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Title: Recent Developments for MCNP6

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Recent Developments for MCNP6

Avneet Sood

(on behalf of MCNP(X) Teams)

JOWOG 6

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Abstract

Recent Development for MCNP6

MCNP5 is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree elliptical tori. Pointwise cross-section data are used.

MCNPX Extends MCNP4C to virtually 34 particles (n,p,e, 5 leptons, 11 baryons, 11 mesons, 4 LI) and energies roughly from 0-100 GeV. MCNPX uses data libraries below ~ 150 MeV (n,p,e,h) and theoretical models otherwise

This presentation reviews some recent features in MCNP5 and MCNPX and gives an overview of the effort to merge both codes.

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This presentation composed with contributions from both MCNP(X) teams

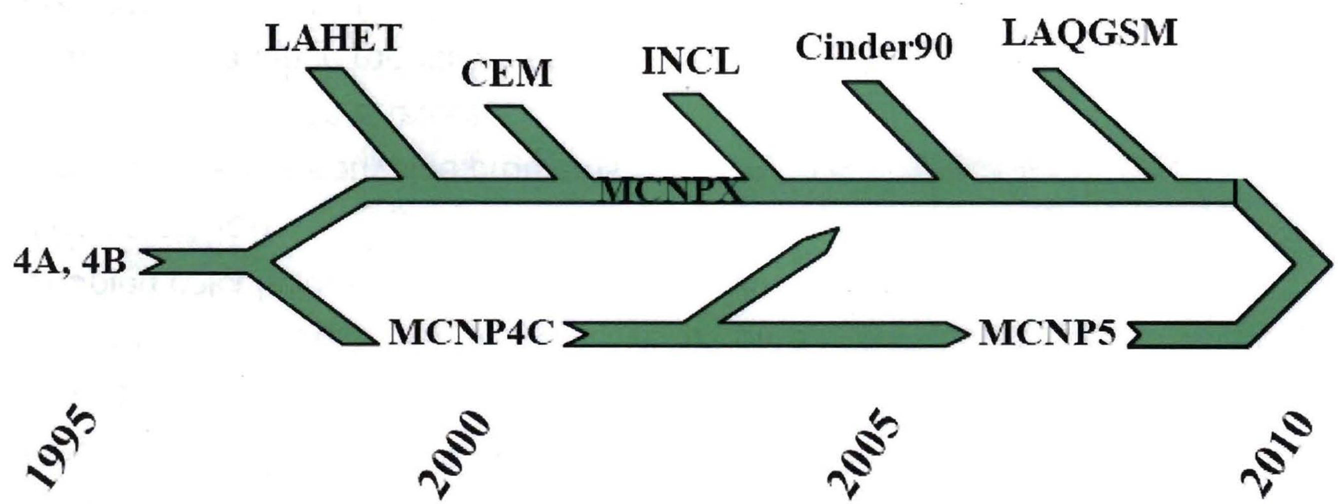
MCNP5

MCNP Overview

Simulate neutron, photon, & electron transport using the Monte Carlo method

- Particles
  - Neutrons, n: 10^{-5} eV - 150 MeV
  - Photons, p: 1 KeV - 100 GeV
  - Electrons, e: 1 KeV - 1 GeV
- Problem modes
  - Single particle type: n, p, or e
  - Coupled calculations: n/p, n/p/e, p/e, e/p
- Many code options
  - Fixed source & eigenvalue problems
  - Generalized source & tallies
  - Numerous variance reduction techniques
  - Forward or multigroup adjoint solutions
  - Time dependent

MCNPX



- Monte Carlo radiation transport code:
  - Extends MCNP4C to virtually all particles and energies
  - 34 particles (n,p,e, 5 leptons, 11 baryons, 11 mesons, 4 LI)
  - Continuous energy (roughly 0-100 GeV)
  - Data libraries below ~ 150 MeV (n,p,e,h) & models otherwise

Applications of MCNP(X)

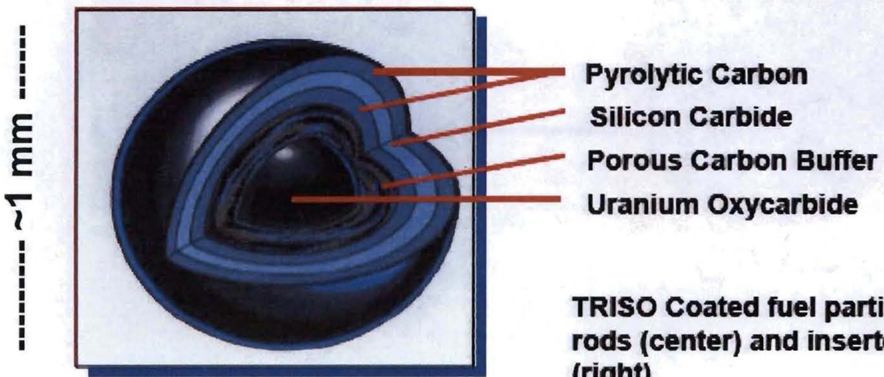
Application	# Groups	Percent
Medical (BNCT, proton therapy, etc.)	50	15
Spacecraft, Cosmic Rays, SEE, propulsion	42	12
Detectors, experiments, Threat Reduction	39	11
ATW, ADS, Energy Amplifiers	37	11
Fuel cycles, beginning to end, including storage	32	9
Accelerator Shielding and Health Physics	28	8
Theoretical Physics	23	7
Neutron Production for Scattering	21	6
Isotope Production	14	4
Radiography	12	4
MCNPX/MCNP code development	11	3
Homeland Security	10	3
Materials studies (IFMIF)	6	2
Radioactive Ion Beams	5	1
Irradiation Facilities	4	1
Neutrino Targets	4	1
Light Sources, electron machines	3	1

New Features in MCNP5 1.40

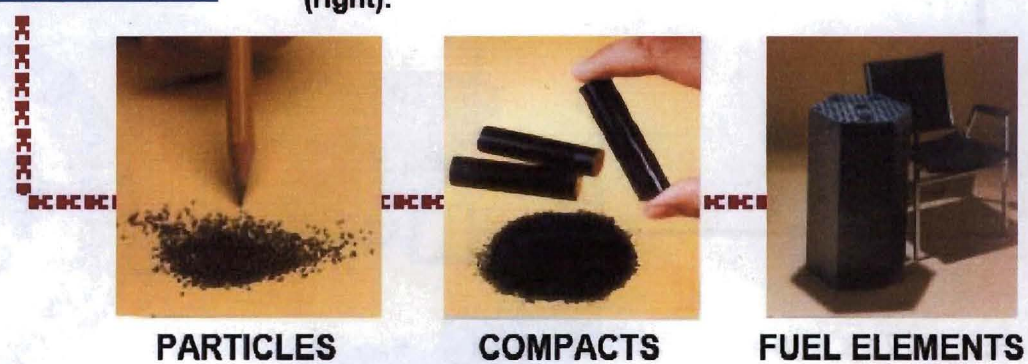
- **RSICC released MCNP5 1.40 in Winter 2006.**
- **MCNP5 1.40 includes these improvements over the previous version [1.30]**
  - Lethargy plots for energy dependent tallies
  - Logarithmic interpolation for input data
  - Fission neutron multiplicity
  - Stochastic geometry
  - Source entropy with plots
  - Mesh tally plotter
  - New electron energy-loss straggling logic
  - Source particle type specification
  - Positron sources

