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Title: MCNPX Upgrades and Validation for Threat Reduction Applications

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Operational Modeling Workshop
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MCNPX Upgrades and Validation for Threat Reduction Applications

Abstract

The MCNP and MCNPX Monte Carlo Radiation Transport codes at Los Alamos have recently been merged, with the product now called MCNP6. This tool integrates the capabilities of both codes, and also includes many DNDOD and DTRA funded improvements. A number of these are aimed at increasing accuracy in simulating active interrogation. In addition, a new user interface called TR-X has been developed to facilitate the calculation of complex scenarios. Our sponsors are also funding several ongoing active interrogation experiments which have been used to validate the appropriate physics in the code. The capabilities of the merged code and interface will be discussed, along with the implications of recent simulations of some active interrogation scenarios.

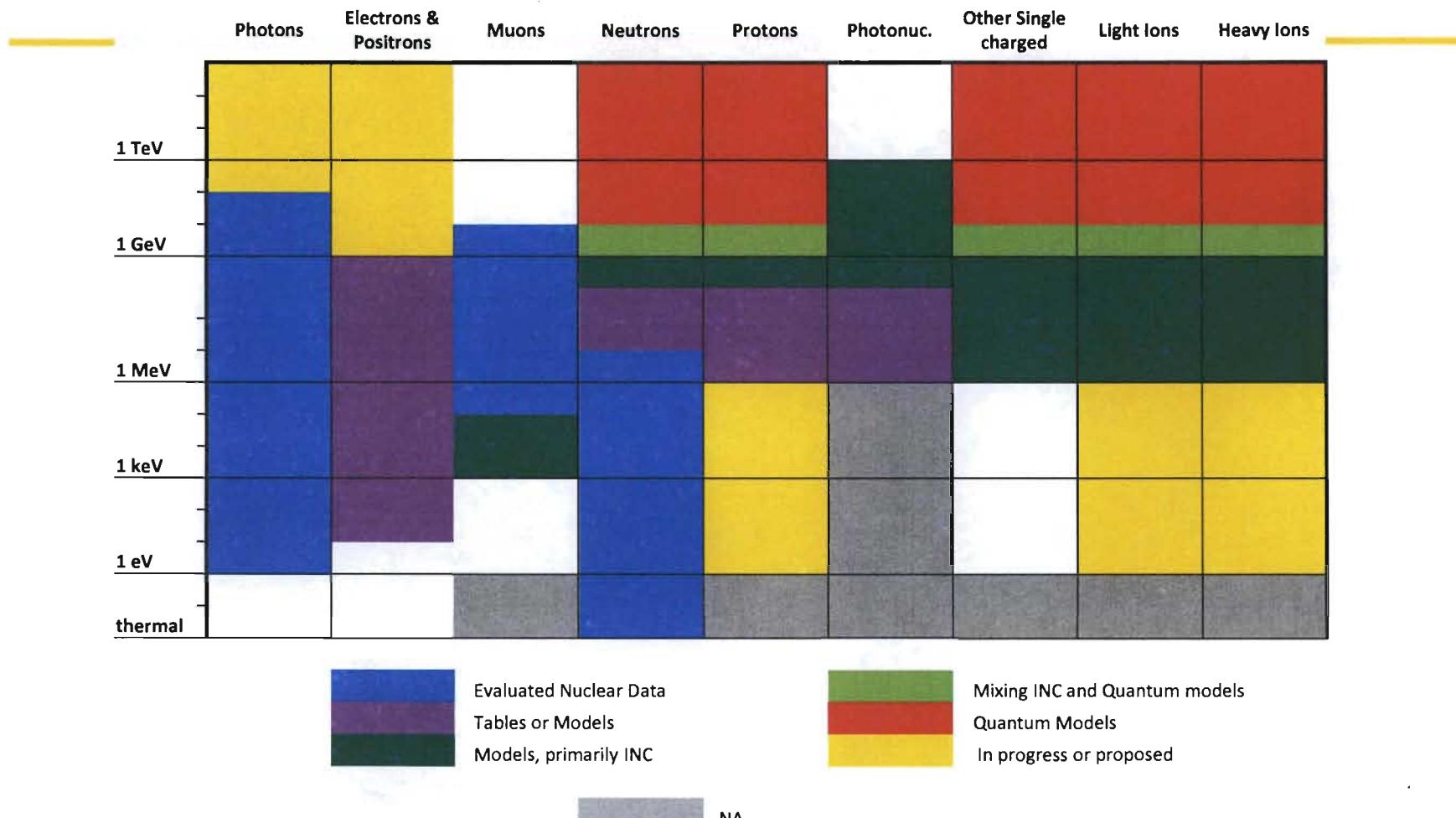
MCNPX Upgrades and Validation for Threat Reduction Applications

Laurie S. Waters, Russell C. Johns
Los Alamos National Laboratory
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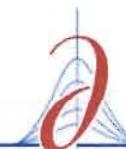
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MCNPX Physics Acceptance Plot



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Slide 1



New Code features funded with Threat Reduction in Mind

Physics Enhancements

- CEM upgrade to 03.02
- Adjustable stopping-power grid
- LLNL photofission multiplicities+upgrade
- LLNL neutron fission multiplicities+upgrade
- Muonic x-ray enhancements
- Delayed neutron spectra, multigroup & exact
- Delayed gamma exact sampling
- NRF data in ACE libraries
- Improved photoatomic form factors
- DG algorithm improvements
- GEF photofission yields
- LAQGSM upgrade to 03.03
- Low Energy Photons and Electrons
- Cerenkov light, reflection, refraction, delta rays
- Electric Fields

Geometry Enhancements

- 'Dynamic Universes'
- Unstructured meshes

Tally Enhancements

- Tally tagging
- LET tally option
- Quality factor tally option
- Cyclic tally binning
- ROC curve tally option
- Residual tally upgrades
- Triple & quadruple coincidences
- Time-dependent pulse-height tallies

