LA-UR- 12-00322

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Title:	MCNPX Upgrades and Validation for Threat Reduction Applications
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Intended for:	Operational Modeling Workshop CACI 4114 Legato Road, Fairfax, VA January 24-26, 2012

Form 836 (7/06)

Operational Modeling Workshop
CACI 4114 Legato Road,
Fairfax, VA
January 24-26, 2012

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 DNDO 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

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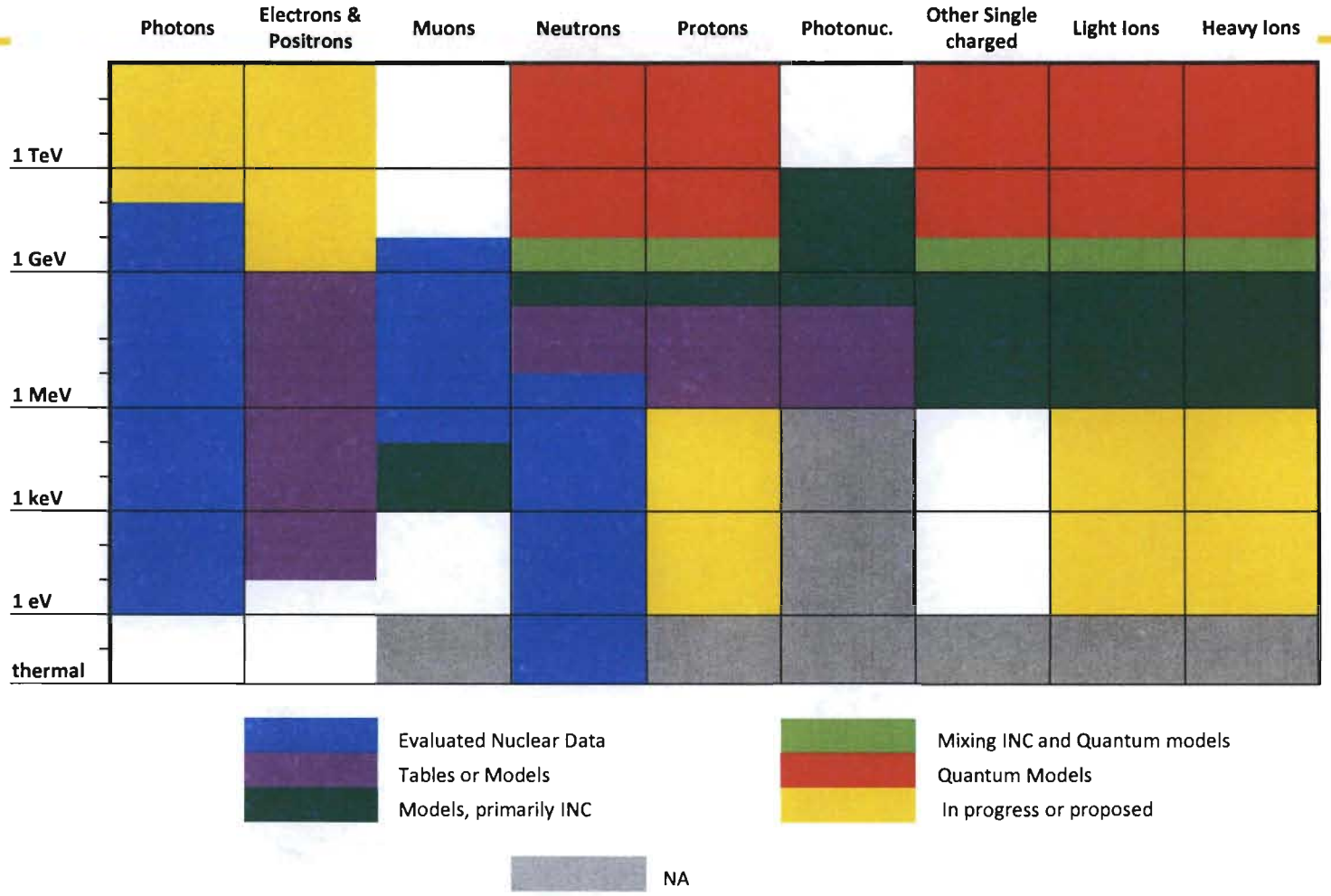
January 24, 2012

