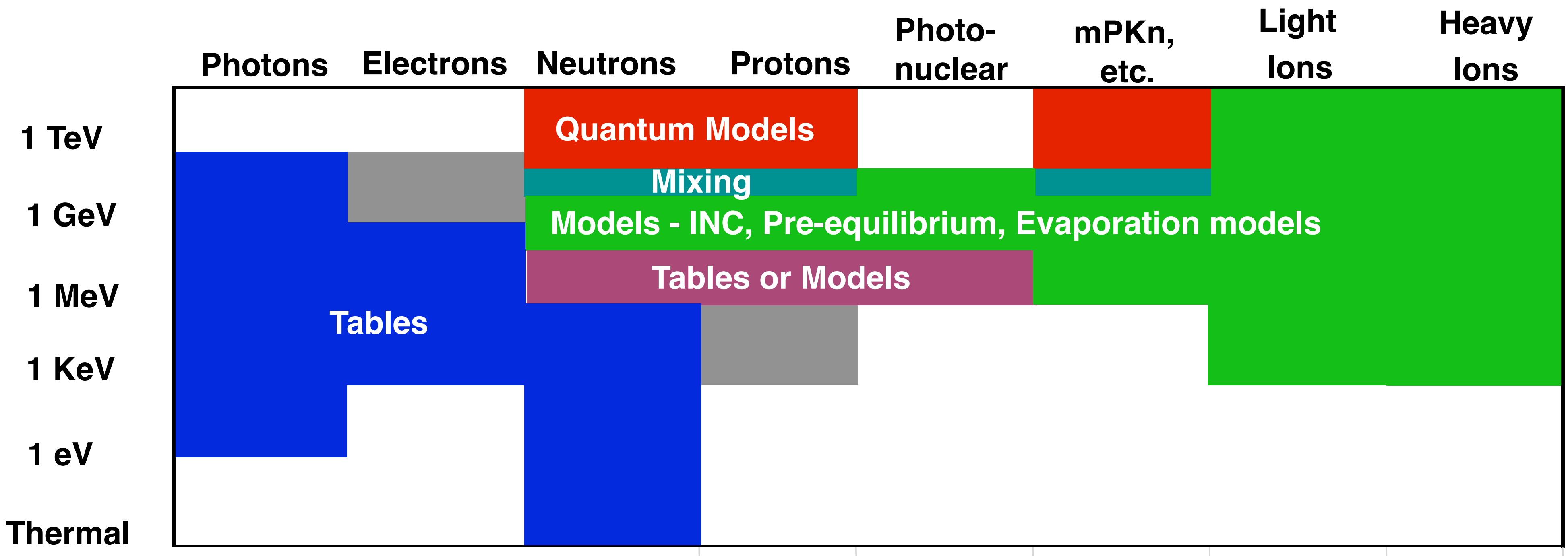
MCNP6 Status (2)

Monte Carlo Codes
XCP-3, LANL

- **MCNP6 contains:**
  - MCNP6 = development version of MCNP at LANL, since 2004
  - Includes:
    - All MCNP5-1.60 capabilities (mpi + threads)
    - All MCNPX 2.7.0 capabilities (mpi)
    - Adjoint-weighted perturbation estimators
    - CINDER 2008 decay & depletion
    - High energy protons & magnetic fields, for proton radiography
    - Unstructured mesh, for linking with ABAQUS
    - Structured mesh, for linking with PARTISN
- **MCNP6 in (very) limited beta release**
  - Recipients are active collaborators and sponsors
  - Full beta access within LANL and LLNL

MCNP6 Status (3)

MCNP6 – all particles & all energies, using best data + models + theory



- **Recent physics improvements:**
  - Photon induced fission multiplicity
  - Characteristic muonic X-rays
  - Exact delayed gamma emissions
  - Visible light
  - Improved photoatomic form factors
  - Upgrades to CEM & LAQGSM 3.03
  - GEF photofission yield