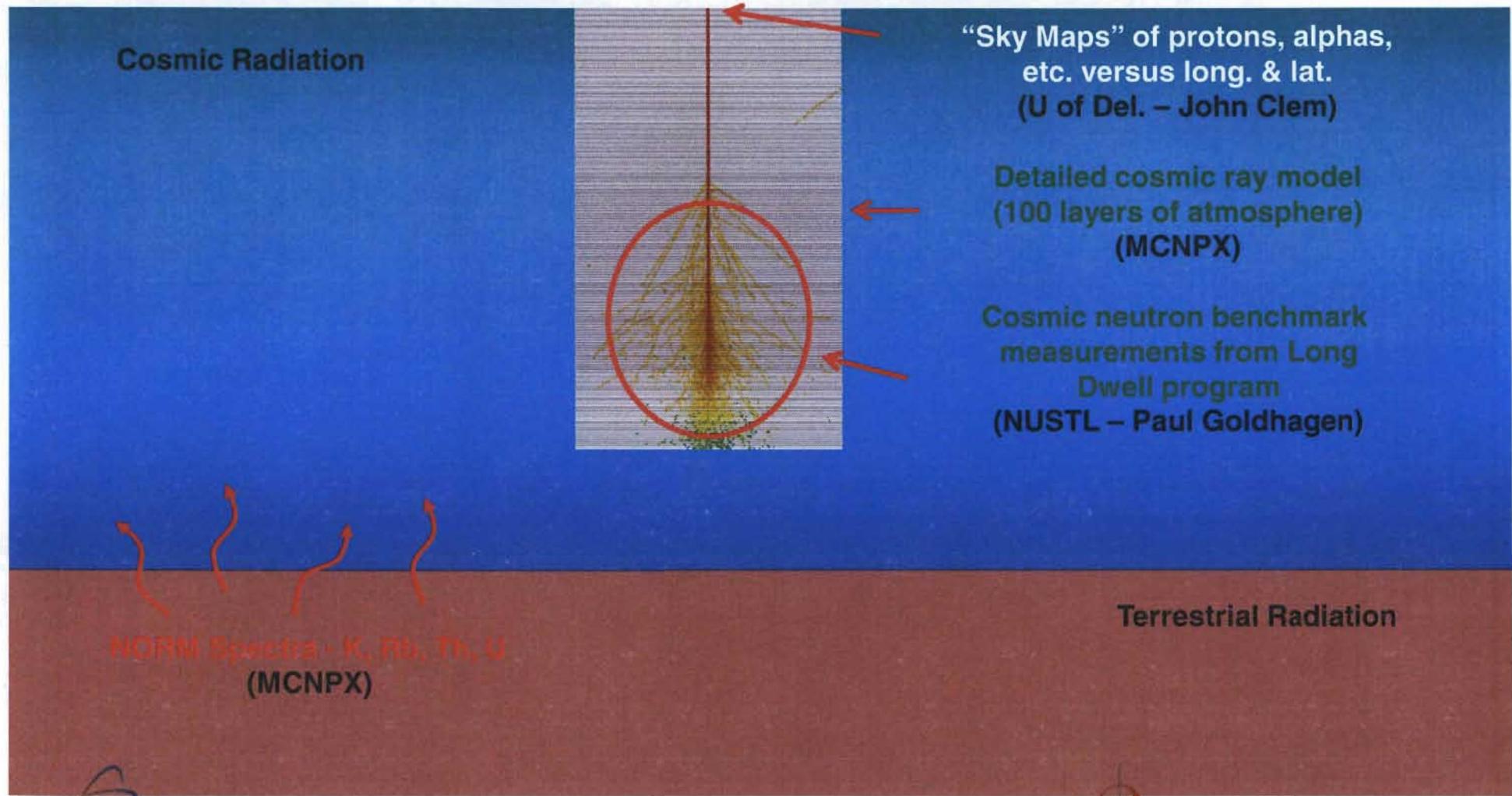
Other Enhancements

- MC PLOT graphics enhancements
- Activation options (ACT card)
- MC PLOT tally manipulations
- Nested READ cards
- Feature-based memory reduction
- M & MX card extensions

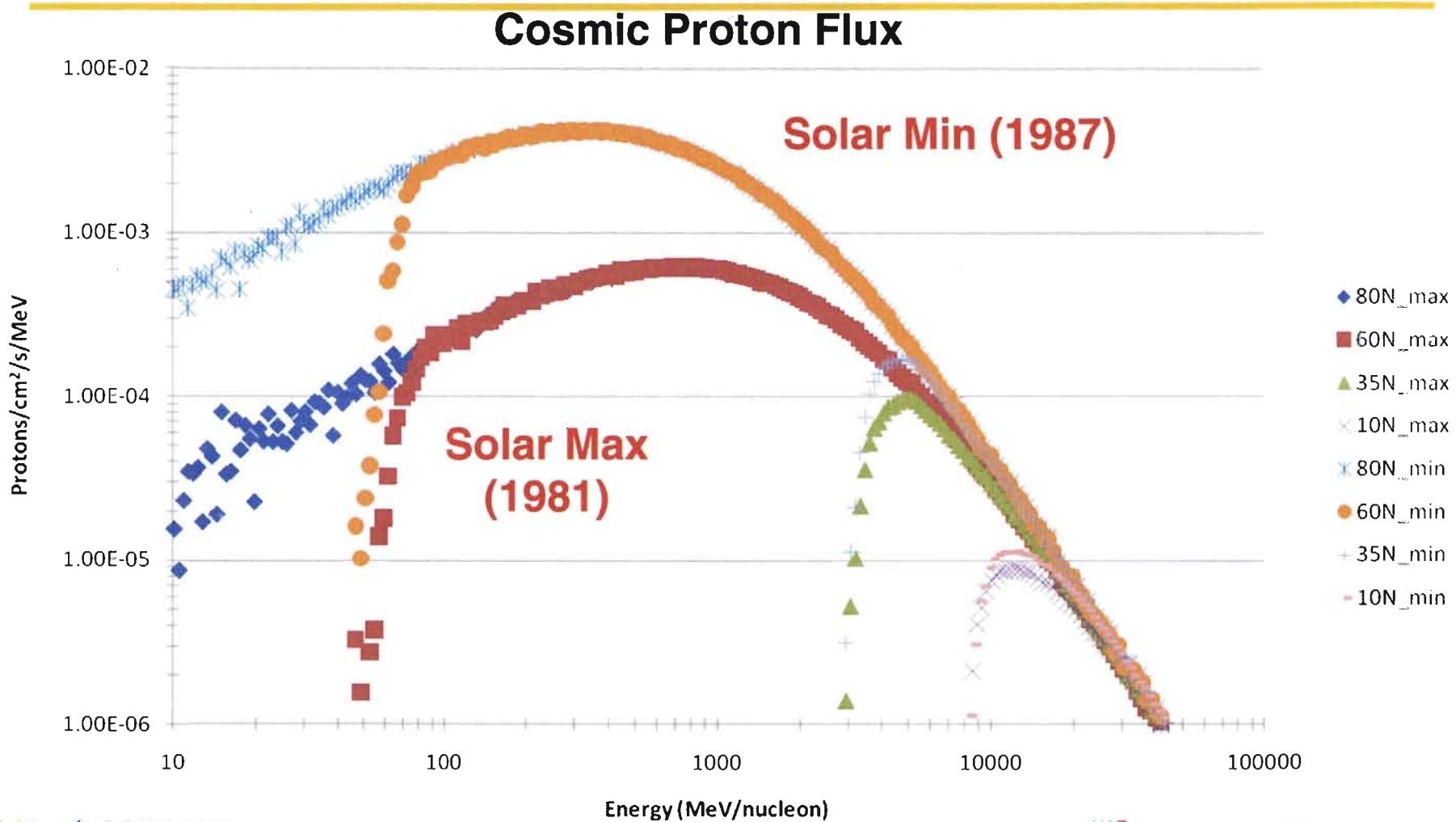
Source Enhancements

- Burnup enhancements
- Pulsed sources
- Beam source options
- Cosmic Ray sources