  - Minor code improvements
  - Numerous bugfixes

Example - Very High Temperature Gas Cooled Reactor

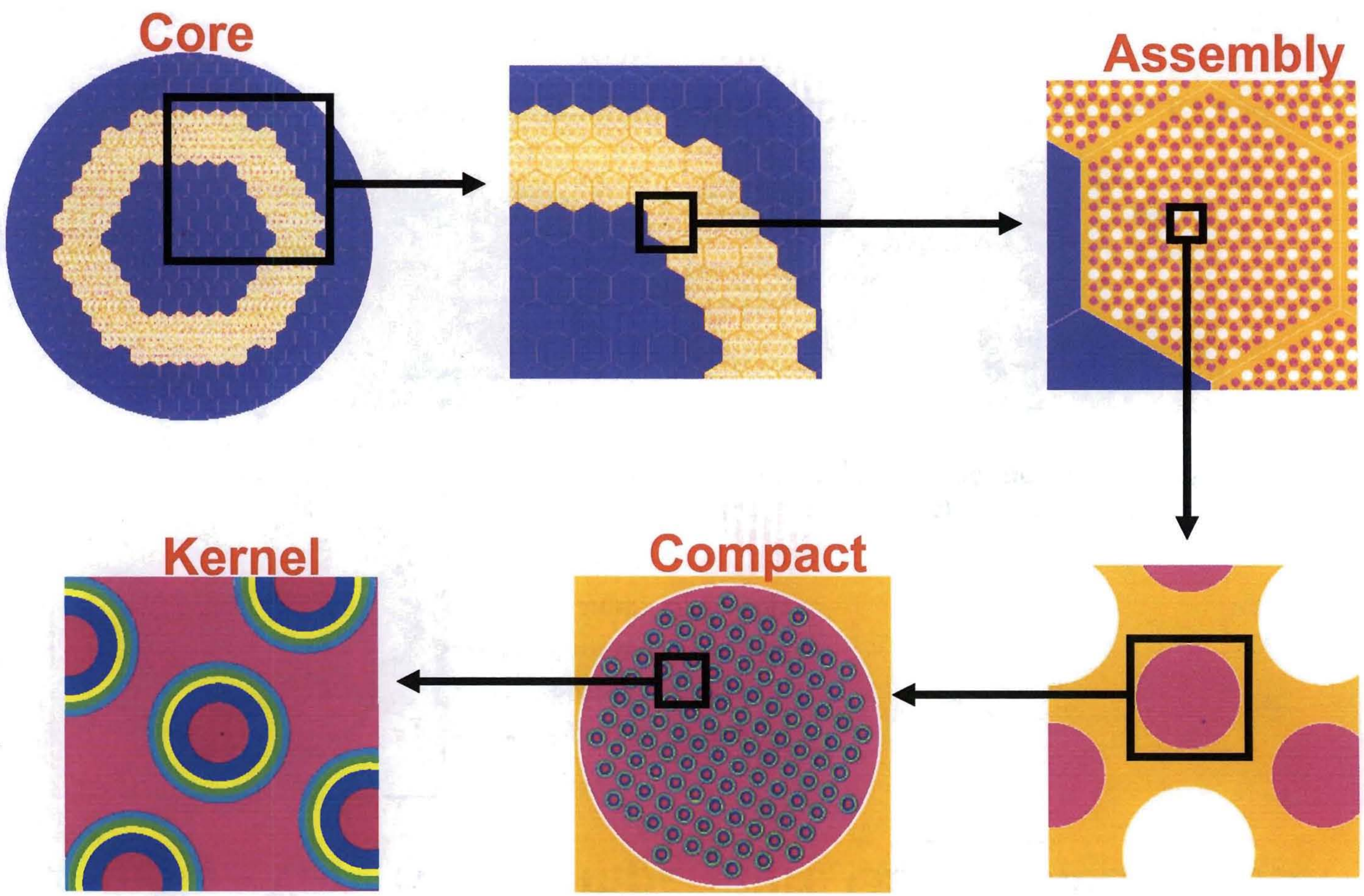


TRISO Coated fuel particles (left) are formed into fuel rods (center) and inserted into graphite fuel elements (right).



P. E. MacDonald, et al., "NGNP Preliminary Point Design – Results of the Initial Neutronics and Thermal-Hydraulic Assessments During FY-03", INEEL/EXT-03-00870 Rev. 1, Idaho National Engineering and Environmental Laboratory (2003).

HTGR Modeling with MCNP5

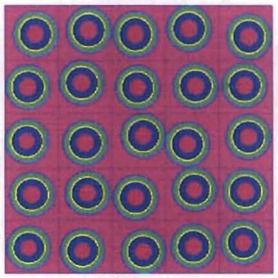


MCNP Models for HTGRs

- **Existing MCNP geometry can handle:**
  - 3D description of core
  - **Fuel compacts or lattice of pebbles**
    - Typically, **hexagonal lattice** with close-packing of spherical pebbles
    - Proteus experiments: ~ 5,000 fuel pebbles
~ 2,500 moderator pebbles
  - **Lattice of fuel kernels** within compact or pebble
    - Typically, **cubic lattice** with kernel at center of lattice element
    - Proteus experiments: ~ 10,000 fuel kernels per pebble
~ 50 M fuel kernels, total
  - Could introduce random variations in locations of a few thousand cells in MCNP input, but **not** a few million.
  - See papers by: Difilipo, Plukiene et al, Ji-Conlin-Martin-Lee, etc.

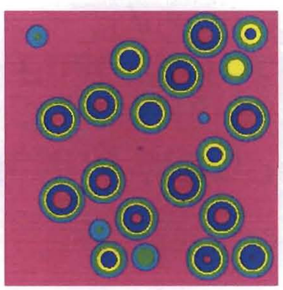
Stochastic Effects

- **MCNP5 stochastic geometry**



Fuel kernels displaced randomly on-the-fly within a lattice element each time that neutron enters

- **RSA placement of fuel kernels**



Fuel kernels placed randomly in job input,
using Random Sequential Addition
Standard MCNP5 - geometry is fixed
for entire calculation
(Does not use stochastic geometry)

Stochastic Effects - Results

MCNP5 Results for Infinite Lattices of Fuel Kernels

Method	K-effective
Fixed 5x5x5 lattice with centered spheres	1.1531 ± 0.0004
Fixed 5x5x5 lattice with randomly located spheres ("on the fly")	1.1515 ± 0.0004
Multiple (25) realizations of 5x5x5 lattice with randomly located spheres	1.1513 ± 0.0004
Multiple (25) realizations of randomly packed (RSA) fuel "box"	1.1510 ± 0.0003

⇒ Small but significant effect from stochastic geometry

⇒ New MCNP5 stochastic geometry matches multiple realizations

⇒ New MCNP5 stochastic geometry matches true random (RSA)

