

MCNPX Models and Applications Hadronic Shower Simulation Workshop

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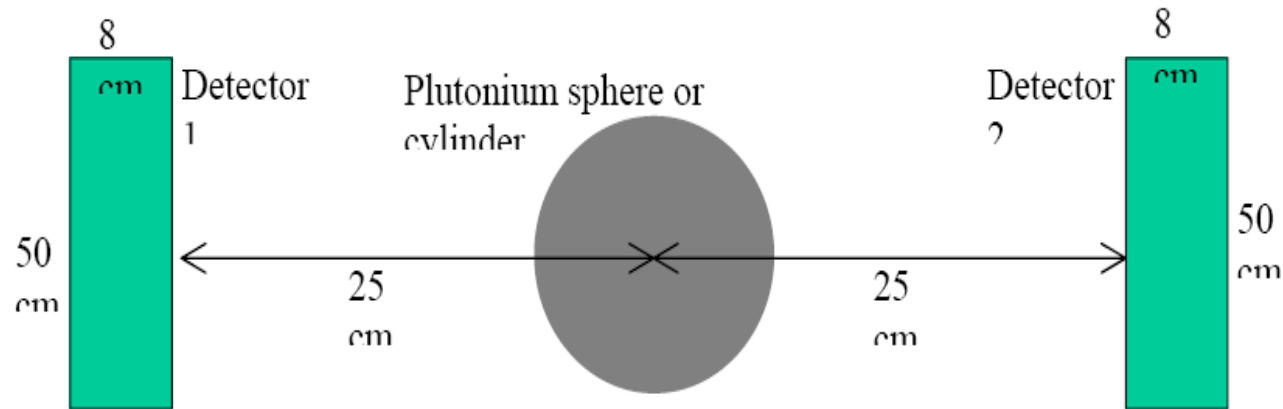
Oak Ridge, TN

HSSW, FNAL, September 6-8, 2006

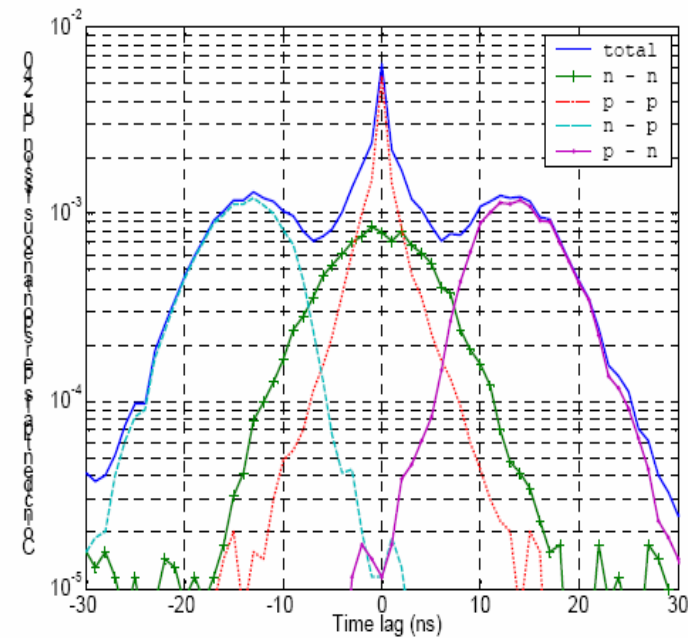
Where MCNPX is very strong

- Neutronics (table-based)
 - Inherent difficulty with correlations (ORNL Polimi patch – need analog processes)
 - Charged particle emission – some hardwired in. $n(\text{He-3},h)t$, $n(\text{He-3},d)d$, $n(\text{Li-6},t)a$, $n(\text{B-10},g)a$
- Criticality
- Transmutation
 - Burnup (Currently KCODE. Fixed source problem is difficult.)
 - Enables delayed particle production, gamma and neutron.
- Variance Reduction
 - Next-event-estimators
- Statistical Convergence Checks (Figure of Merit = $1/(T\sigma^2)$)
 - 10 separate checks (not just the standard deviation)
- Ease of Use
 - Don't have to code anything
 - All standard shapes + torus, lattices, repeated structures, basically no limit on geometry. (no formally released magnetic fields)
 - 2 Commercial GUIs
- Quality Assurance, Security, Support
- Extension outside of traditional neutronics arena
 - 30 particles, 4 light ions, all heavy ions
 - Models in addition to libraries (solves the correlation problem)

MCNP-PoliMi



Sara A. Pozzi, Enrico Padovani, John T. Mihalczo, "MCNP-POLIMI Evaluation of Time Dependent Coincidence Between Detectors for Fissile Metal Vs. Oxide Determination", BWXT Y-12 Report No: Y/LB-16,131



Tallies

- F1 - Current = W_i
- F2 - Surface Flux = $W/(|\mu|*A)$
- F4 - Flux = $W*\lambda/V$
- F5 – Detector Fluence = $W*p(\mu)*\exp(-s)/2\pi R^2$
- F6 – Energy Deposition – $W*\lambda*\sigma_T(E)*H(E)*\rho_a/m$
 - +F6, mean to be used in model region,
adds dE/dx + recoil + cufoff energies
- F7 – Fission Energy Deposition – $W*\lambda*\sigma_F(E)*Q*\rho_a/m$
- F8 – Pulse Height – W_s in bin $E_d * W/W_s$
 - Pulse height light coincidence tally