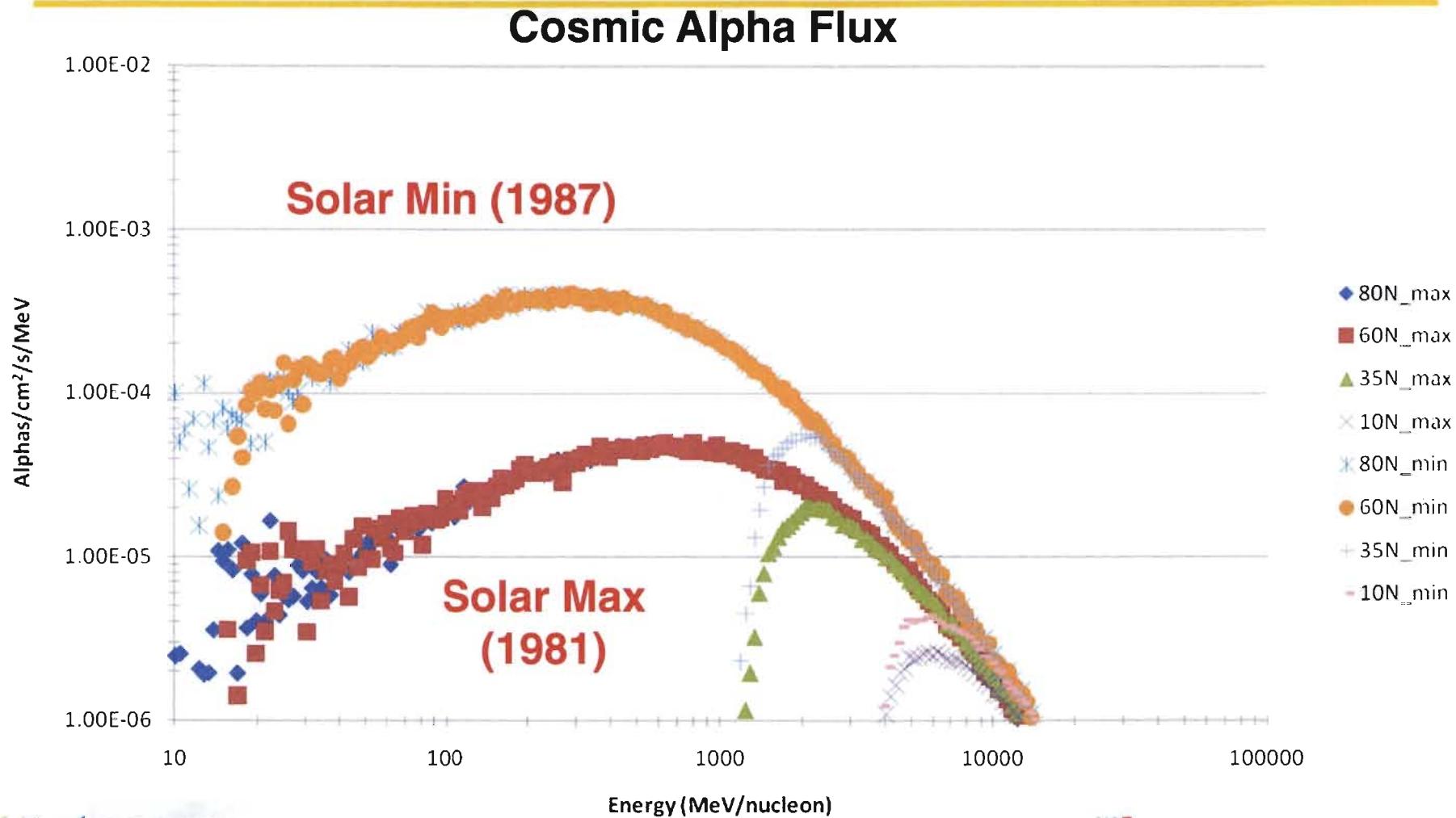
Collaborations are underway to improve background spectra – simulations to be combined with measurements



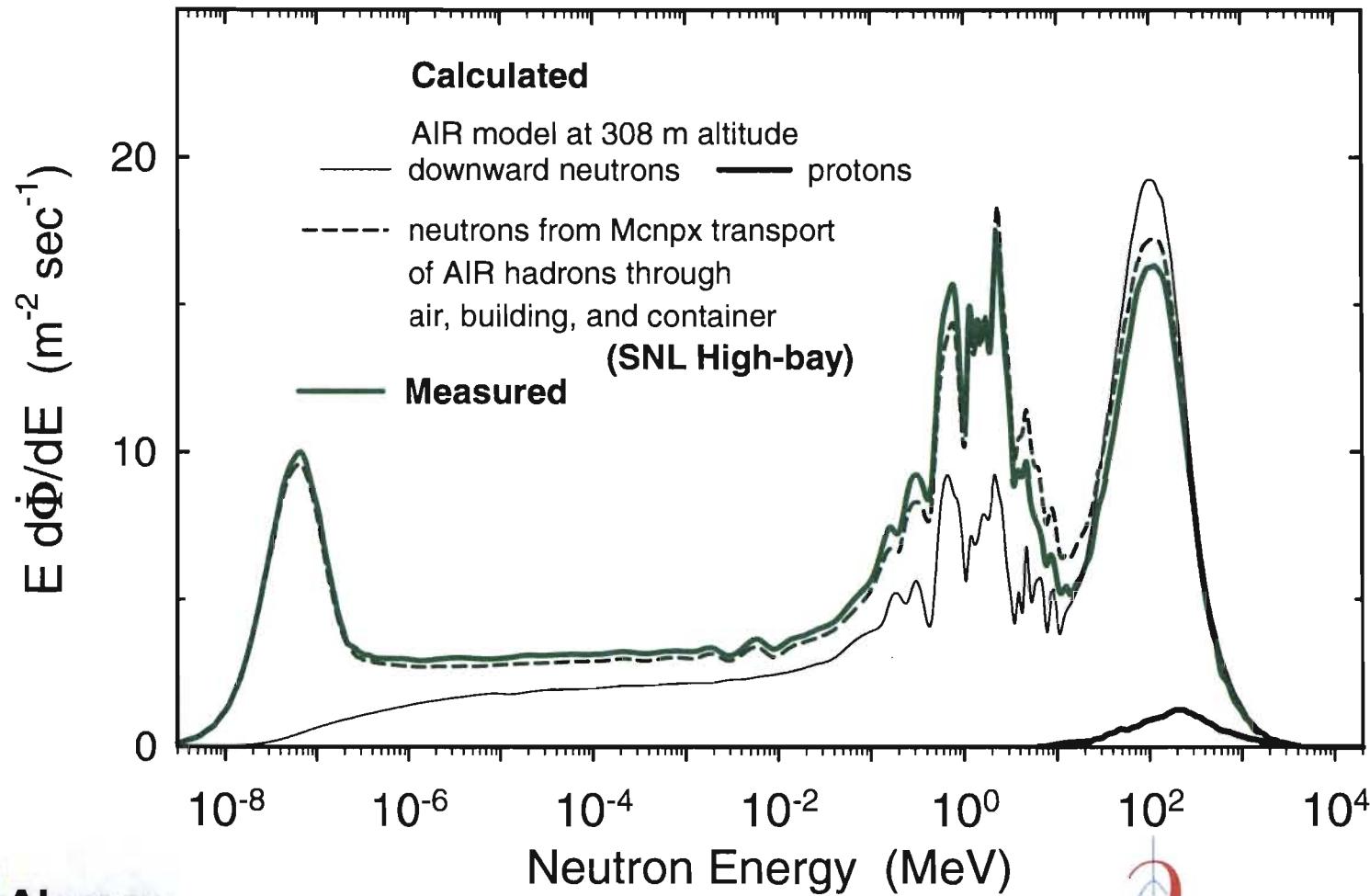
GCR spectra are produced by U of D computer code – accounts for terrestrial modulation & angle of incidence