Operational Modeling Workshop
CACI, Jan 24-26, 2012

MCNPX Physics Acceptance Plot



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

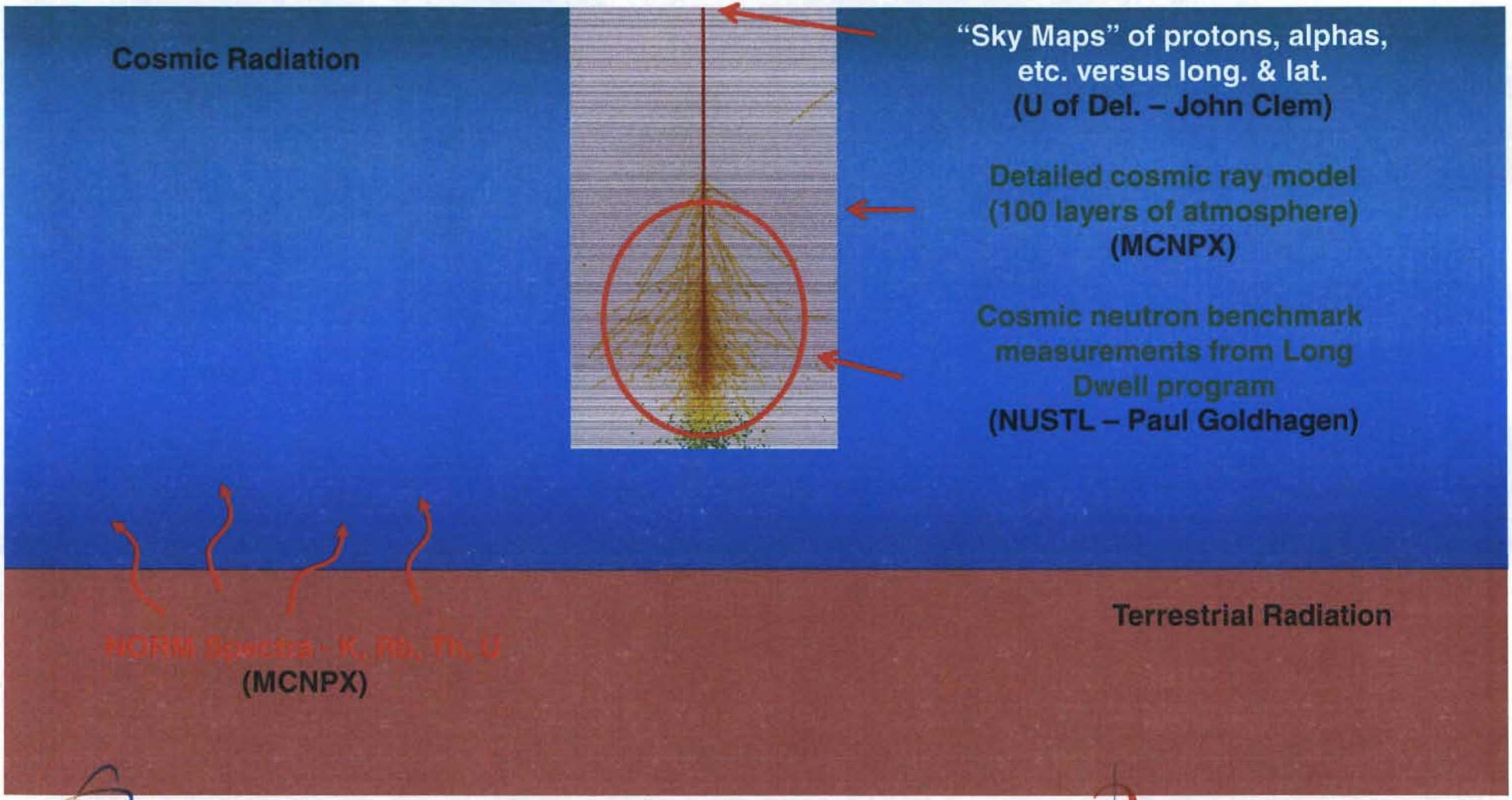
Geometry Enhancements
'Dynamic Universes'
Unstructured meshes