- **Incorporates other codes:**

CINDER	burnup & decay	LANL
ITS	electron transport	SNL
LAHET	high energy transport	LANL
CEM	high energy transport	LANL
LAQGSM	high energy transport	LANL
MARS	high energy transport	FNAL
HETC	high energy transport	ORNL

MCNP6 Status (4)

- **MCNP & MCNPX teams have adopted MCNP6 as the base for all future development**

- **To go from Beta release to Production release:**
  - Assurance of reliability and accuracy for criticality
  - Assurance of reliability and accuracy for other apps
  - Comparable performance
  - Complete documentation

- **Future Work**
  - Cleanup coding style
  - Remove duplicate features
  - Extend parallel threading capability to new features
  - New Features

- **General release through RSICC**
  - 2012

Verification / Validation (1)

- **MCNP V&V Suites -- Focus**
  - **Physics-based V&V**
  - **Compare to experiment or exact analytic results**
  - Part of MCNP permanent code repository & RSICC distribution
  - Automated - easy to run & collect results, compare to experiments

- **Continuous Test System for MCNP6**
  - **3 platforms - Linux 32, Linux 64, Windows 64**
  - **5 compilers - Intel 10+11, PGI 7, Pathscale 3, gfortran**
  - **Serial, mpi, omp, mpi+omp**
  - **Array bounds checking**
  - **875 problem input files**
  - **Total: 10,000 runs each night**

Verification / Validation (2)

Monte Carlo Codes
XCP-3, LANL

- **Testing + V&V Suites**

REGRESSION	- 66 installation & regression test problems
VALIDATION_CRITICALITY	- 31 ICSBEP Handbook cases
VERIFICATION_KEFF	- 75 analytic problems, exact results
VALIDATION_SHIELDING	- 19 shielding/dose problems vs experiment
KOBAYASHI	- void & duct streaming, point detectors
POINT_KINETICS	- adjoint weighted Rossi-α, β_{eff}, Λ_{eff}

- **Recently added V&V Suites**

VALIDATION_CRIT_EXPANDED	-119 ICSBEP Handbook experiments
Rossi Alpha Val. Suite	- 12 ICSBEP Handbook experiments
VALIDATION_LANL_SB-CS	-194 ICSBEP Handbook experiments
VALIDATION_SHIELDING	- improved models & experiment results

High-E proton, heavy ion
Delayed n & γ spectra
Subcritical multiplication
Perturbation verification
Production / depletion

Verification / Validation (3)

- **MCNP5 & MCNP6 continue to be used extensively in the development & testing of ENDF/B-VII.0 and ENDF/B-VII.1 nuclear data libraries:**

> **"As noted there were a number of additional "first-ever" features of the ENDF/B-VII.0 validation effort. There was almost total reliance on continuous-energy Monte Carlo methods. Because these methods can handle even the most complex geometry features of the benchmark models and provide "rigorous" treatment of the neutron physics, the calculational errors are reduced essentially to the statistical errors of the computation and the errors due to nuclear data. And it is now practical to run sufficient neutron histories in the computation to make the former errors negligibly small relative to the latter. Furthermore, the validation calculations relied almost totally on a single code system (NJOY/MCNP). This dominance of a single code system is not viewed as limiting the validation effort given (i) the general acceptance and universal recognition of the high quality of this physics tool and (ii) the availability of sufficient, both historical and current, independent verification of the ENDF/B-VII.0 validation results by other independent code systems, primarily with results of the U.S. Naval Reactor Labs code RACER [281, 282] and RCP01 [283] and the Argonne National Laboratory code VIM [284]."**

M.B. Chadwick, et al., *ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology,* Nuclear Data Sheets, Vol. 107, No. 12, pp 2931-3060 (2006)

User Support & Training (1)

Monte Carlo Codes XCP-3, LANL

- **11,586 copies of MCNP distributed by RSICC, Jan 2001 – Oct 2011**
- **Classes**
  - **Theory & Practice of Criticality Calculations with MCNP5**

    FY 2011: Hanford/PNNL, LANL, Y-12

    FY 2012: INL, PNNL/Hanford, ?