GCR spectra are produced by U of D computer code – accounts for terrestrial modulation & angle of incidence



Use U of D cosmic spectra with MCNPX to produce starting spectrum for NUSTL spectrometer deconvolution

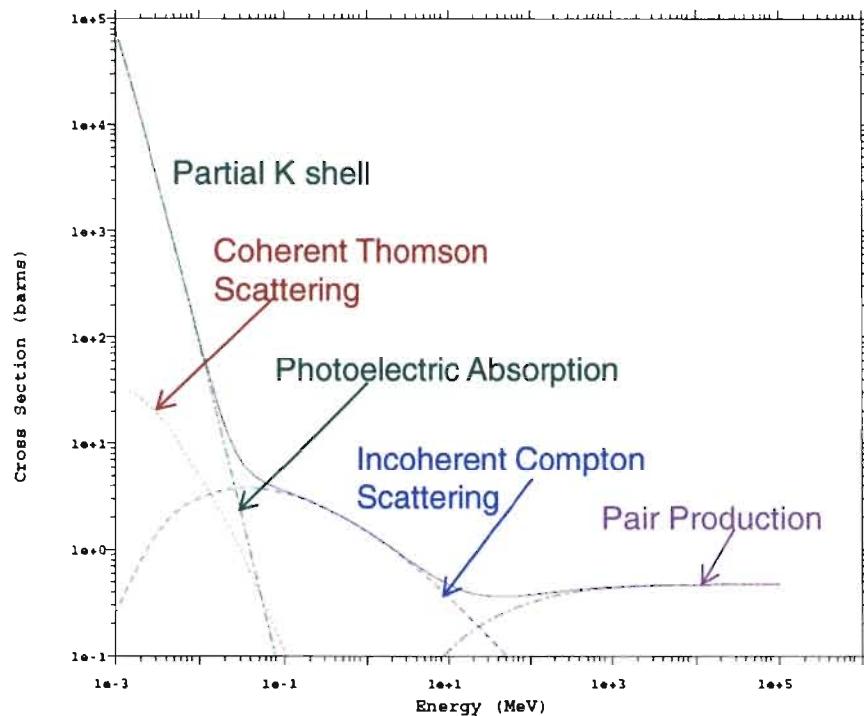


EPDL photon cross section upgrade

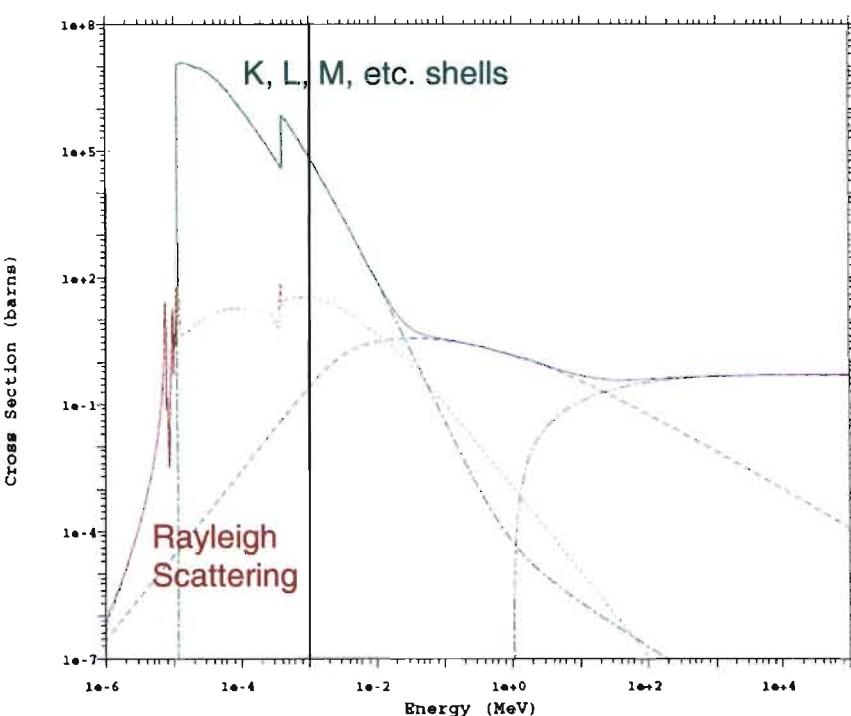
Extension to ENDF/BVI.8 EPDL photon cross sections

Coherent and Incoherent scattering, Photoelectric Absorption capture, fluorescence, Pair Production