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

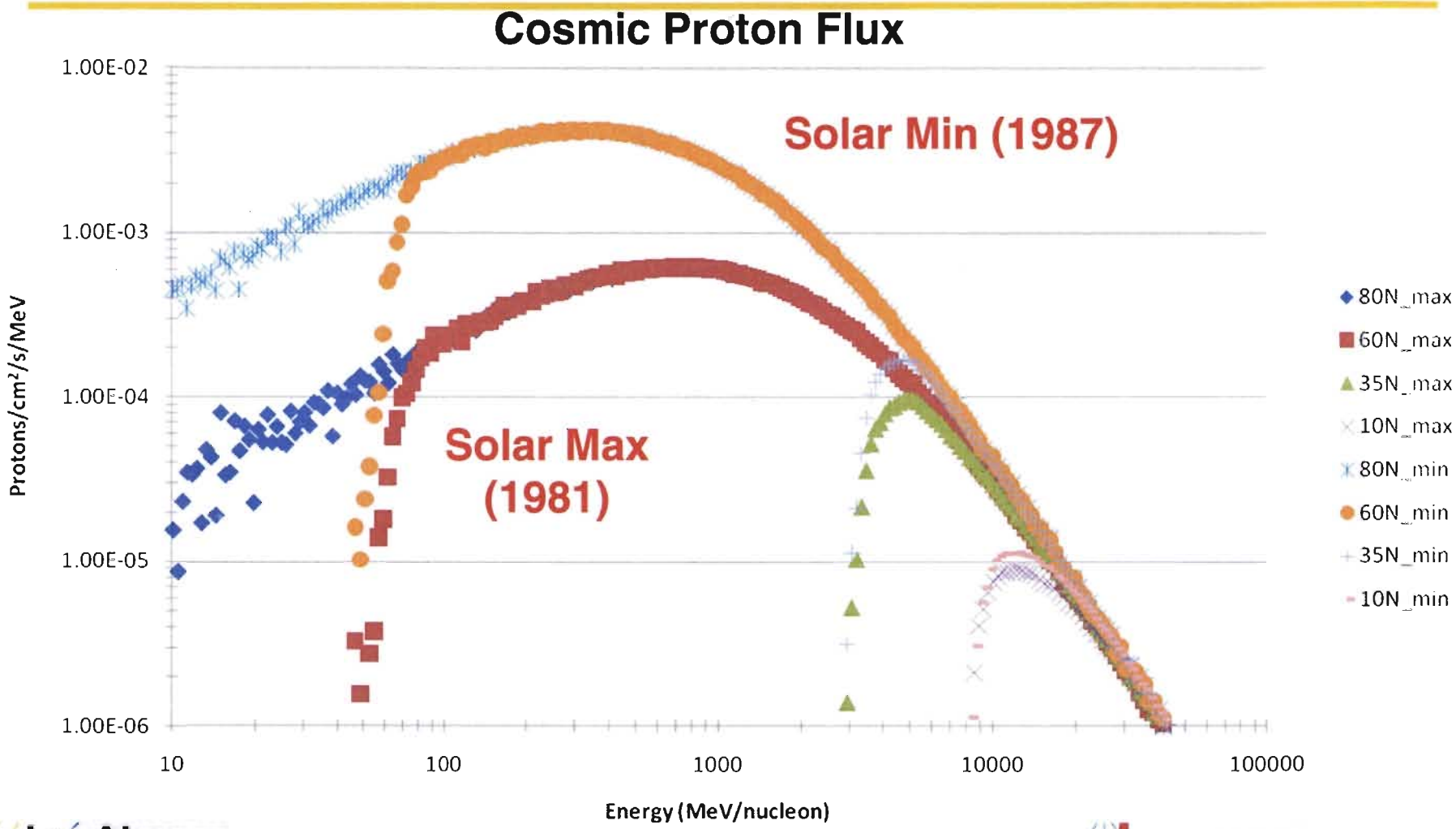
Other Enhancements
MCPLOT graphics enhancements
Activation options (ACT card)
MCPLOT tally manipulations
Nested READ cards
Feature-based memory reduction
M & MX card extensions