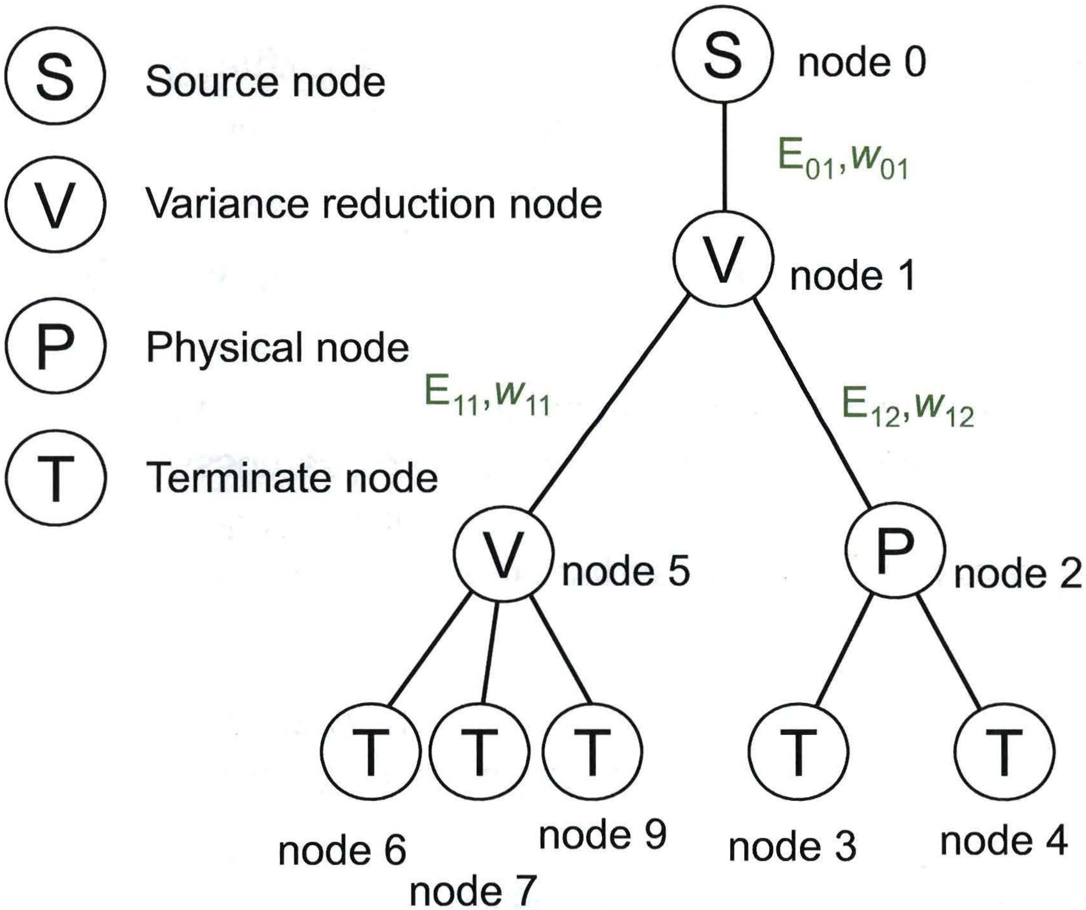
MCNP5 1.50

- **RSICC released MCNP5 1.50 in Winter 2008.**
- **MCNP5 1.50 includes these improvements**
  - Pulse Height Tally Variance Reduction
  - Temperature dependent cross sections
  - Long Filenames
    - up to 256 characters; Unix/Linux path names
  - Improved Annihilation gamma treatment
- ENDF/B-VII.0 data libraries in ACE format

Pulse-Height Tally Variance Reduction

- Pulse-height (F8) tallies depend on collections of particles (e.g., the entire particle history)
  - Two 1 MeV photons deposited in one cell registered as one 2 MeV count, not two 1 MeV counts
  - Assumes both photons have weight one.
  - Not the case when using variance reduction
- Create "trees" to keep track of relationship between individual particles
  - Weight assigned to branches of the tree
  - Energy deposited and weight stored for each branch

Pulse Height Tally Trees



Pulse height tallies require knowledge of the entire particle history

E_{ij} is the energy deposited on branch_{ij}.

w_{ij} is the weight multiplier for branch_{ij}.

Pulse Height Tally Variance Reduction

- Variance Reduction Options
  - Geometry splitting, Energy splitting, Time splitting
  - Weight Window
  - Exponential Transform
  - Forced Collision
  - DXTRAN
  - Weight Cutoff, Implicit Capture
- Future Variance Reduction Options
  - Neutrons
  - Electron specific variance reduction
    - Controls types and how many specific types of electrons are produced
      - bremsstrahlung
      - photon-induced secondary electrons
      - electron-induced x–rays
      - knock-on electrons

Temperature-Dependent Cross Sections

- **Traditional MAKXSF functions**
  - Convert cross-section libraries to/from ASCII & binary
  - Copy entire libraries to new files
  - Copy selected nuclide tablesets to new libraries
  - Create new **xsdir file for the new libraries**
- **Create nuclide table-sets at new temperatures**
  - Doppler broaden resolved resonance data to higher temperature
  - Interpolate unresolved resonance probability tables to new temperature
  - Interpolate $S(\alpha, \beta)$ thermal data to new temperature
- **Create new *xsdir* file which includes all of the above changes**

Doppler & Interpolation Routines

- **Taken from "doppler" code by MacFarlane, taken from NJOY**
  - References:
    1. R.E. MacFarlane & P. Talou, "DOPPLER: A Utility Code for Preparing Customized Temperature-Dependent Data Libraries for the MCNP Monte Carlo Transport Code", unpublished (Oct 3, 2003)
    2. R.E. MacFarlane & D.W. Muir, "The NJOY Nuclear Data Processing System, Version 91", LA-12740-M (1994).

- **Doppler Broadening**
  - Doppler broaden the resolved resonance data to new (higher) temperature
  - Temperatures can be specified in degrees-K or in MeV
  - Only need base cross-section, at lower temperature

- **Interpolation**
  - For S(α, β) thermal data or unresolved resonance probability table data
  - Must have existing datasets at BOTH lower & higher temperature

Testing - Kritz Benchmarks

- Mosteller, MacFarlane, Little, White, "Analysis of Hot and Cold Kritz Benchmarks With MCNP5 and Temperature-specific Nuclear Data Libraries", LA-UR-03-7071 (2003).
  - Separate nuclear data sets were generated at 245 C using DOPPLER and NJOY
  - Basic data were taken from ENDF/B-VI Release 6 (ENDF66)
  - MCNP5 calculations were performed for the hot 2-D benchmarks, and the results were compared
  - Each calculation employed 550 generations with 10,000 neutron histories per generation
  - Results from first 50 generations were discarded, giving 5,000,000 active histories for each case

Case	Library	keff	Δk (vs NJOY)
Kritz:2-1	NJOY	0.9914 ± 0.0003	—
	DOPPLER	0.9911 ± 0.0003	-0.0003 ± 0.0004
	new MAKXSF	**0.9913 ± 0.0003**	**-0.0001 ± 0.0004**
Kritz:2-13	NJOY	0.9944 ± 0.0003	—
	DOPPLER	0.9942 ± 0.0003	-0.0002 ± 0.0004
	new MAKXSF	**0.9940 ± 0.0003**	**-0.0004 ± 0.0004**
Kritz:2-19	NJOY	1.0005 ± 0.0003	—
	DOPPLER	1.0009 ± 0.0003	0.0004 ± 0.0004
	new MAKXSF	**1.0004 ± 0.0003**	**-0.0001 ± 0.0004**