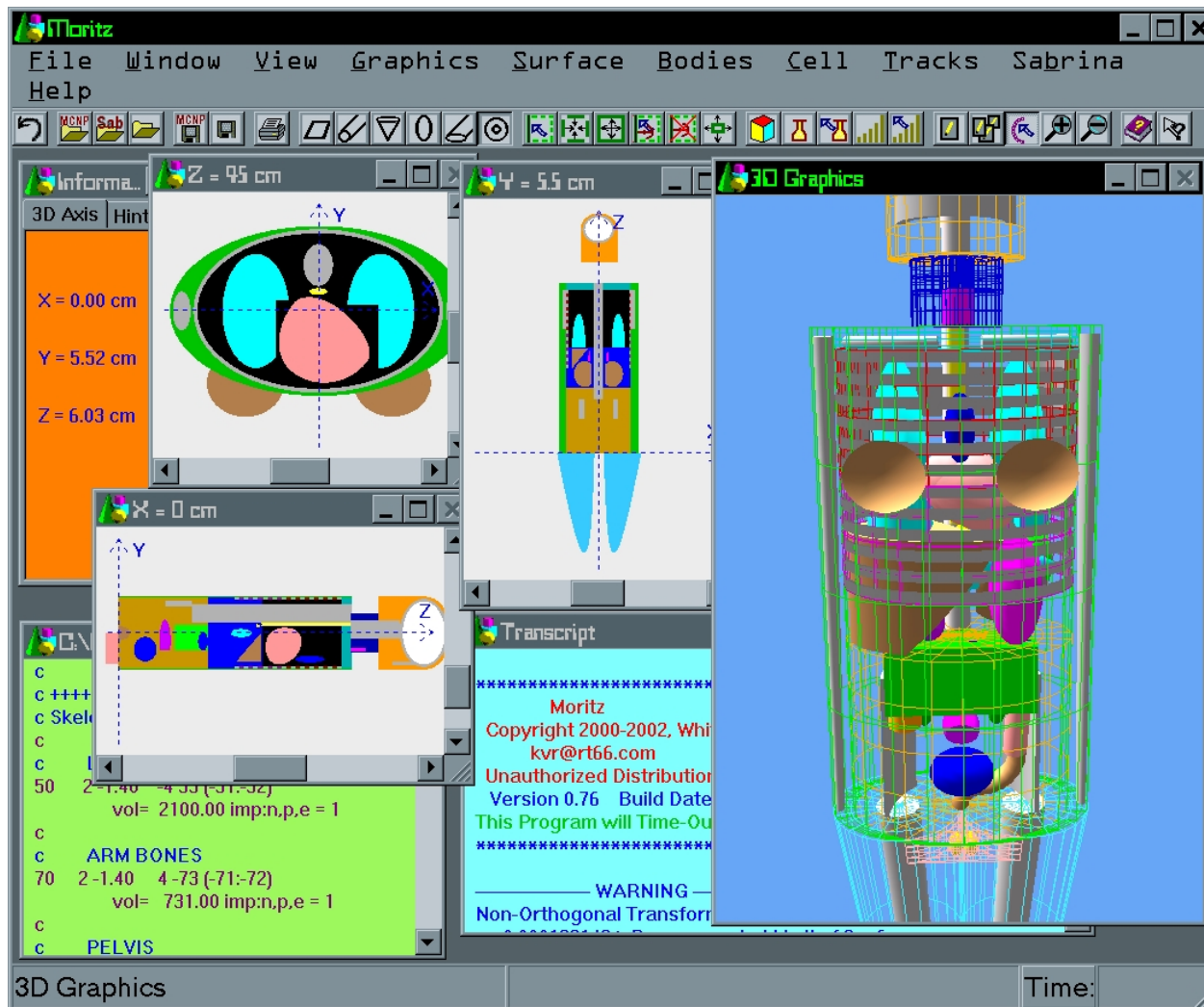
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UNCLASSIFIED



Moritz



MCNPX Particle and Energy Acceptance

MCNPX Code Acceptance								
	Photons	Electrons	Neutrons	Protons	Photonuclear	Other single μ Π K ν , etc	Light Ions d t s a	Heavy Ions
1 TeV			Quantum Models			Models		
1 GeV			Mixing					
1 MeV			Models INC, Pre-equilibrium, Evaporation models Tables or Models					
1 keV			Tables				In progress	
1 eV								
Thermal								

Selecting Tables or Models in MCNPX

mode n h p d t s a

m1 1001 1 1002 1 1003 1 6012 1 20040 1 nlib .24c

mx1:n j model j 6000 20000

mx1:h j model 1001 j j

mx1:p 0 6012 0 j j

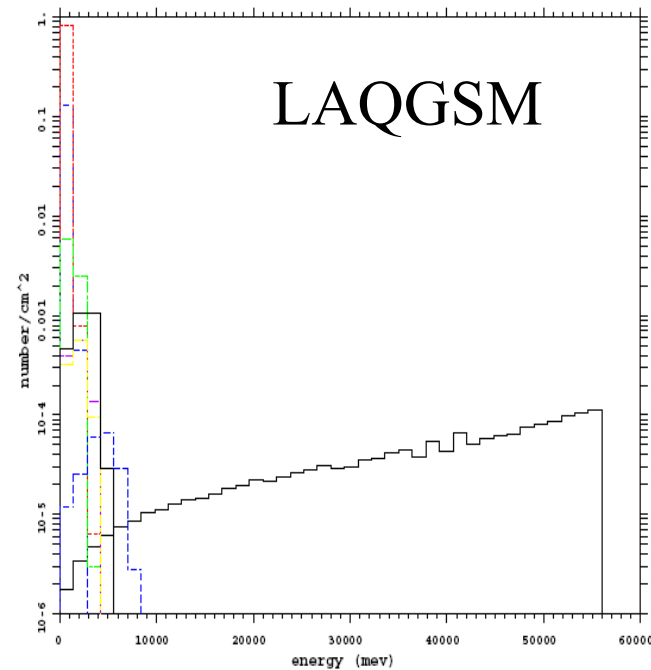
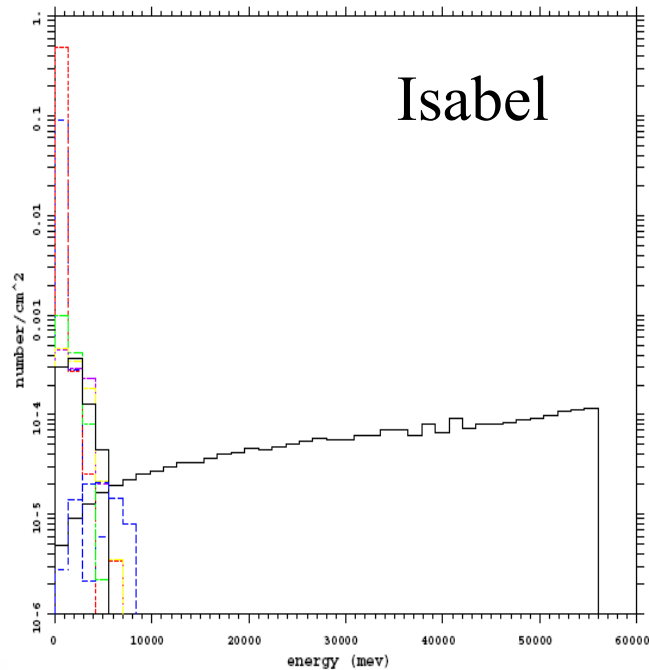
Heavy Ions

mode #

SDEF par=# or par=6012

F1:# 4

FT1 ZAD 8016 20040 26000 92238



Charged Particle Transport (not electrons)