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



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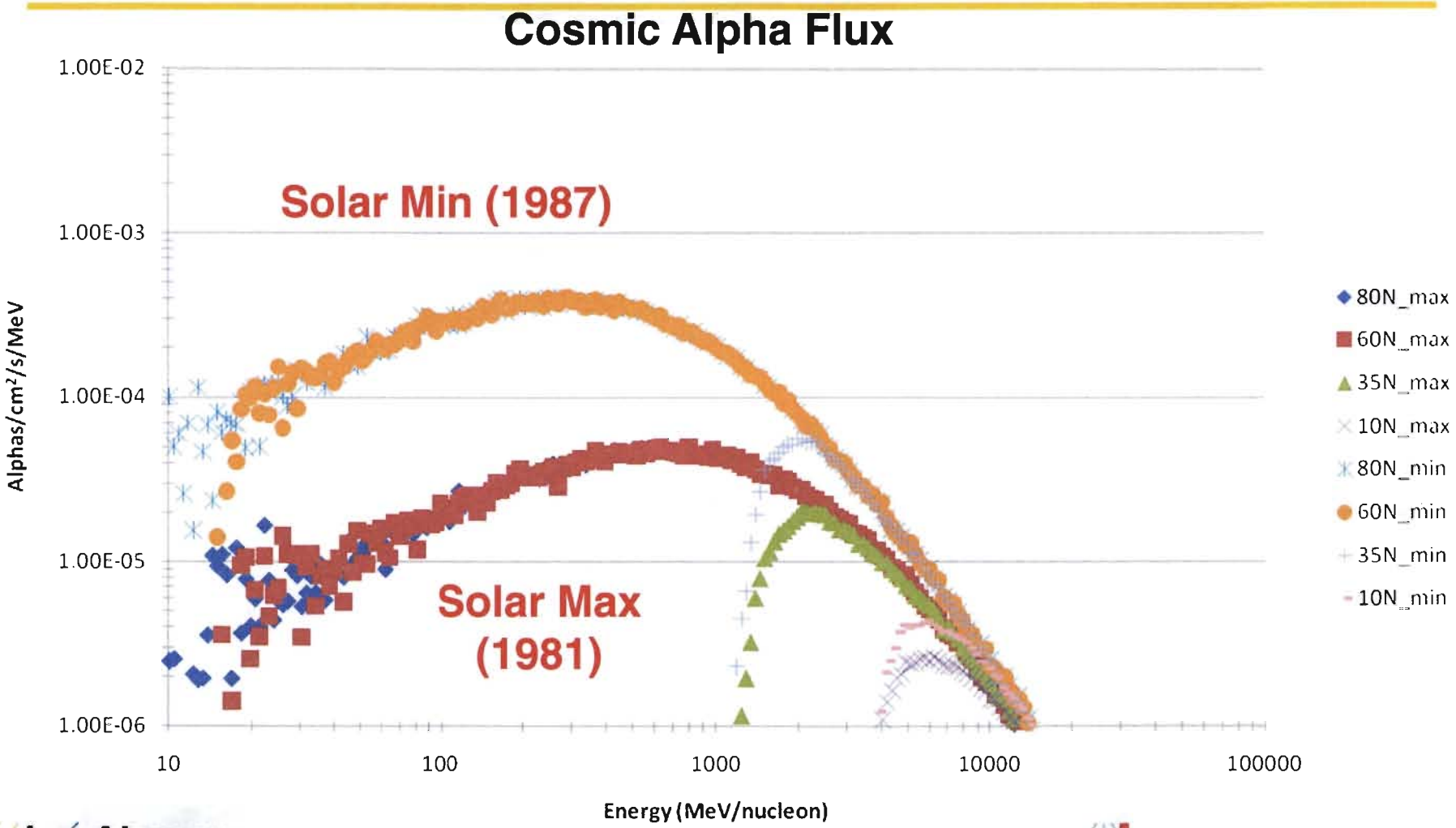
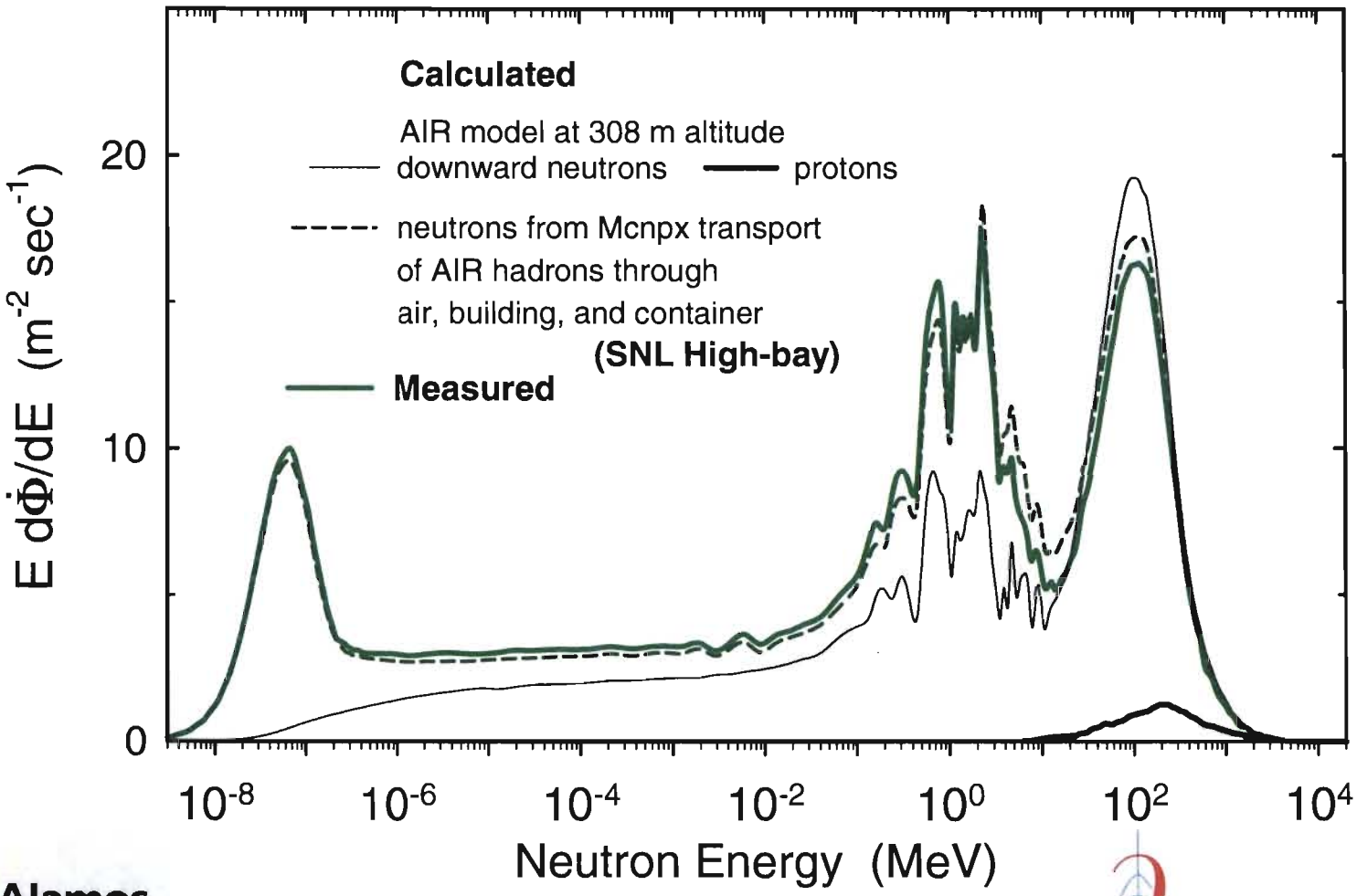