MCNPX

MCNPX 2.6.0

- Transmutation using Cinder90 (BURN card)
  - Several keywords of options (MAT, POWER, etc.)
  - Automatic updating of material atom densities
- Long file names (40 vs. 8 characters)
- STOP card - terminate tallies at desired precision
- Corrections/enhancements/extensions
  - Proton step size control (HSTEP on M card)
  - New $S(\alpha,\beta)$ scattering law
  - Differential data tallies extended to table physics
  - Separate printout of induced fission multiplicity
- Spherical weight windows
- Delayed neutrons & gammas
  - ~1000 nuclides treated with gamma line data
- Photon tally tagging

Fuel Burnup Calculations

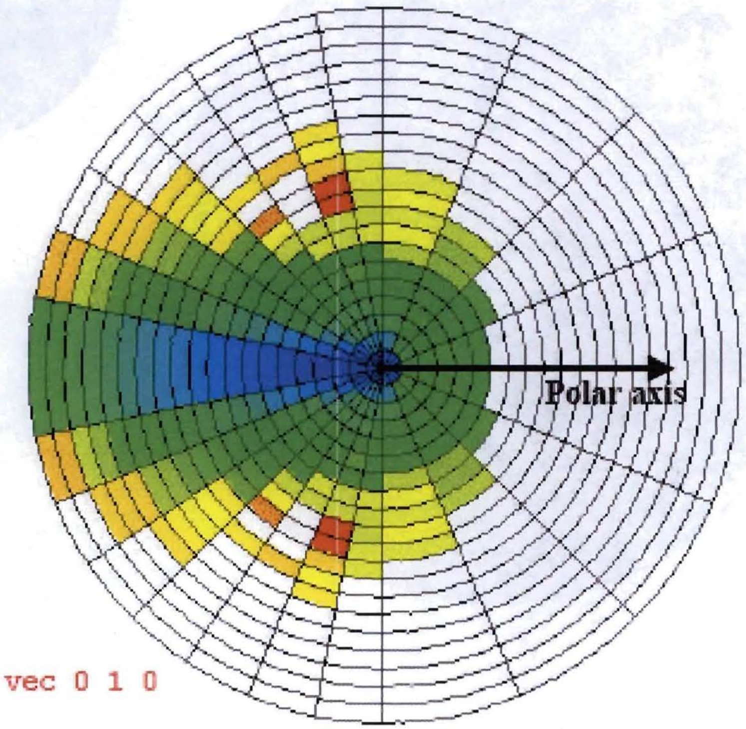
- **During operation of a nuclear system, the isotopic concentration will change as isotopes consume neutrons and undergo various nuclear reactions**
  - (n,f), (n,alpha), (n,beta), (n,p), etc.
- **Changes in the isotopic concentration over time will result in changes in performance parameters**
  - Core Reactivity/ Power Distribution/ SDM/ Poison Concentration
- **MCNPX currently only tracks depletion information for certain isotopes**
  - Materials listed on material card(s)
  - Fission products selected from a specified fission product tier
  - Nuclides created from the isotope generator algorithm
- **CINDER90 does track isotope concentrations for 3456 isotopes**
  - Only those isotopes utilized in the steady state transport calculation contain isotope abundance data in the output file

Variance Reduction: Spherical Weight-Windows

- Variance reduction techniques exchange user time for computational efficiency
  - Computational times often reduced by factors of 100 – 1000
  - Several techniques available
- Mesh-based weight-windows technique allows user to subdivide phase space for determining importance functions
  - Spatial mesh: Cartesian, cylindrical meshes
  - Energy, time
  - Spherical mesh

Spherical-mesh weight-windows

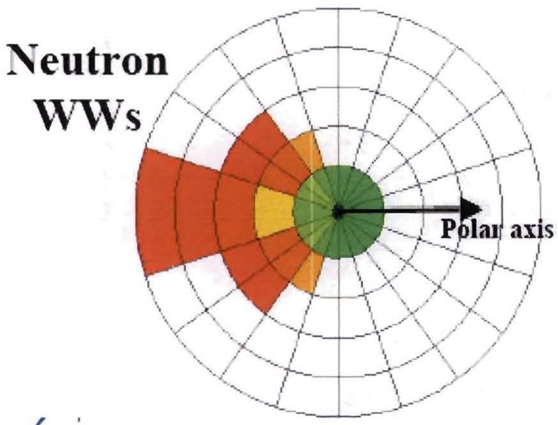
```
10 MeV photons into 1m H2O surrounding HEU
1  1  -19.0    -1     imp:p=1
2  2  -1.0     +1 -2 imp:p=1
3  0           +2 -3 imp:p=1
4  0              -3 imp:p=0

1 sph 0 0 0  3
2 sph 0 0 0  100
3 sph 0 0 0  200

mode p
sdef erg=10 pos=-105 0 0 rad=d1 axs=1 0 0 ext=0
     vec=1 0 0 dir=d2
si1  0 10
sp1  -21 1
si2  0 1
sp2  0 1
m1   92235 .5 92238 .5
m2   1001 2 8016 1
nps 100000
f4:p 1
wwg 4 0
mesh geom rpt origin=0 0 0 ref=-99 1 1 axs 1 0 0 vec 0 1 0
     imesh  101.   iints  20
     jmesh  .25 .5 jints  4 8
     kmesh   1      kints  1
```