Old Nitrogen Cross Sections

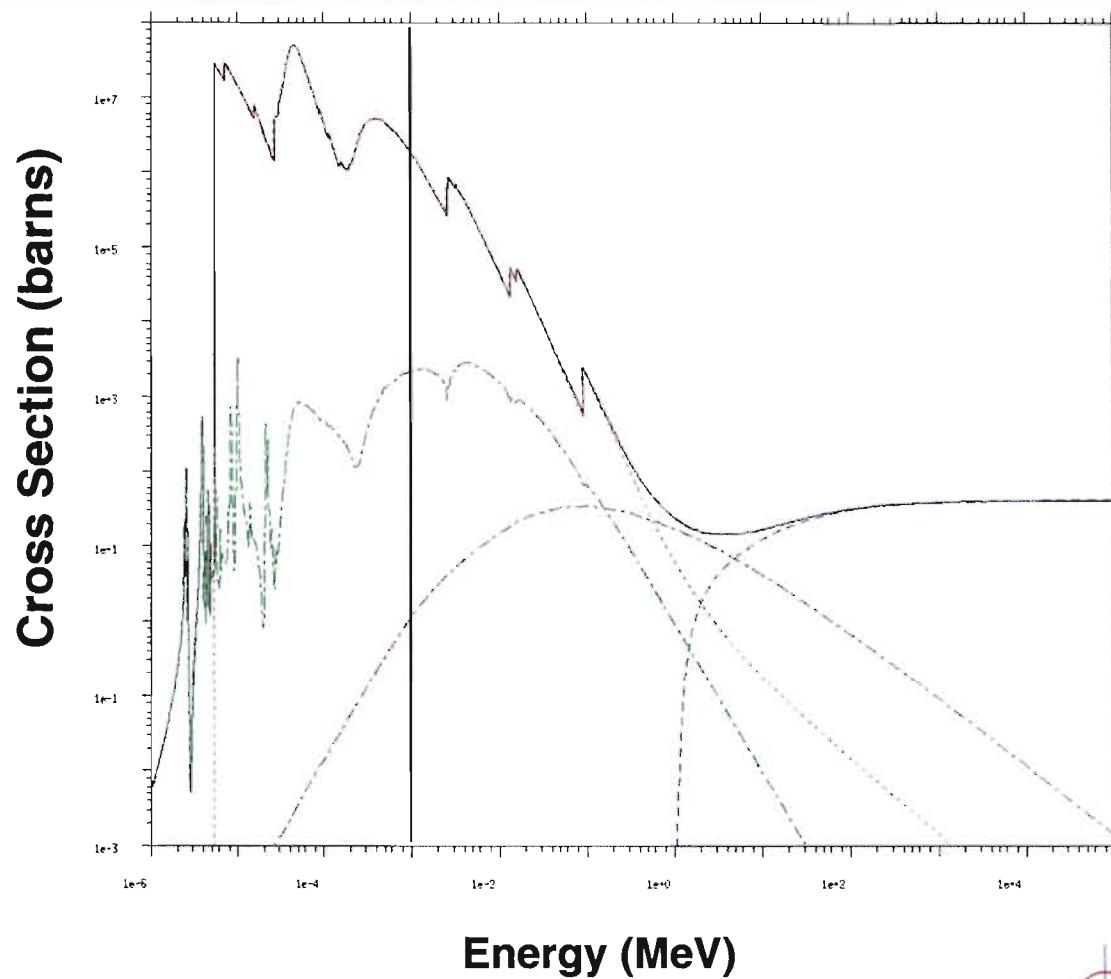


New Nitrogen Cross Sections



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Cross Sections for Lead



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Beta decay nuclides now in MCNPX – exact generation of neutrons

No18 1.67 s	Ne19 ⁺ 17.22 s	Ne20 90.48	Ne21 ⁺ 0.27	No22 9.25
β^- 3.42, γ 1011, --	β^- 2.24, γ 109.3 (1011, 1316), --	β^- 0.07, 40	β^- 7.3 γ 11.8	β^- 048.30 γ 120.3 (80)
E 1.45	E 3.23	19.9944	20.0024	
F17 ⁺ 64.5 s	F18 ⁺ 1.830 h	F19 ⁺ 100	F20 ⁺ 11.00 s	F21 ⁺ 4.16 s
β^- 1.34	β^- 0.36	β^- 3.40, γ 1633, --	β^- 5.4, γ 350, 7, 1316, --	
E 2.7869	E 1.54	19.994229	E 2.016	E 5.680
O16 99.76	O17 ⁺ 0.04	O18 0.20	O19 ⁺ 26.9 s	O20 13.5 s
β^- 19 mb, 4 mb	β^- 26.31 γ 4 mb	β^- 18 mb, 26 mb	β^- 3.3, 4.60, γ 137.1, 1316, --	β^- 2.76, γ 1016, --
11.99401603	10.994134	17.994160	E 4.890	E 5.514
N16 0.37	N16 ⁺ 7.13 s	N17 ⁺ 4.17 s	N18 ⁺ 0.62 s	N19 ⁺ 0.35
β^- 4.21, 10.64, γ 6128, 71.15, --	β^- 2.7, γ 1.171, 323, γ 27.6, 2194 (1011)	β^- 0.1, γ 221.1, γ 1016, --	β^- 1.681.9, 1651.5, γ 221.1, γ 1016, --	β^- 0.6, γ 3130, 705, γ 1016, --
11.9941603	E 5.514	E 4.89	E 12.90	E 12.54
C14 5730 s	C15 ⁺ 2.45 s	C16 ⁺ 0.75 s	C17 20 ms	C18 0.07 s
β^- 1.91 γ 1016	β^- 4.51, 9.82, γ 5297.8, --	β^- 0.1, 1.71	β^- 1.371, 1849, 1906	β^- 0.1
β^- 1.68		E 4.15	E 11.80	

Z < 20, over 3

Z < 70, over 10

Li9	177 msec	Co72, Co73, Co 74, Co 75
Be12	24 msec	Ni73, Ni74, Ni75, Ni76, Ni77, Ni78
B13	17.4 msec	.
B14	14 msec	Br87 55.9 sec
C16	.75 sec	Br88 16.4 sec
C17	20 msec	Br89 4.37 sec
C18	.07 sec	Br90 1.9 sec
N17	4.17 sec	Br91 0.54 sec
N18	0.62 sec	Br92 0.34 sec
	.	.
	.	.
	.	.

Eu165 (Z=63)

The TR-X/MOAB Code

TR-X is a new code project at Los Alamos with several goals:

- Move to modern software engineering
 Make problem setup, run, and analysis using MCNP codes easier with the user of 'Wizards'
- Build some intelligence to warn the user when mistakes are likely
- Take full advantage of all MCNP features
- Rethink the way input files are set up – The Template concept. Input files are formed by manipulating templates.
- TR-X is a standalone program.
- Developed using the Qt C++ libraries & C++.
- Works natively under Windows, Mac, and Linux/Unix operating systems
- Works
- Can be expanded to other radiation transport codes.
- Comes with installer.