- Energy Loss
 - Bethe -Bloch
 - The ionization potentials have been enhanced to the values and interpolation procedures recommended in ICRU Report 37 (ICR84), bringing the model into closer ICRU compliance.
 - The density effect correction now uses the parameterization of Sternheimer and Peierls (STE71).
 - For high-energy protons and other light charged projectiles, the approximate SPAR model (ARM73) has been replaced with a full implementation of the maximum kinetic energy transfer.
 - For intermediate energies, the shell corrections to the stopping power have been adapted from Janni (JAN82).
 - A continuous transition in the stopping power between the ranges 1.31 MeV/AMU (Atomic Mass Unit) for the high-energy model, and 5.24 MeV/AMU (the low energy SPAR model) is achieved with a linear interpolation between the two models.
 - No very very low (Lindhard-Scharff or Anderson-Ziegler) model is included.
 - Student has started this.

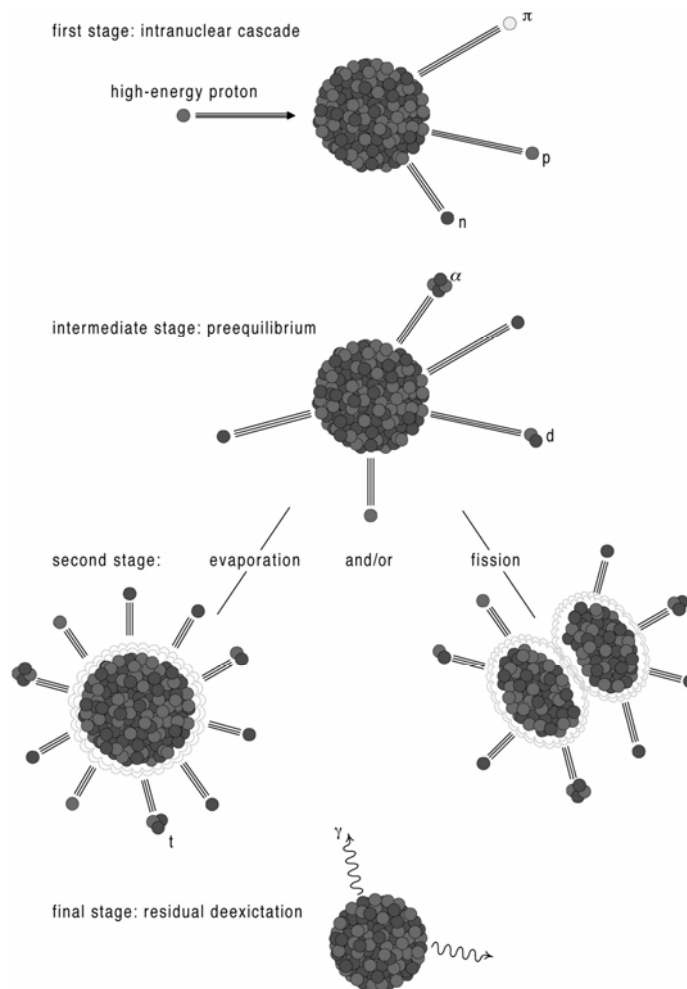
Charged Particle Transport (not electrons)

- Small angle Coulomb Scattering
 - Rossi-Greisen scattering algorithm (Rossi, B. & Griesen, K., “Cosmic-Ray Theory”, Rev. Mod Phys 13, Oct 1941 pp 262-268)
 - Overpredicts large angle, high-Z Coulomb scattering
 - MCNPX does not yet accommodate transverse displacements in charged-particle substeps

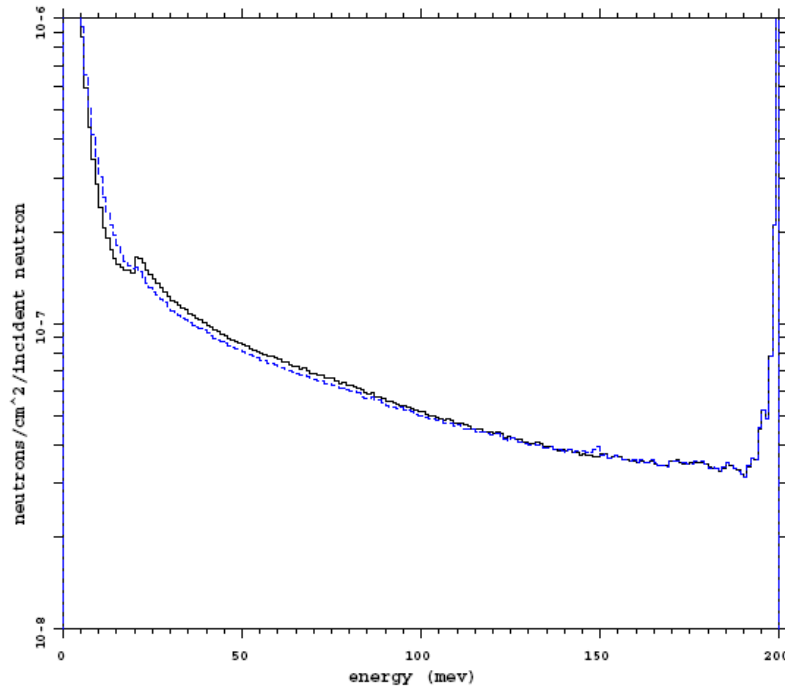
Charged Particle Transport (not electrons)

- Energy Straggling
 - At low energies and large step sizes, the Vavilov distribution approaches a Gaussian.
 - At very high energies, or small step sizes (and for electrons in almost all circumstances), the Vavilov distribution approaches a Landau distribution.
 - The module implemented in MCNPX to represent the Vavilov model does not currently account for the Gaussian and Landau limits
 - Updated logic applies the Vavilov algorithm to each substep and to each partial substep, and makes a better estimate of the continuous-slowng-down energy loss (mean energy loss) across energy-group boundaries.