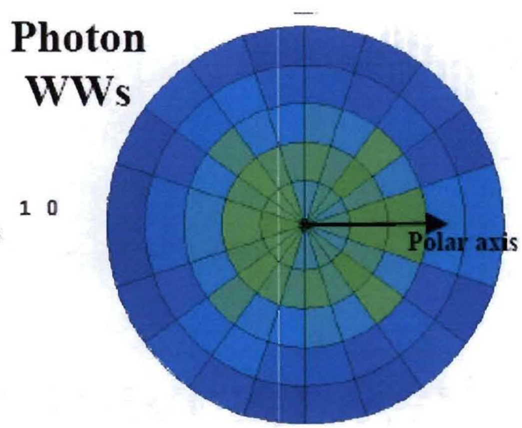


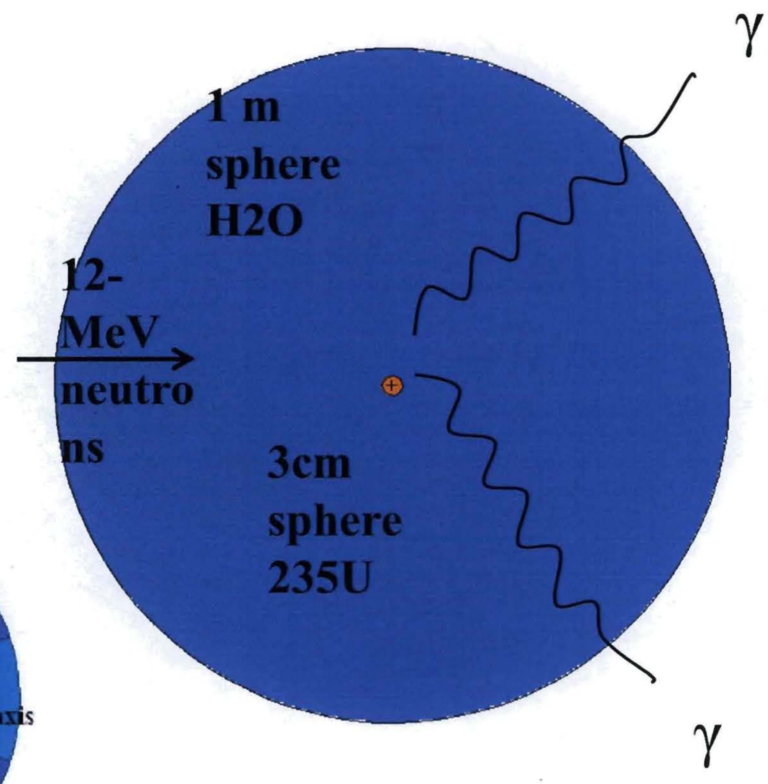
Delayed Particle Production: Neutrons and Gammas

•Delayed gammas signatures due to:
- •decay of radioactive fission products created by neutron- or photon-induced fission, or
- • residual nuclides created by neutron library interactions and all model interactions

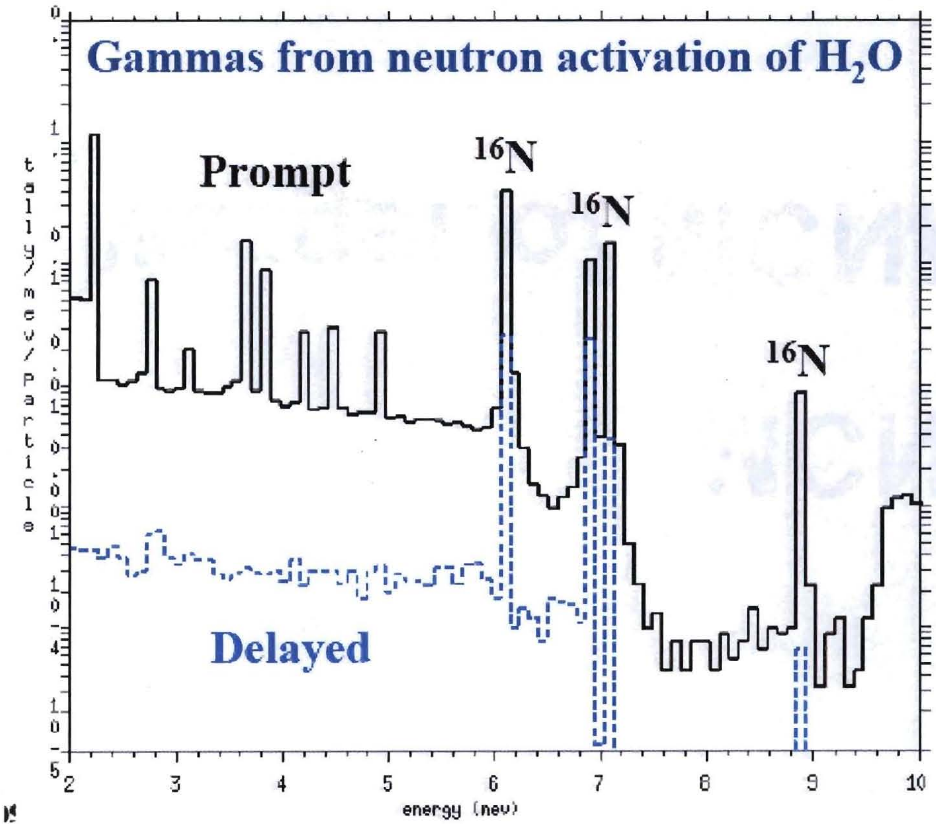
•Delayed neutron production due to:
- •Fission

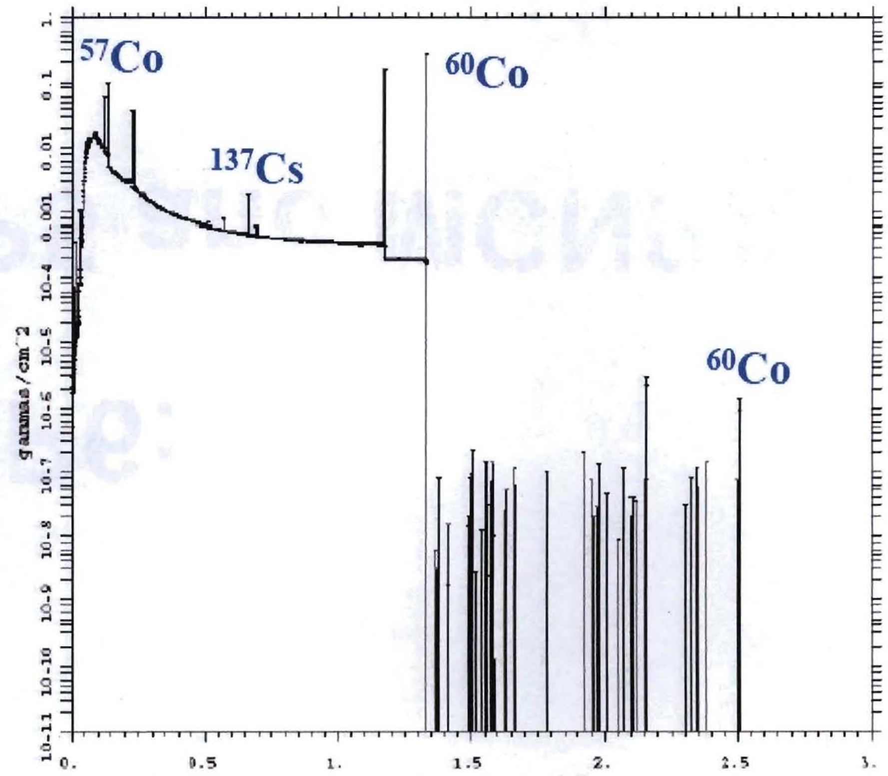






Activation Neutrons,Gammas ; Background Radiation Sources





MCNP6:

Merger of MCNP5 and MCNPX

MCNP6: Merger of MCNP5 and MCNPX

Phase 1
- Move MCNPX variables to MCNP6
- (reconcile particles, common, etc.)