Introduction – Ease of Use

MCNP & MCNPX

- Text only input
- Small geometry changes can lead to large number of input modifications
- Data analysis limited
 - Tallies
 - Cross Sections
 - Plotting available only with x-windows
- Mistakes are common and may be hard to spot
- Running on Clusters confusing

TR-X

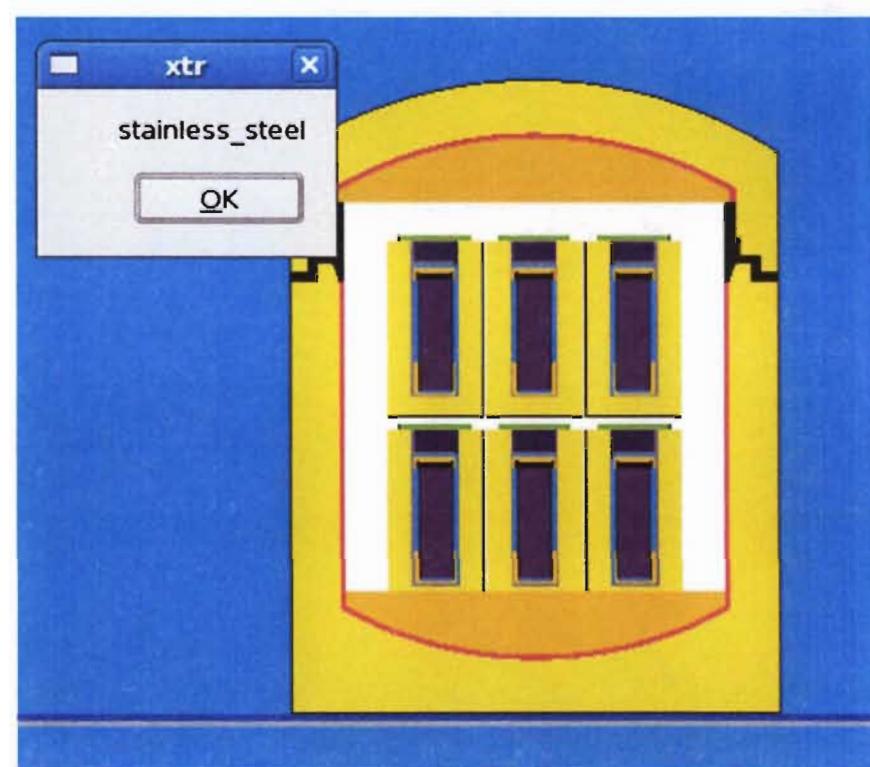
- Graphic point and click interaction
- Geometry manipulation simplified with templates
- Data handling expanded
 - OUTP tables parsed & plotted
 - Export to Excel format
 - Comparison of cross section plots
 - Runs natively under Widows, Mac, or Linux/Unix
- Wizards to check for common mistakes
- Tools to automate running on local and remote machines

Introduction - Standardization

- MCNP(X) is used to investigate different approaches to solving a problem.
- There can be difficulty in comparing approaches modeled by different users.
- TR-X helps with standardization.
 - Library of standardized objects
 - Library of standardized materials
 - Standardized analysis tools
- Changes to standardized objects and materials are reported to the user by TR-X.
- Wizards help users to be constant in approach.

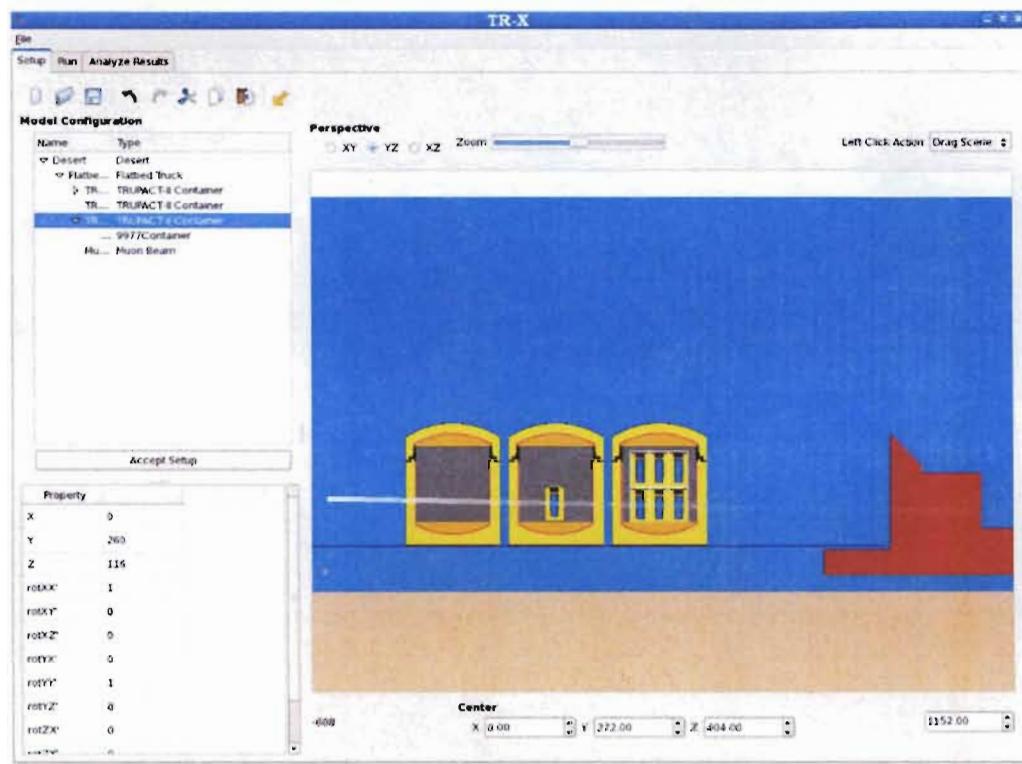
TR-X: Templates

- Templates tie together multiple possible aspects of an object
 - Predefined geometry
 - Materials
 - Position
 - Sources
 - Tallies
 - Variable parameters
 - Level of a gas tank
 - Circumference of a sphere
 - Inter object interaction
 - Type
 - Fillable spaces
 - Gravity Vector
 - Collision detection
- Smart templates



TR-X Page 1: Scenario Setup

- Scenario geometry is done on the setup page of TR-X.
- Scenarios are set up by combining templates to form a hierarchical tree.
- The user interacts with scenarios through both mouse and keyboard input.



TR-X: Wizards

- A Wizard is a series of dialogs that guides a user through a process.
- TR-X uses Wizards help users through complex tasks.
- Wizards included in TR-X
 - Template Wizard
 - Material Wizard
 - Tally Wizard
 - Physics Wizard
 - Machine Wizard
 - Run Wizard
- Wizards do not provide for the use of MCNP(X) as black box. Instead, TR-X enables a more effective use of MCNP(X).