    Previous: Y-12, PNNL, INL, ANL, LLNL, SRL, LANL
  - **Introduction to MCNP5** – 4 classes/year at LANL
  - **Advanced Variance Reduction** – 1-2 classes/year at LANL
- **Conference Papers & Presentations**
  - PHYSOR 2010: Monte Carlo workshop
  - SNA+MC-2010: plenary talk + 3 papers (crit, perturb, parallel)
  - ANS Winter 2010: 1 paper (V&V for perturb)
  - M&C 2011: 1 paper (statistical tests)
  - ANS Summer 2011: 3 papers (stats, V&V, crit suite)
  - ICNC 2011: 6 papers (V&V,status,methods)
  - NS&E journal: paper on adjoint-weighted tallies
  - PNST Journal: 4 papers

User Support & Training (2)

- **MCNP Forum**
  - User-group – beginners & experts, ~1,000 members
  - Feedback, bug reports, guidance
- **Reference collection**
  - DVD with 1000+ MB of references on Monte Carlo & MCNP, ~600 items
  - Web browser based
  - All MCNP6, MCNP5, & previous MCNP code documentation
  - Criticality, V&V, adjoints, electrons, detectors, parallel, benchmarks, …..
  - Includes 8 half-day Monte Carlo workshops
- **University collaborations**
  - Michigan, New Mexico, Wisconsin, Oregon State, MIT, RPI
  - Summer students at LANL
- **Participated in ANS 10.7 Standards committee**

R&D Work in Progress (1)

Perturbation Theory

- **MCNP computes perturbations to k using two methods:**
  - **Differential operator/Taylor series**
  - **Adjoint-based** (new 2010, MCNP6)
    - Allows applications such as additions of impurities, cross-section library comparisons, & material substitutions that were not possible with differential operator
- **V&V efforts show:**
  - Good agreement when Δ*k*'s in same direction
  - When both are apply, methods are complementary (neither is always better)
  - Difficulties with scattering cross section perturbations observed

Continuous-Energy Sensitivity Coefficients

- **MCNP6 can produce sensitivity coefficients in continuous-energy**
  - Uses adjoint-weighted perturbation techniques
  - Verified against multigroup results
  - Good performance for capture and fission
- **Scattering needs improvements**
  - In theory need double-differential scattering cross sections
  - Approximate extensions with scattering laws should be straightforward
  - Exact is theoretically possible, but costly

R&D Work in Progress (2)

Boundary Sensitivity Coefficients

- **Boundary interface locations (e.g., radius of a sphere) can be uncertain**
- **Favorite showed theory of computing sensitivity coefficients to interface locations**
- **Should be extendable to continuous-energy Monte Carlo**
  - Necessarily uses "exact" method for scattering sensitivities
  - Work in progress, results to be presented

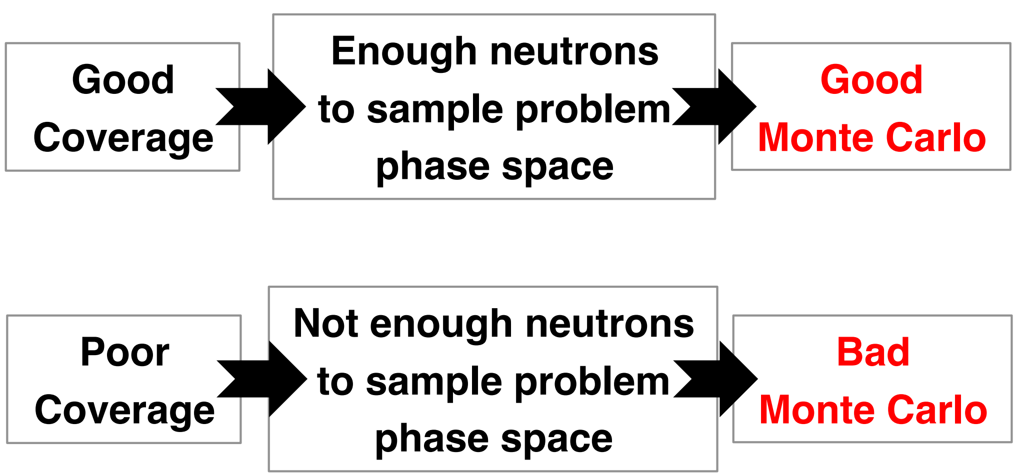
Reliability of Large Collections of Tallies