Phase 2
- First half of IMCN (card reading)

Phase 3
- Second half of IMCN
- (geometry, tallies materials)

Phase 4
- XACT (Read / process cross sections,
- proton library, heating)

Phase 5
- MCRUN - particle transport

Phase 6
- MCRUN – sources and tallies

Phase 7
- Tally and cross section plots

Phase 8
- Geometry plot

Phase 9
- MCNPX 26 C, D, E, F, … upgrade

Phase 10
- Debug
- Quality control
- Documentation

MCNP6: Merger of MCNP5 and MCNPX

- July 2006: Began Merger ~2.25 FTEs (MCNPX 2.6.B)
- Sept 2007: Continue Merger ~2.0 FTEs (MCNPX 2.6.C)
- April 2008: (MCNPX 2.6.0)
- Sept 2008: Continue Merger ~ 1.8 FTEs,
  - All MCNPX 2.6.B capabilities complete, 340 test problems integrated
- October 2008: (MCNPX 2.7.A)
- November 2008: 340 test suite passes (with caveats)
- December 2008: Upgrade to MCNPX 26C complete

- December 2008
  - Add 0.75 FTE to Merger Effort

MCNP Merger Current Status

- **Jan 2009: Incorporate Current 427-problem MCNPX test set;**
- **Jan 2009: Super-patch to bridge 26D, 26E, 26F, 260, and 27A versions of MCNPX complete.**
  - ***We anticipate full functionality with current MCNPX (27B ?) by June 1, 2009.***
  - ***We anticipate final obsolescence of MCNPX by Oct 1, 2009.***
- **Correct expedient coding**
  - **Many routines lack consistent style and F90 conventions.**
  - **Eliminate shadow routines**
- **Parallel constructs - MPI and threading**
- **Remove duplicate capabilities:**
- **Performance - speed and storage**
- **Documentation**
- **V&V**

MCNP:

Nuclear Survivability and Weapon Effects

(Work is done by Tim Goorley, X-3 MCC)

MCNP for Nuclear Survivability and Weapon Effect Modeling

- Survivability
  - Fission Heating
  - Intrinsic Radiation
- Weapon Effects
  - Prompt & Delayed Dose
  - Radioisotope production
  - Electron Currents & Ion Positions

•MCNP Capabilities

•3D Geometry; Energy, Time and Space dependant source terms

•Fully coupled Neutron, Photon, Electron Continuous Energy Monte Carlo Transport (First Principles)

•not ray-tracing of point kernels

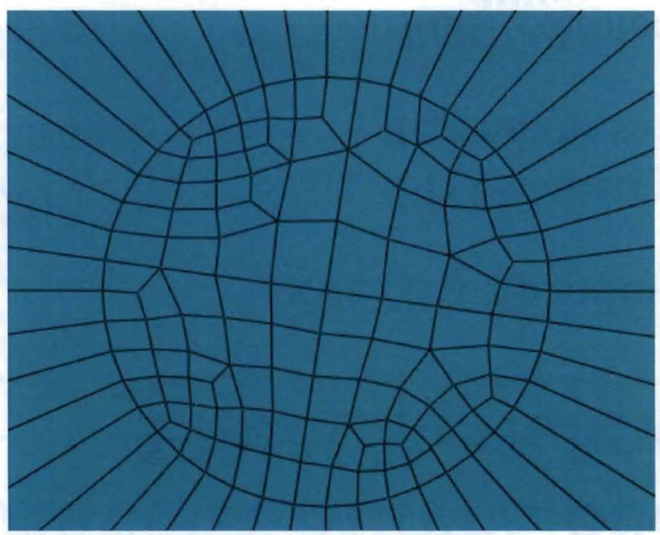
•Variance Reduction Techniques to speed calculations

•Support massively parallel & desktop

•Variety of quantities of interest (fluxes, currents, events, convolution)

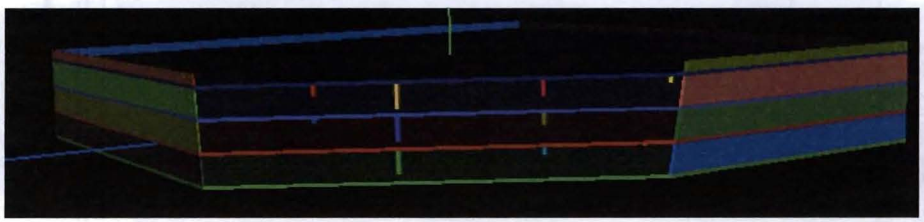
MCNP for Nuclear Survivability

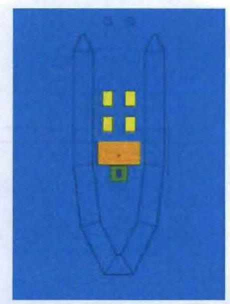
- MCNP has the ability to do radiation transport on ABAQUS unstructured meshes with linear and bilinear elements and calculate fluxes and heating on these meshes.
- These values are passed back on same mesh into ABAQUS for thermal and mechanical response analysis.
- For example, fission heating and intrinsic radiation.

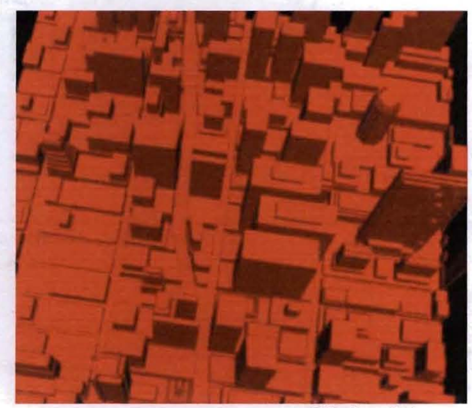


MCNP: 3-D geometries

- Locations & Structures of Interest
  - Small individual structures
  - Detailed vehicles & people
  - Large 3D (satellite based) geometries – specific cities