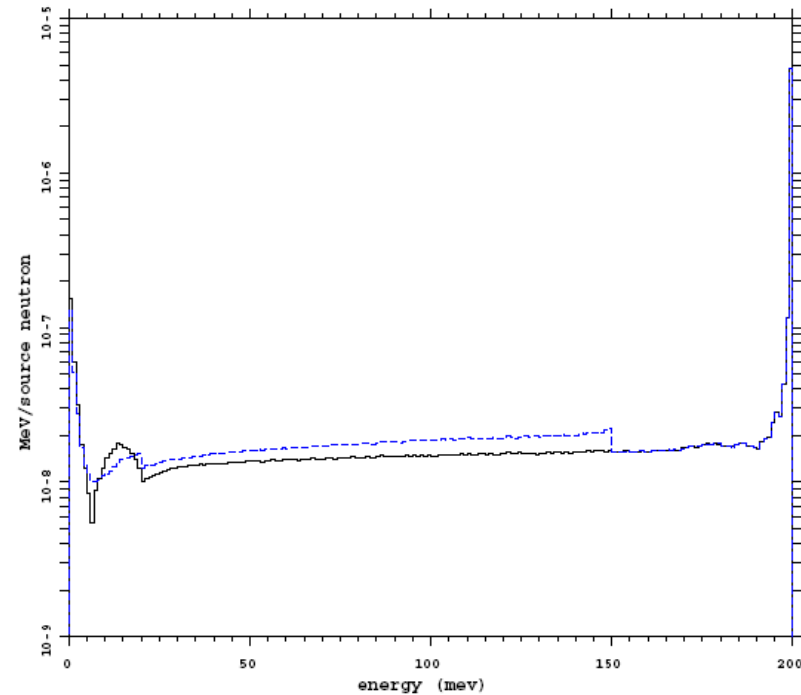
Model Choices in MCNPX



Matching Tables and Models



Neutrons in aluminum, flux



Neutrons in aluminum, energy deposition

Black- 20 MeV library, Blue, 150 MeV library

Physics Process	Bertini	ISABEL	CEM2k	INCL4
Monte Carlo Technique	“spacelike”	“timelike”	“spacelike”	“spacelike”
Intranuclear Cascade Model	Bertini	Isabel INC	Improved Dubna INC	Liège INC
Nuclear Density Distribution	$\rho(r) = \rho_0 / \{\exp[(r-c)/a] + 1\}$ $c = 1.07A^{1/3} \text{ fm}$ $a = 0.545 \text{ fm}$ $\rho(r) = \alpha_i \rho(0); i=1, \dots, 3$ $\alpha_1=0.9$ $\alpha_2=0.2$ $\alpha_3=0.01$	$\rho(r) = \rho_0 / \{\exp[(r-c)/a] + 1\}$ $c = 1.07A^{1/3} \text{ fm}$ $a = 0.545 \text{ fm}$ $\rho(r) = \alpha_i \rho(0); i=1, \dots, 16$	$\rho(r) = \rho_0 / \{\exp[(r-c)/a] + 1\}$ $c = 1.07A^{1/3} \text{ fm}$ $a = 0.545 \text{ fm}$ $\rho_n(r)/\rho_p(r) = N/Z$ $\rho(r) = \alpha_i \rho(0); i=1, \dots, 7$ $\alpha_1=0.95, \alpha_2=0.8, \alpha_3=0.5,$ $\alpha_4=0.2, \alpha_5=0.1, \alpha_6=0.05,$ $\alpha_7=0.01$	$\rho(r) = \rho_0 \{\exp[(r-R_0)/a] + 1\}$ $R_{\max} = R_0 + 8a$ $R = (2.745E-4 A_T + 1.063) A_T^{1/3} \text{ fm}$ $a = 0.510 + 1.63E-4 * A_T$ fm $r\text{-}p \text{ correlations}$ $R(0)=0 \text{ and } R(p_F)=R_{\max}$ diffuse surface
Nucleon Potential	$V_N = T_F + B_N$	Nucleon kinetic energy (T_N) dependent potential $V_N = V_i(1 - T_n/T_{\max})$	$V_N = T_F + B_N$	$V_0 = 45 \text{ MeV}$
Pion Potential	$V_\pi = V_N$	$V_\pi = 0$	$V_\pi = 25 \text{ MeV}$	

Physics Process	Bertini	ISABEL	CEM2k	INCL4
Mean Nucleon Binding Energy	$B_N = 7 \text{ MeV}$	Initial B_N from mass table; the same value is used throughout the calculation	$B_N = 7 \text{ MeV}$	
Elementary Cross Sections	Standard Bertini INC (old)	Standard ISABEL (old)	New CEM97, last update March 1999	
Pauli Blocking				Statistical blocking factors
Light and Heavy ion sources	Not considered	All allowed	Not considered	Light ions
γA interactions	Not considered	Not Considered	Allowed	Not considered
Condition for passing from the INC stage to evaporation	Cutoff energy $\sim 7 \text{ MeV}$	Different cutoff energies for p and n, as in VEGAS code	$P = W_{\text{mod}} - W_{\text{exp}} / W_{\text{exp}}$ $P = 0.3$	$t_{\text{stop}} = f_{\text{stop}} t_0 \left(\frac{A_T}{208} \right)^{0.16}$ $f_{\text{stop}} = 1$
Nuclear Density Depletion	Not considered	considered	Not considered	Collisions forbidden between spectators

Physics Process	Bertini	ISABEL	CEM2k	INCL
Pre-equilibrium stage	MPM (LAHET) model	MPM (LAHET) model	Improved MPM (CEM97)	
Evaporation Model	Dresner model for n, p, d, t, ^3He , α emission (+ fission) (+ γ emission) (note, 19 particle emission is possible but not implemented)	Dresner model for n, p, d, t, ^3He , α emission (+ fission) (+ γ emission)	CEM97 model for n, p, d, t, ^3He , α emission (+ fission) (+ γ emission)	ABLA Weisskopf-Ewing model
Fission	ORNL RAL ($Z \geq 71$)	ORNL RAL ($Z \geq 71$)		Refined fragment mass distribution function, friction through fission delay recipe
Level Density	$1/D = C e^{2(aE)^{.5}}$ Ignatyuk model Julich model HETC model	$1/D = C e^{2(aE)^{.5}}$ Ignatyuk model Julich model HETC model	CEM97 models for $A = a(Z, N, E^*)$	
Multifragmentation of light nuclei	Fermi Breakup for $A < 17$. Only 2- and 3-body breakup channels considered. (could go up to 7-body breakup)	Fermi Breakup for $A < 17$	Fermi Breakup for $A < 17$	