- **Criticality alarm design & accident assessment require global flux or dose fields**
  - High resolution, >100K mesh elements
  - Can results be trusted?
- **Some MCNP statistical checks extended**
  - Observe convergence of moments of relative variances
  - Minimal memory cost or compute time
  - Sensitive to large scores in a few mesh
    - Suggests undersampling of problem
- **Applications in criticality safety, reactor physics, shielding, etc.**

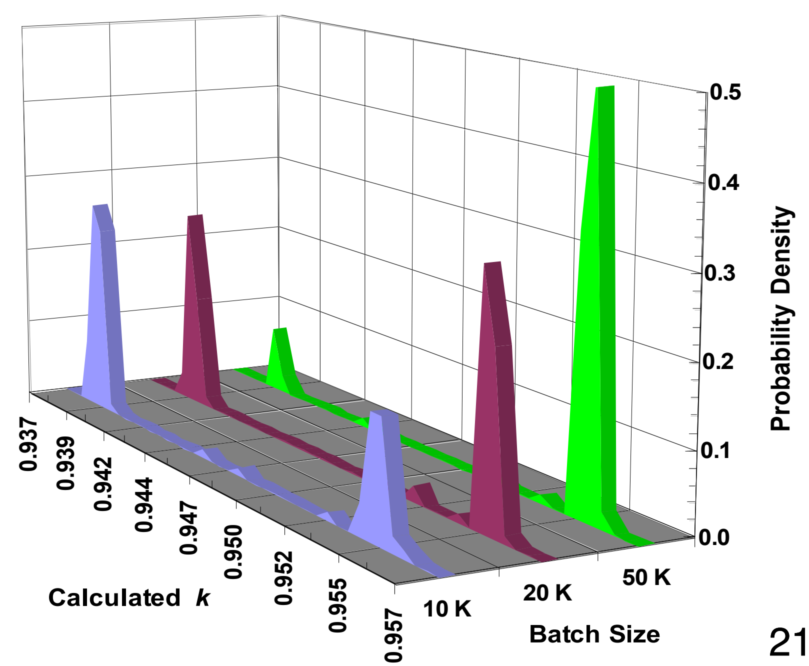
R&D Work in Progress (3)

Statistical Coverage

- **Implicit assumption in criticality calculations that all regions of problem are adequately covered**
  - Easy to satisfy for typical reactors
  - May be difficult for certain criticality safety problems
    - Multiple regions, loosely coupled
    - Some regions more/less reactive
    - Asymmetric coupling between regions



- **Revised k_{eff} of the World problem**
  - 9x9x9 array of Pu spheres in water
  - Central sphere larger, cadmium coated
  - Loose, asymmetric coupling
- **Results of 100 independent trials:**
  - Starting guess uniform in all spheres
  - keff and H_{src} always converged
  - 10K particles per cycle:
    - 60% chance of **getting wrong k**



R&D Work in Progress (4)

Monte Carlo Codes
XCP-3, LANL

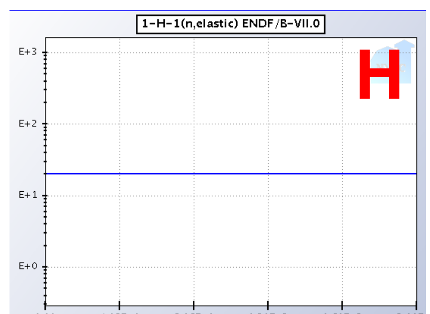
Continuous S(α, β) Scattering For Thermal Neutrons