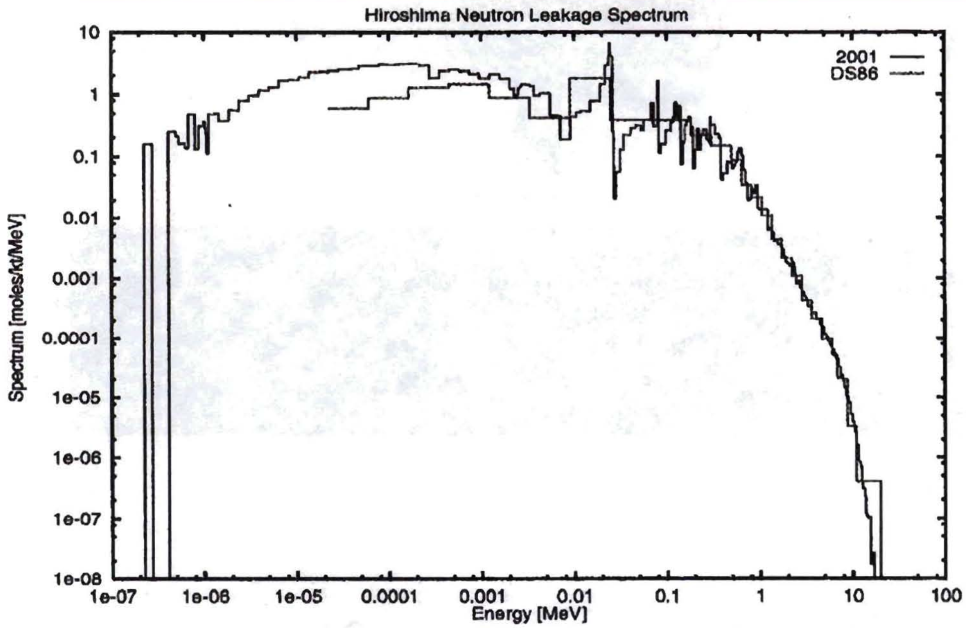


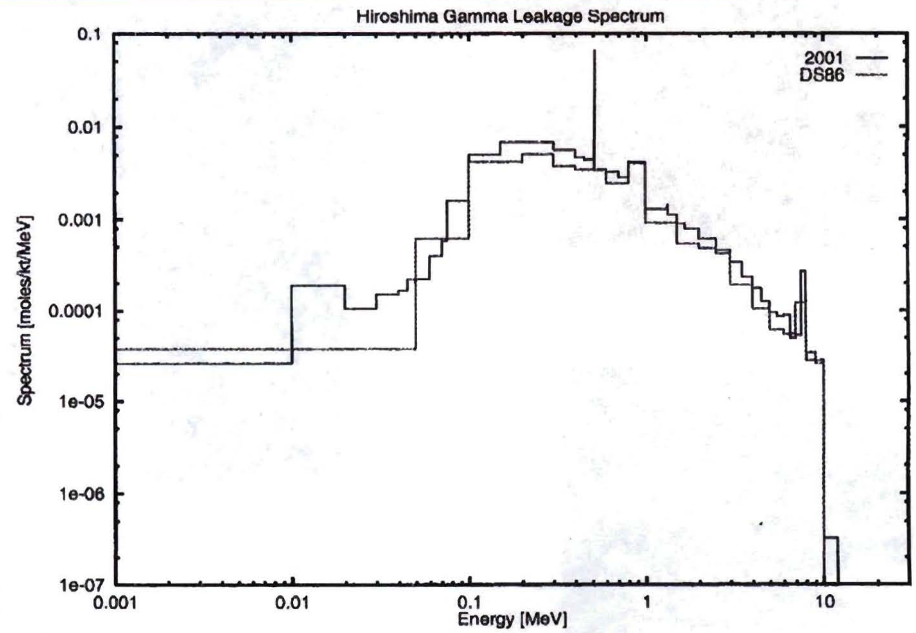




Slide 34

Hiroshima Sources



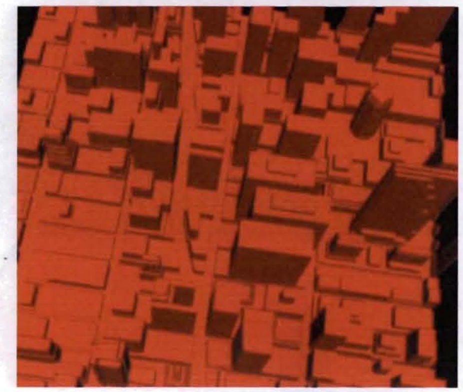


From: Reassessment of the Atomic Bomb Radiation Dosimetry for Hiroshima and Nagasaki, DS02

Source Term Evaluations, Steve White, Paul Whalen, Alexandra Heath.

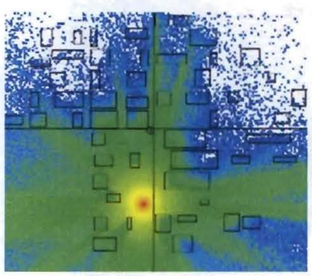
Total n	**0.1768**	**Moles/kt**
Average n energy	**0.3106**	**MeV**
Total γ	**0.0066**	**Moles/kt**
Average γ energy	**1.3979**	**MeV**
Yield Range	**15-18**	**kt**

New York City – Times Square

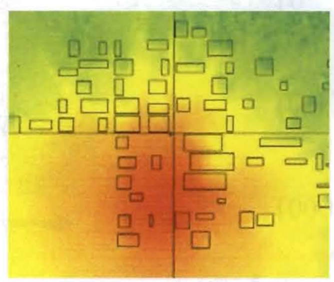


1 km

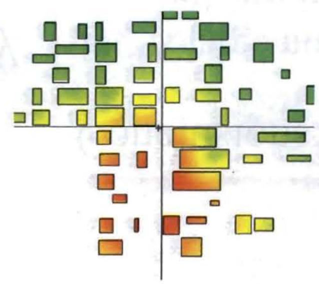
MCNP Results



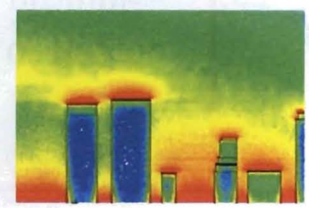
Electron flux/current for EMP source term