INCL4 Transition time from INC to Evaporation

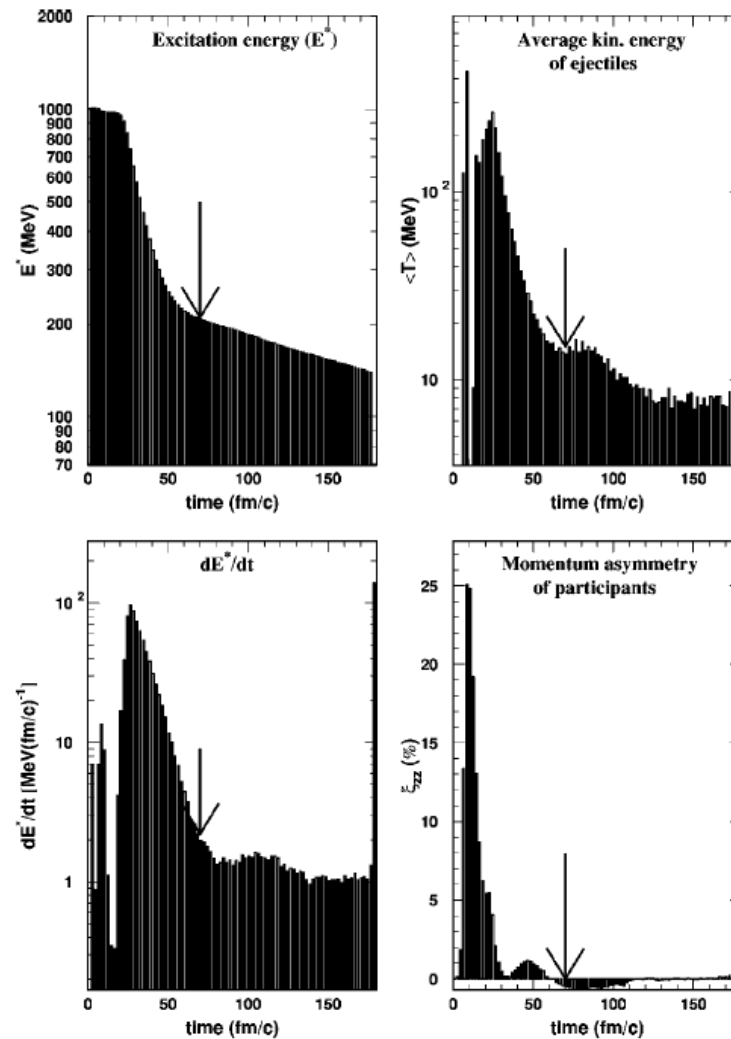
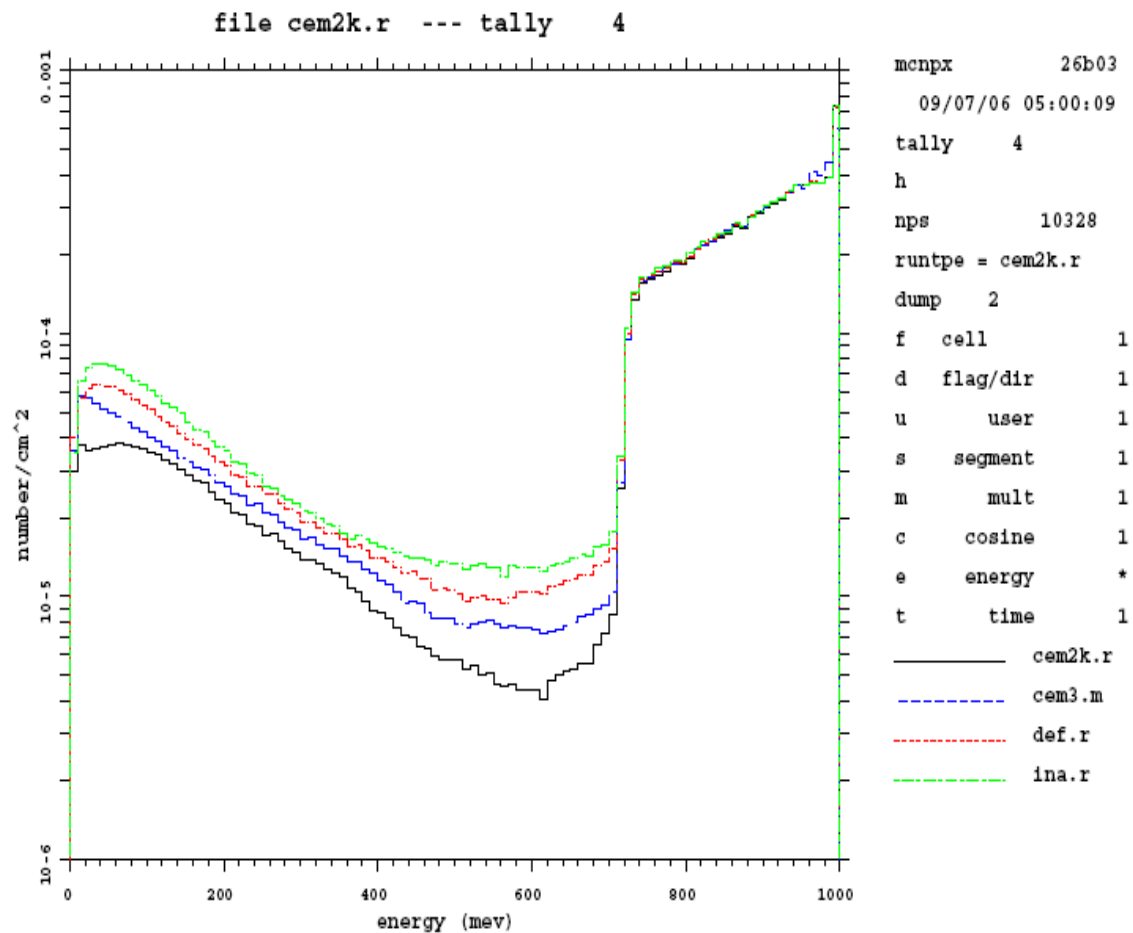
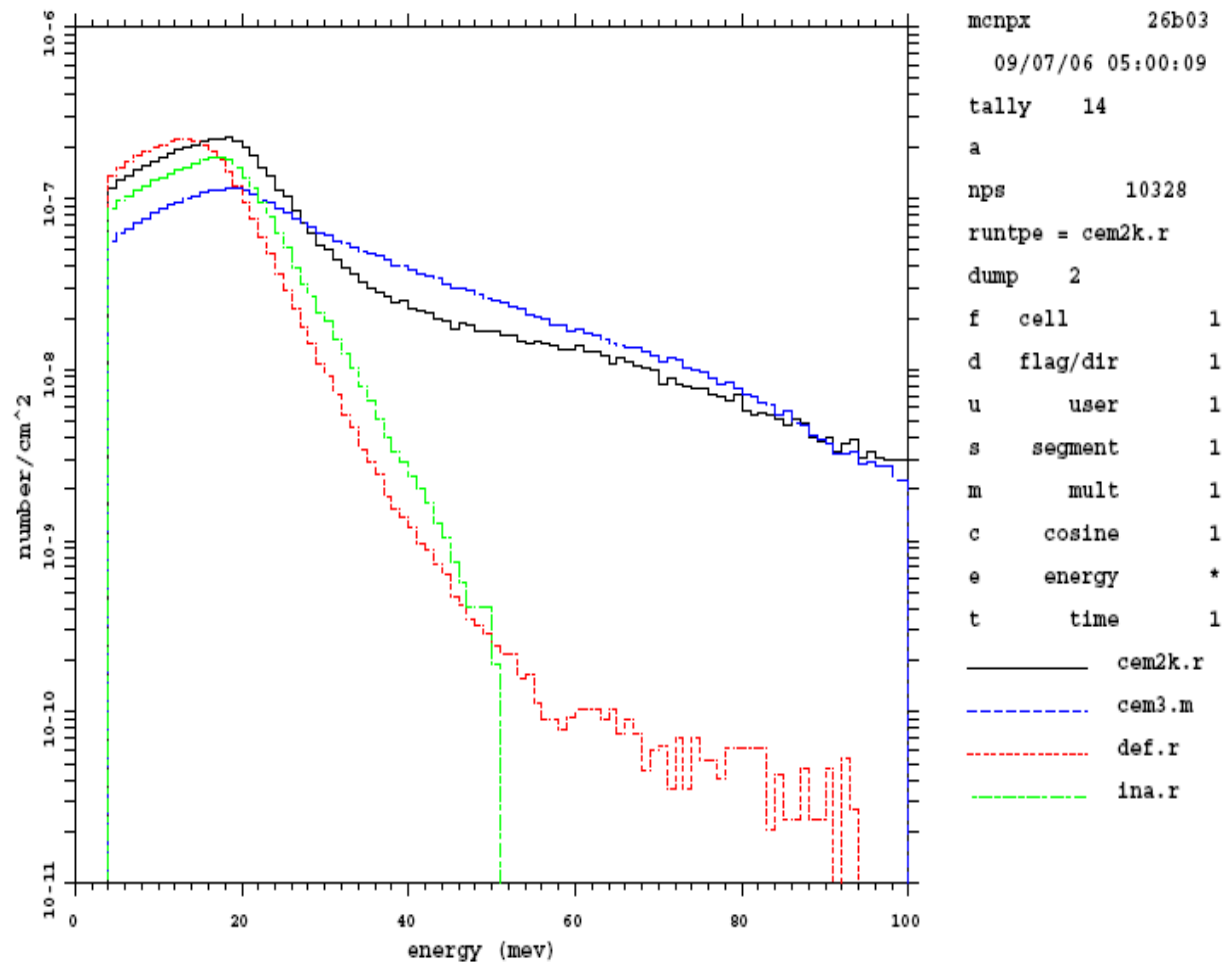