TR-X: Input Wizards

Template Wizard

- Walks the user through the creation of a template from MCNP(X) cell and surface definitions.
- Prompts the user for additional information needed to make a complete template
 - Bounding box
 - Fillable cells
 - Gravity vector
 - Materials
 - Tallies
 - Intrinsic sources

Material Wizard

- Helps the user define new materials.
- Allows users to define materials through one of several methods
 - Mixture of isotopes
 - Elemental breakdown
 - Combination of other materials
- Reduces the chance of confusion of weight or atom fractions.
- Provides users with a means of checking availability of cross section libraries.

TR-X: Input Wizards – Continued

Physics Wizard

- Wizard to help users select the proper physics options and avoid common mistakes
 - Suggests which particles need to be tracked.
 - Sets particle energy and time cutoffs in a intuitive format.
 - Helps users select the proper library or model based on scenario conditions.
 - Assists user in selecting proper physics options for each particle.
- A solid understanding of physics is still necessary for proper use of this Wizard.

Tally Wizard

- Helps users with tasks associated with implementing tallies in MCNP(X).
- Presents the user with definitions of tally functions.
- Allows users to place tallies not already included in a template.
- Provides help in selecting variance reduction techniques for the scenario.



Example Wizard Page: General Physics Options

Dialog - [Preview]

General Physics Options

Move the cursor over the parameter for an explanation
Items marked in green may be changed
Items in red need particular attention

Neutrons ON	Maximum Energy = 1000 MeV Minimum Energy = 0.0 MeV Time cutoff = Very Large Shakes WC1 = 0.50 WC2 = -0.25 SWTM = minimum source weight	EAN = 0.0 IUNR = 0 DNB = -1 TABL = -1 FISM = 0 RECL = 0	Mass = 949.58 MeV Average Lifetime = 897.0 Sec Neutrons tracked Antineutrons tracked
Photons ON	Detailed treatment < 1000 MeV Minimum Energy = 0.001 MeV Time cutoff = Very Large WC1 = 0.50 WC2 = -0.25 SWTM = minimum source weight	EMCPF = 0.0 EDES = 0 NOCOH = -1 ISPAN = -1 NODOP = 0 DGB = 0	Mass = 949.58 MeV Average Lifetime = 1e29 Sec
Electrons ON	Maximum Energy = 1.0 GeV Minimum Energy = 0.001 MeV Time cutoff = Very Large Weight Cutoff 1 = 0.50 Weight Cutoff 2 = -0.25 SWTM = minimum source weight	IDES = 0 IPHOT = 0 IBAD = 0 ISTRG = 0 XNUM = 1 RNOK = 1 ENUM = 1 NUMB = 1	Mass = 0.511008 MeV Average Lifetime = 1e29 Sec Electrons tracked Positrons tracked
Protons ON	Maximum Energy = 1000 MeV Minimum Energy = 1.0 MeV Time cutoff = Very Large WC1 = 0.50 WC2 = -0.25 SWTM = minimum source weight	EAN = 0.0 TABL = -1 ISTRG = 0 RECL = 0	Mass = 938.2723128 MeV Average Lifetime = 1e29 Sec Protons tracked Antiprotons tracked
Alphas ON	Maximum Energy = 1000 MeV Minimum Energy = 1.0 MeV Time cutoff = Very Large	ISTRG = 0	Mass = 938.2723128 MeV Average Lifetime = 1e29 Sec

OK Cancel

- One example of a Wizard sub-page is the General Physics Options page.
- This page presents users with options from the “PHYS” and “CUT” cards from MCNP(X) and brings users attention to new and misused options.
- The values on this page are generated by TR-X based upon the choices made on the first page of the Wizard.
- Changes made to this page are constrained to prevent the user from entering values that are not allowed.
- Further checking on the values is done to make sure that values entered are logical in the overall context of the problem

TR-X: Runtime Wizards

Machine Wizard

- Tool to gather needed information for running MCNP(X) on a remote machine
 - Machine name and path
 - Credentials to use for login
 - Type of credential verification
 - Number of processors on the machine
 - Submission process used to start jobs
- Does not set up the remote machine, the user must provide information on existing settings.
- The use of TR-X on remote machines requires MCNP(X) to be installed, but not TR-X.

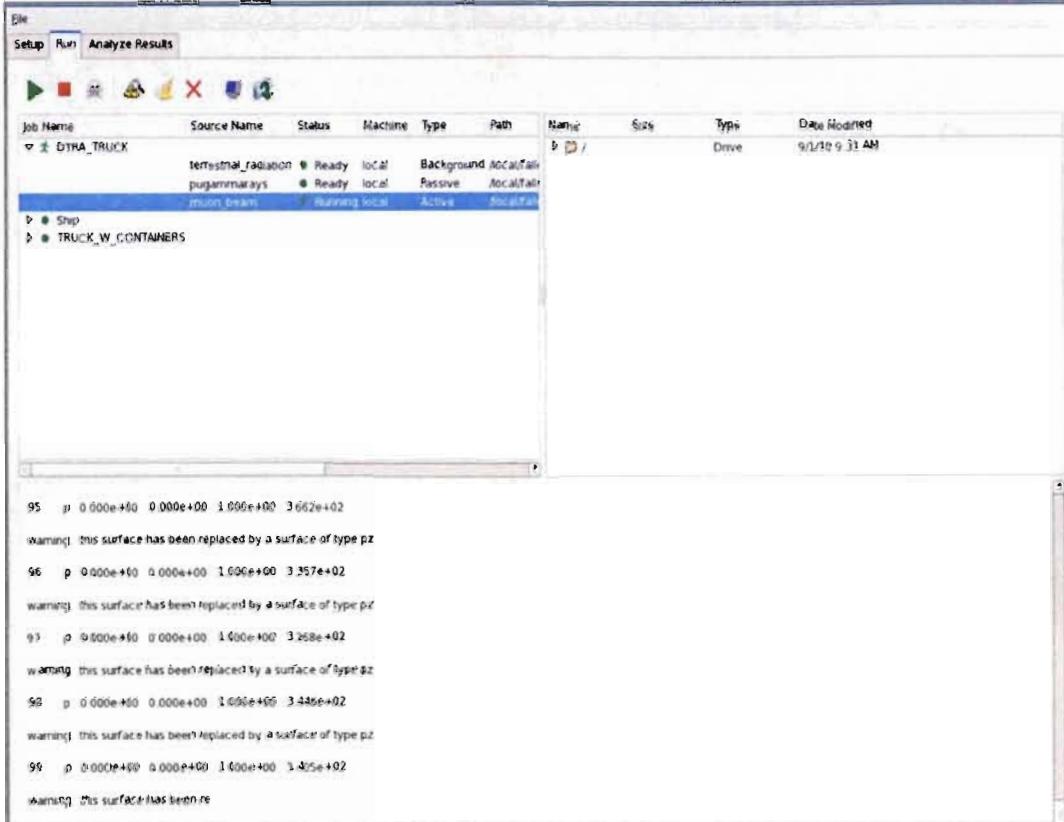
Run Wizard

- Walks the user through the final steps needed before a scenario can be run in MCNP(X).
- Gathers information on how the scenario is to be run.
 - Number of source particles
 - Number of processors to use
 - Location to store generated files
 - Other information based on type of run
- Presents options from multiple MCNP(X) cards in an accessible fashion.
 - Debugging options
 - How often to dump the RUNTPE file
 - Starting values for the random number generator
 - Code rendezvous options for multiprocessing runs