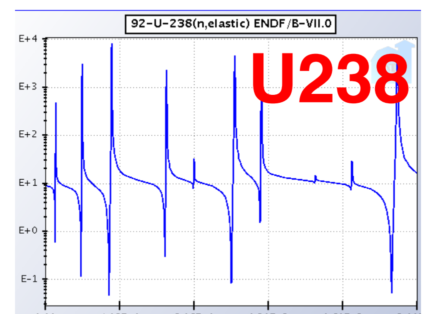
- **S(α, β) thermal neutron scattering**
  - Accounts for temperature, chemical-, & molecular-binding on collision physics
  - Traditional NJOY-MCNP uses discrete energy-angle data, gives ray effects for problems with only a few scatters
- **Continuous S(α, β) treatment**
  - Developed by MacFarlane in early 2000s
  - Implemented in MCNP5-1.51 & 1.60
  - Never adequately verified/validated
- **Recent V&V effort**
  - A. Pavlou (U.Mich), 2011
  - Thorough V&V with ICSBEP benchmarks
  - Conclusion: valid for use in crit-safety
  - Continuous S(α, β) data to be included with MCNP ENDF/B-VII.1 data libraries

Free-gas Resonance Scattering For Epithermal Neutrons

- **Free-gas scattering model**
  - For neutrons with energies of a few eV to a few 100 eV, used to account for target nuclide thermal motion
  - Traditional: assume constant $\sigma_{scatter}$
- **Resonance scatter can be important for free-gas model**

sig-scatter, 1 eV – 200 eV





- **MCNP mods to include resonance scattering in free-gas model**

R&D Work in Progress (5)

Monte Carlo Codes
XCP-3, LANL

On-The-Fly Doppler Broadening

- **US DOE NEUP project with Univ. Michigan, ANL, LANL (2011-2012)**
  - W.R. Martin & students (U.Mich)
  - G. Yesilyurt (ANL)
  - F.B. Brown (LANL)
- **Provide general temperature treatment for MCNP**
  - OTF Doppler broadening
  - OTF interpolation for S(a,b) thermal
  - OTF interpolation for unresolved resonance probability tables
  - Provides continuous termperature capability, without precomputing thousands of cross-section datasets

CMFD & Fission Matrix Convergence Acceleration

- **Hybrid methods to improve convergence of fission source distribution for criticality**
  - Use low-order deterministic method to accelerate global convergence of MC source distribution
  - Parameters for low-order solution obtained from accurate MC
- **CMFD / MC**
  - Coarse-Mesh Finite Difference method used for low-order
  - Low-order solutions used to bias source sampling in MCNP
- **Fission matrix**
  - Computed directly during MC
  - Fission matrix eigenvector used to bias source sampling in MCNP

R&D Work in Progress (6)

Improvements to Parallel MPI & Threading

- **For criticality calculations**
  - Reduce the amount of data exchanged at MPI rendezvous
- **MPI improvements**
  - Automatic chunking of large transfers
  - Convert from buffered MPI message arrays to in-place
  - Asynchronous MPI messages
  - Improve Fortran/C interface
- **OpenMP threading improvements**
  - Replace private thread-safe storage for certain large arrays by OpenMP critical section
  - Use OpenMP atomic operations with shared tally arrays

Parallel MC for Exascale Computers

- **Exascale computers are coming**
  - Millions of cpu cores
  - Reduced memory/cpu-core
- **Need new parallel approach**

Parallel on particles

+

Distributed data

- Particles distributed among nodes
- Fetch data remotely from other nodes as needed by particles (do not move particles to data)
- Eliminate synchronization & particle motion among compute nodes

Future Release Plans

- MCNP6 = MCNP5 + MCNPX merger
- Impact on Criticality Calculations → none
  - All KCODE criticality features same as for MCNP5
  - Matches results with MCNP5 for criticality suites
- Monte Carlo team will support MCNP6,
  no new features or releases of MCNP5 or MCNPX
- MCNP6 is coming
  - Beta-0 release: 1Q CY 2011 – very limited distribution
  - Beta-1 release: 4Q CY 2011 – general beta testing
  - Production release: CY 2012 – RSICC release

We need to plan for MCNP5 → MCNP6 transition over the next few years

Questions ?