FIG. 2. Time variation of the average value of a few physical quantities, within our INC model. The panels refer, in a clockwise order, starting from the upper left, to the excitation energy, the average kinetic energy of the ejectiles, the asymmetry of the participant momentum distribution, and the time derivative of the excitation energy, respectively. The results correspond to collisions of 1-GeV protons with Pb nuclei with an impact parameter of 4 fm. The arrows indicate the chosen stopping time.

Protons (1 GeV h + 20 cm cylinder of 208Pb)



Alphas (1 GeV h + 20 cm cylinder of 208Pb)



p + Pb and p + Zr, 800 MeV

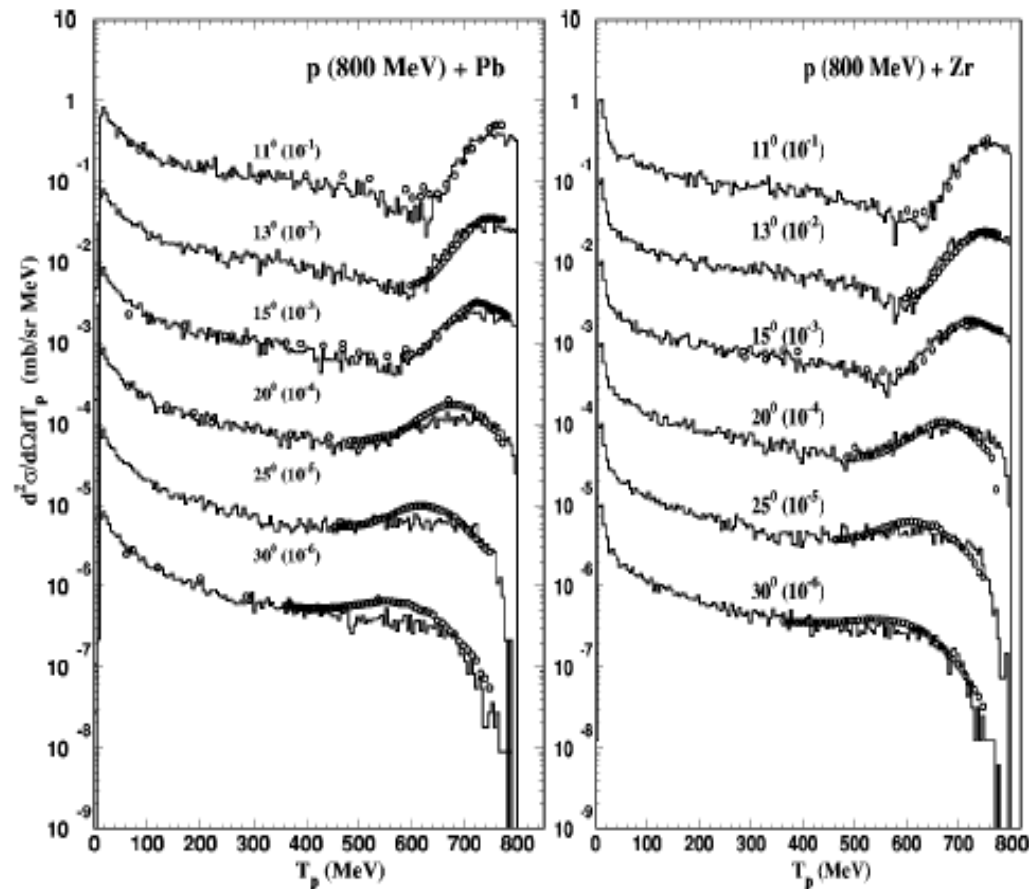
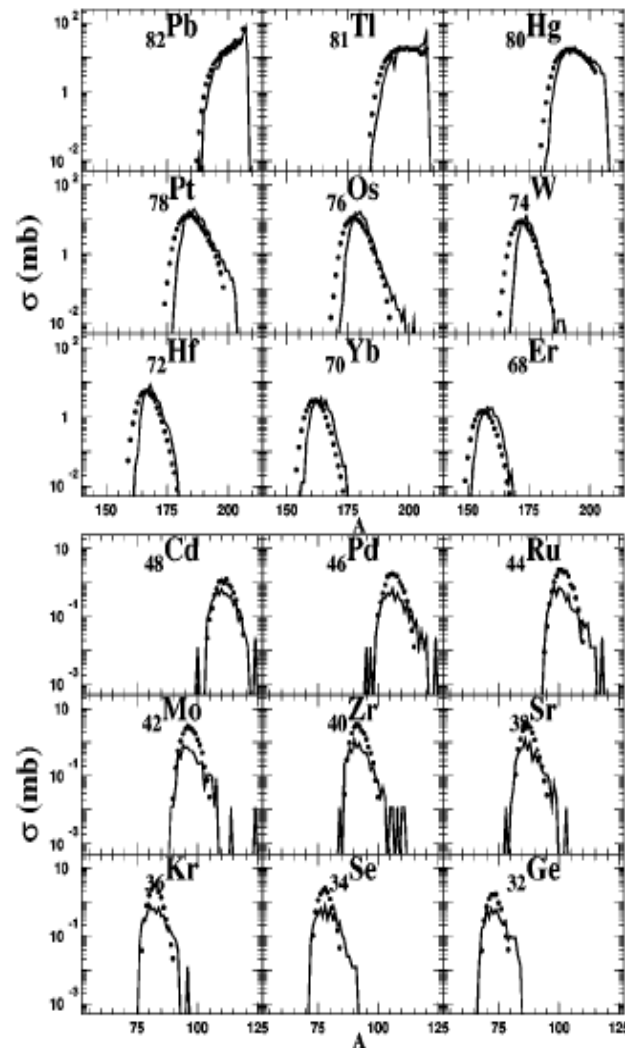


FIG. 12. Proton double differential cross sections for proton-induced reactions on a Pb target (left panel) and on a Zr target (right panel) at 800 MeV incident energy. The predictions of the INCL4+KHSv3p model are given by the histograms. Data (circles) are from Refs. [52,53].

INCL/ABLA Pb + p fragments 1 GeV/n



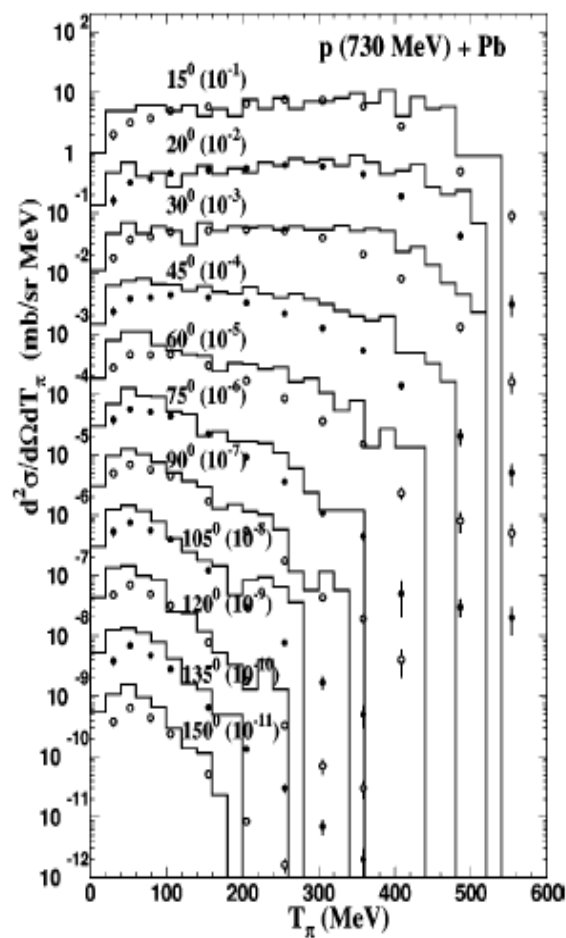
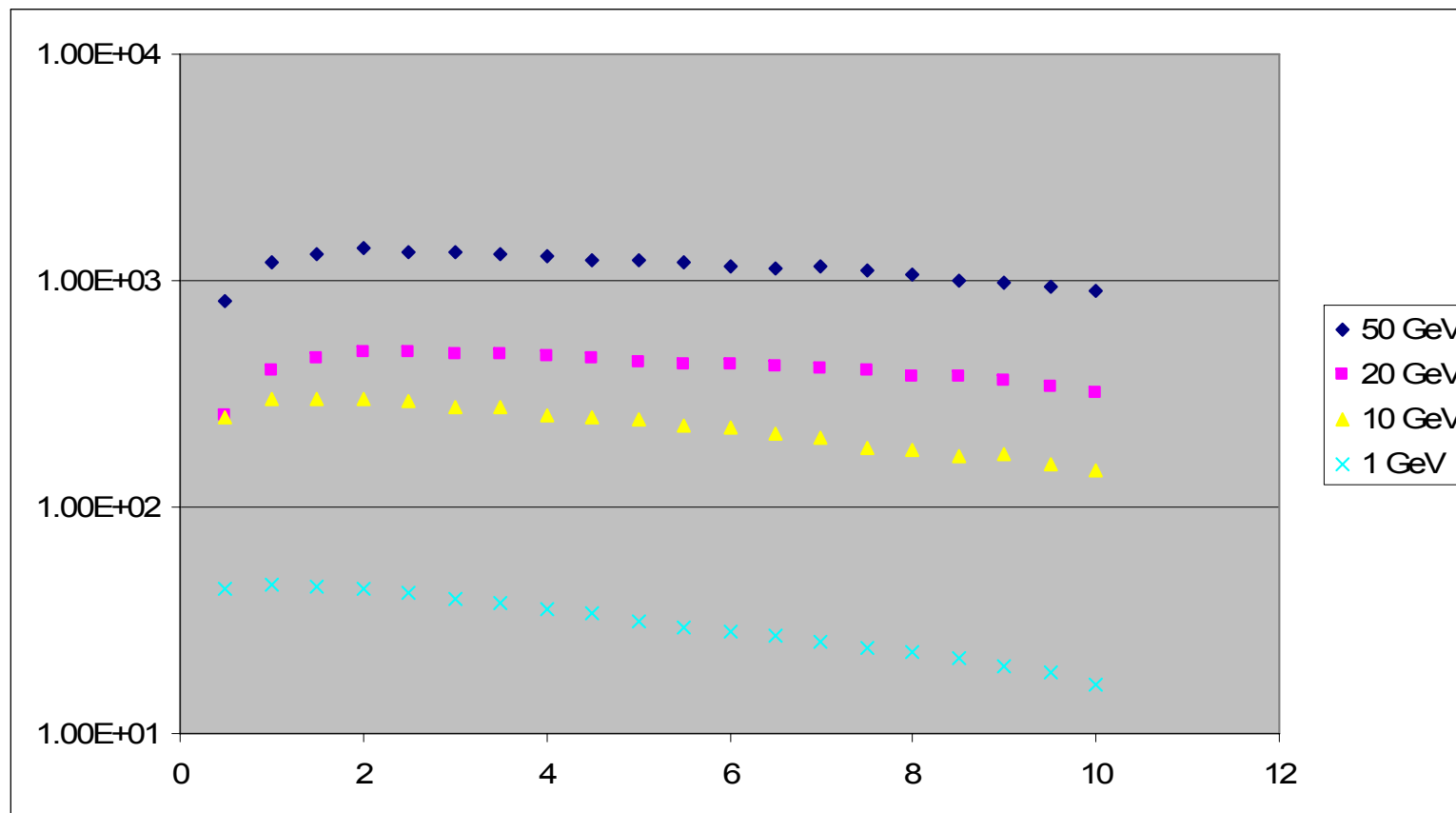