Dose for acute radiation affects assessment

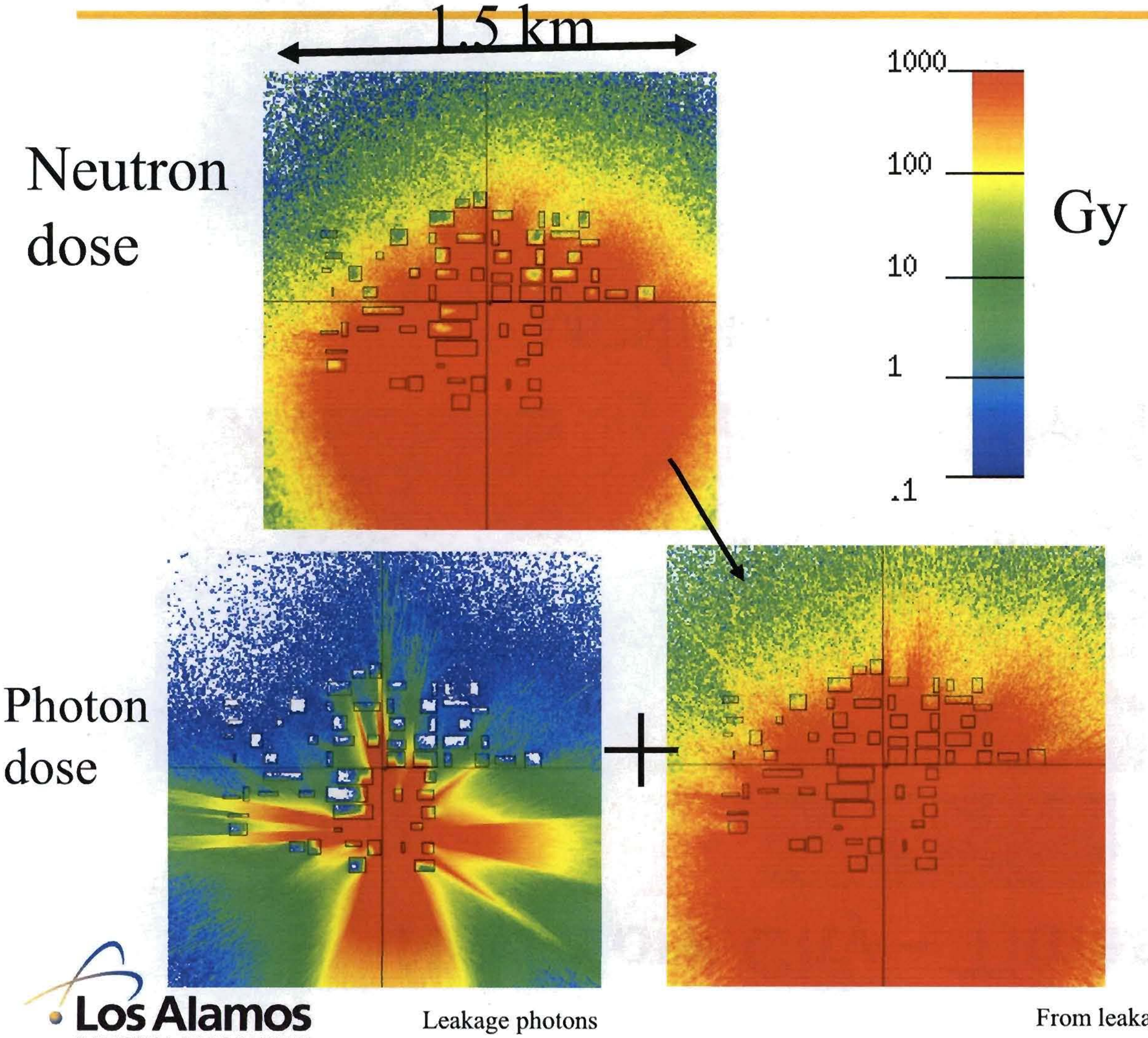


Radioisotope Production



Dose from Radioactive Fallout

New York City – Times Square Hiroshima Bomb detonation @ 1 meter – prompt dose



Conclusions:

1) A large number of people will survive the prompt nuclear radiation.

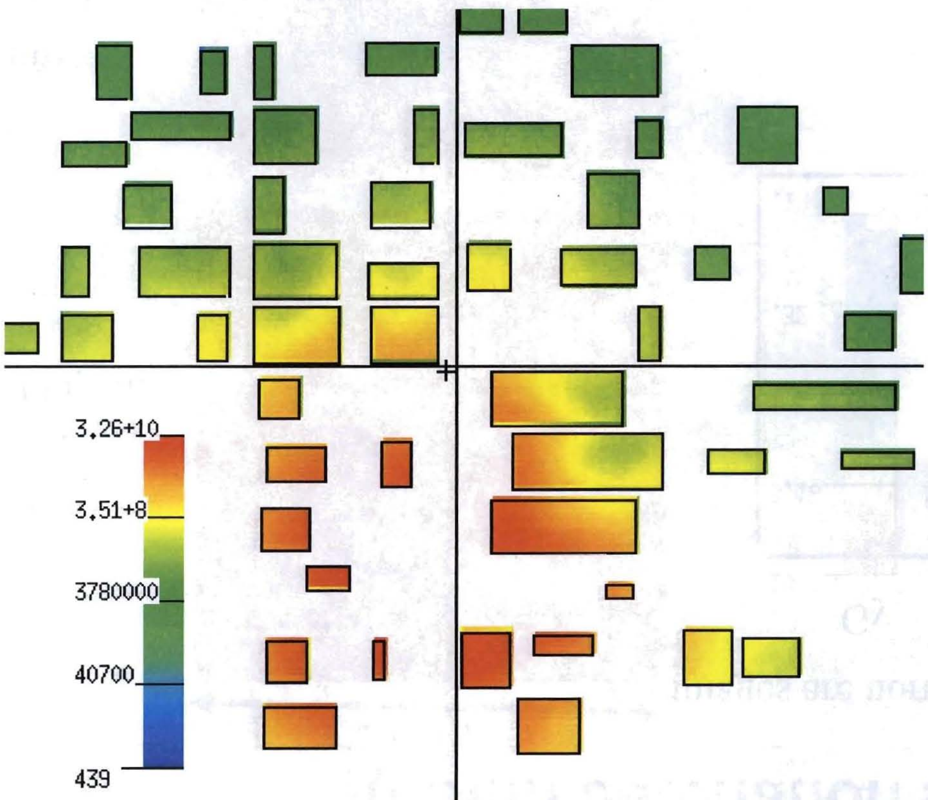
2) Presence of air & buildings makes a large difference in dose. (Model with more buildings needs to be created)

3) Larger scale simulation (2-3 km) also recommended to determine extent of high dose areas.

4) Need way to convolve with building occupancy data.

New York City – Times Square
Hiroshima Bomb detonation @ 1 meter – radioisotope production

^{28}Al Production



^{28}Al atoms in 2x2x5 m of material

^{27}Al has a 0.23 barn xs, and is present in many common materials.

It produces ^{28}Al, which has a short half-life (2.25 min) and has a high γ 1.7 MeV.

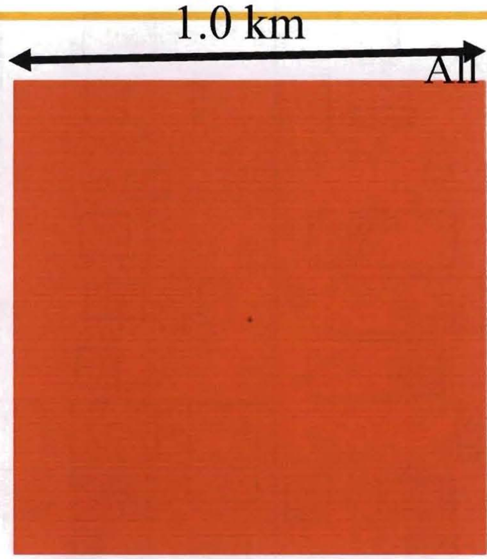
Conclusions:

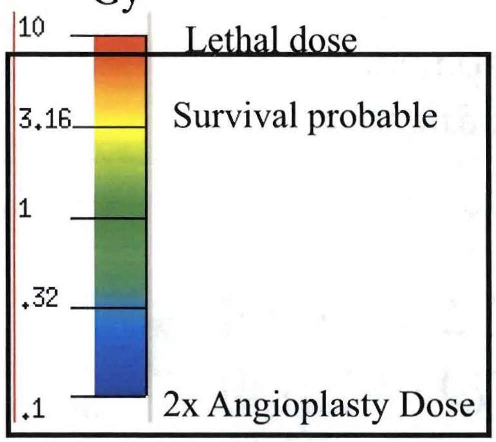
1) A large amount of radioactive material will be produced.
2) Use as source term for dose calculations after "rubbelization"
3) Can be used to identify where burnup is necessary.

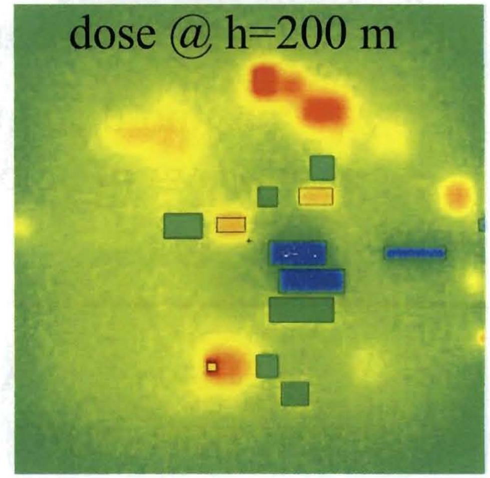
New York City – Times Square Radioactive Fallout over city – Dose (bomb detonation several km away)

All images are normalized to same scale

Open Field 10 Gy/hr







Times Square Ground level dose