TR-X Page 2: Scenario Execution

- MCNP(X) runs are initiated, controlled, and viewed from the TR-X Run Page.
- Runs input files either created by TR-X or imported from other sources
- TR-X executes the necessary steps for running on remote machines.
- The current status of runs is easily visible to users.
- Users can interrupt and restart a run.
- Visualizations of the OUTP file information is available during execution.



The screenshot shows the 'Run' tab of the TR-X interface. A table lists the status of various jobs:

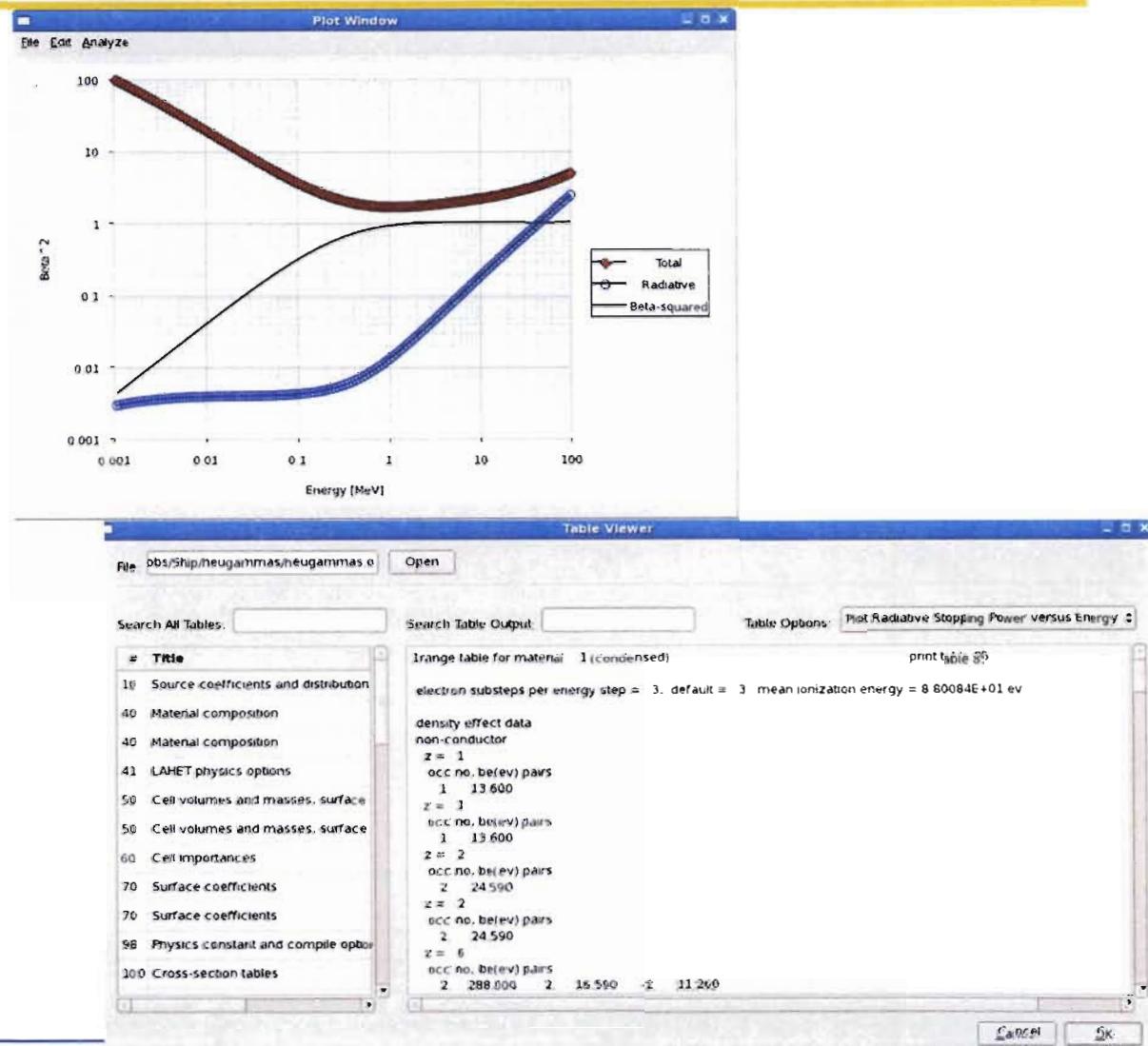
Job Name	Source Name	Status	Machine	Type	Path	Name	Size	Type	Date Modified
DYNA_TRUCK									
	terrestrial_radiation	Ready	local	Background	local,full				
	pugammarays	Ready	local	Passive	local,full				
	zircon_bream	Running	local	Active	local,full				

Below the table, a log window displays the contents of an OUTP file:

```
95  p  0.000e+00  0.000e+00  1.000e+00  3.662e+02
warning: this surface has been replaced by a surface of type pz
96  p  0.000e+00  0.000e+00  1.000e+00  3.357e+02
warning: this surface has been replaced by a surface of type pz
97  p  0.600e+00  0.000e+00  1.000e+00  3.268e+02
warning: this surface has been replaced by a surface of type pz
98  p  0.000e+00  0.000e+00  1.000e+00  3.448e+02
warning: this surface has been replaced by a surface of type pz
99  p  0.000e+00  0.000e+00  1.000e+00  3.405e+02
warning: this surface has been replaced by a surface of type pz
```

TR-X: Analysis – Page 3

- New tools are available for visualizing OUTP file data produced by a run.
- Tools are provided to analyze tally convergence.
- TR-X can compare data from other runs or databases.
- Data is exportable to formats readable by Microsoft Excel and other programs
- The user can add algorithms to analyze data.



Conclusions

Questions?

TR-X development is sponsored
by DTRA.