FIG. 13. Positive pion double differential cross sections for proton-induced reactions on a Pb target at 730 MeV incident energy. The predictions of the INCL4+KHSv3p model are given by the histograms. Data (circles) are from Ref. [54].

TABLE II. Neutron multiplicities, obtained by integration of the experimental double differential cross sections in proton-induced reactions on Pb nuclei (second column), compared with the predictions of our model (third column) and those from other models. See Sec. VI for more details. Note that ISABEL cannot be run in LAHET above 1 GeV.

Energy	Expt.	INCL4 KHSv3p	TIERCE Cugnon	LAHET Bertini	LAHET ISABEL	LAHET Bertini-preq
Pb $T_{lab}=800$ MeV						
0–2 MeV		3.3	4.9	5.61	5.13	5.37
2–20 MeV	6.5 ± 1.0	6.8	6.9	8.63	6.63	7.12
20 MeV- E_{max}	1.9 ± 0.2	2.5	2.2	1.75	1.92	2.13
Total		12.5	14.0	16.0	13.7	14.4
Pb $T_{lab}=1200$ MeV						
0–2 MeV		3.4	5.8	6.35		6.02
2–20 MeV	8.3 ± 1.0	8.1	8.9	11.44		9.86
20 MeV- E_{max}	2.7 ± 0.3	3.1	2.8	2.45		2.83
Total		14.7	17.4	20.2		18.7

Benchmark Task 7



Input file for Task 7

task 7 energy dep profile in a thick target for proton beam

```
1 1 -19.3 -1 u=1
2 0      1 u=1
3 0     -2 lat=1 fill=1 u=2
4 0     -3 fill=2
5 0      3 -4
6 0      4
```

```
1 rcc 0 0 0 0 0 .5 1
2 rpp -2 2 -2 2 0 .5
3 rcc 0 0 0 0 0 10 2
4 so 100.0
```

mode n p h d t s a | / z k l + -

Imp:n 1 1 1 1 1 0

phys:n 1000.0

phys:p 1000.0 j j 5

phys:h 1000.0

lca 8j 1

sdef x=0 y=0 z=-10 vec 0 0 1 dir 1 par=h erg=1000.

m1 74180 .12 74182 26.3 74183 14.28 74184 30.7 74186 28.6

```
+f6 (1<3[0 0 0]<4) (1<3[0 0 1]<4) (1<3[0 0 2]<4) (1<3[0 0 3]<4)
      (1<3[0 0 4]<4) (1<3[0 0 5]<4) (1<3[0 0 6]<4) (1<3[0 0 7]<4)
      (1<3[0 0 8]<4) (1<3[0 0 9]<4) (1<3[0 0 10]<4) (1<3[0 0 11]<4)
      (1<3[0 0 12]<4) (1<3[0 0 13]<4) (1<3[0 0 14]<4) (1<3[0 0 15]<4)
      (1<3[0 0 16]<4) (1<3[0 0 17]<4) (1<3[0 0 18]<4) (1<3[0 0 19]<4) T
```

MCNPX Applications

- Reactors
 - Materials damage
 - Criticality and burnup
 - ASCI, GNEP
- Intermediate Energy Accelerators
 - APT, SNS

MCNPX Applications

- Medical
 - Design of proton therapy facilities
 - Heavy ions
- Space
 - Space power reactors
 - Cosmic ray shielding
 - Cosmic ray backgrounds, SEE
 - Cosmochemistry
- Threat Reduction
 - Active Interrogation
 - Detector design and performance, espec. neutrons
 - Signal backgrounds
 - Nonproliferation
 - Wide variety of applications