Use U of D cosmic spectra with MCNPX to produce starting spectrum for NUSTL spectrometer deconvolution

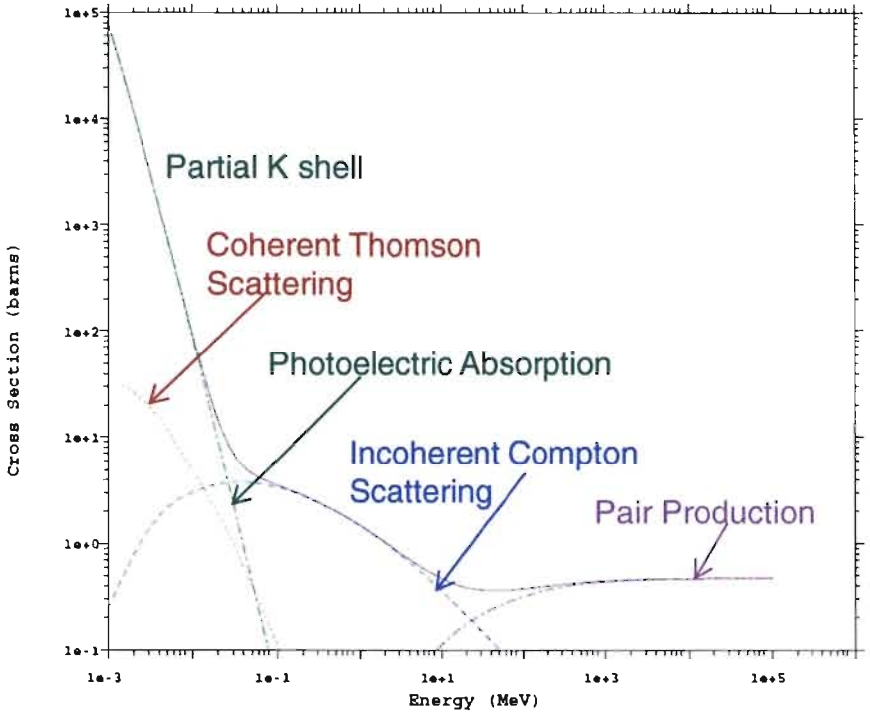


EPDL photon cross section upgrade

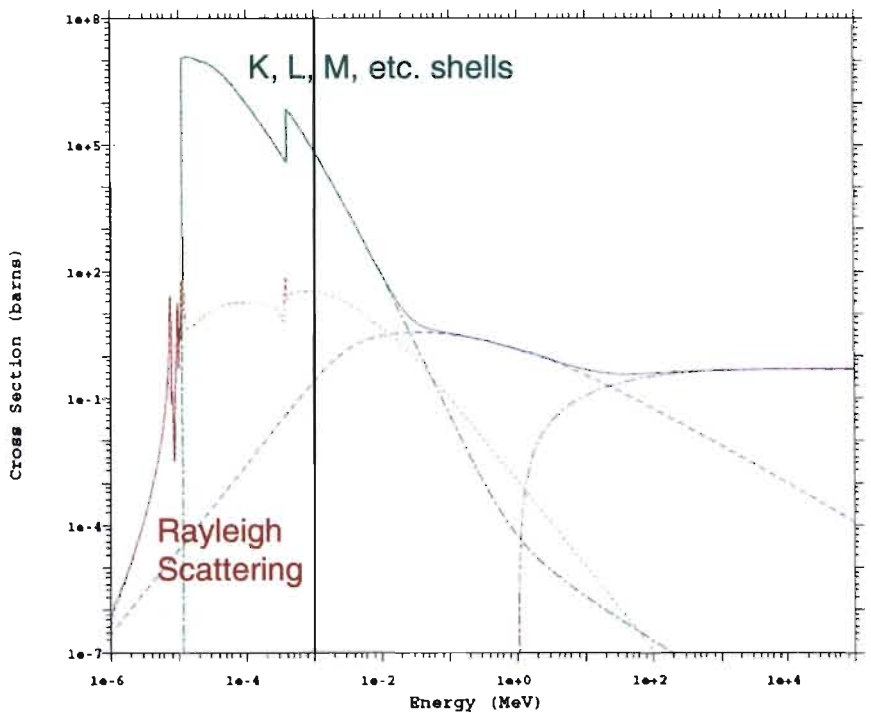
Extension to ENDF/BVI.8 EPDL photon cross sections

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

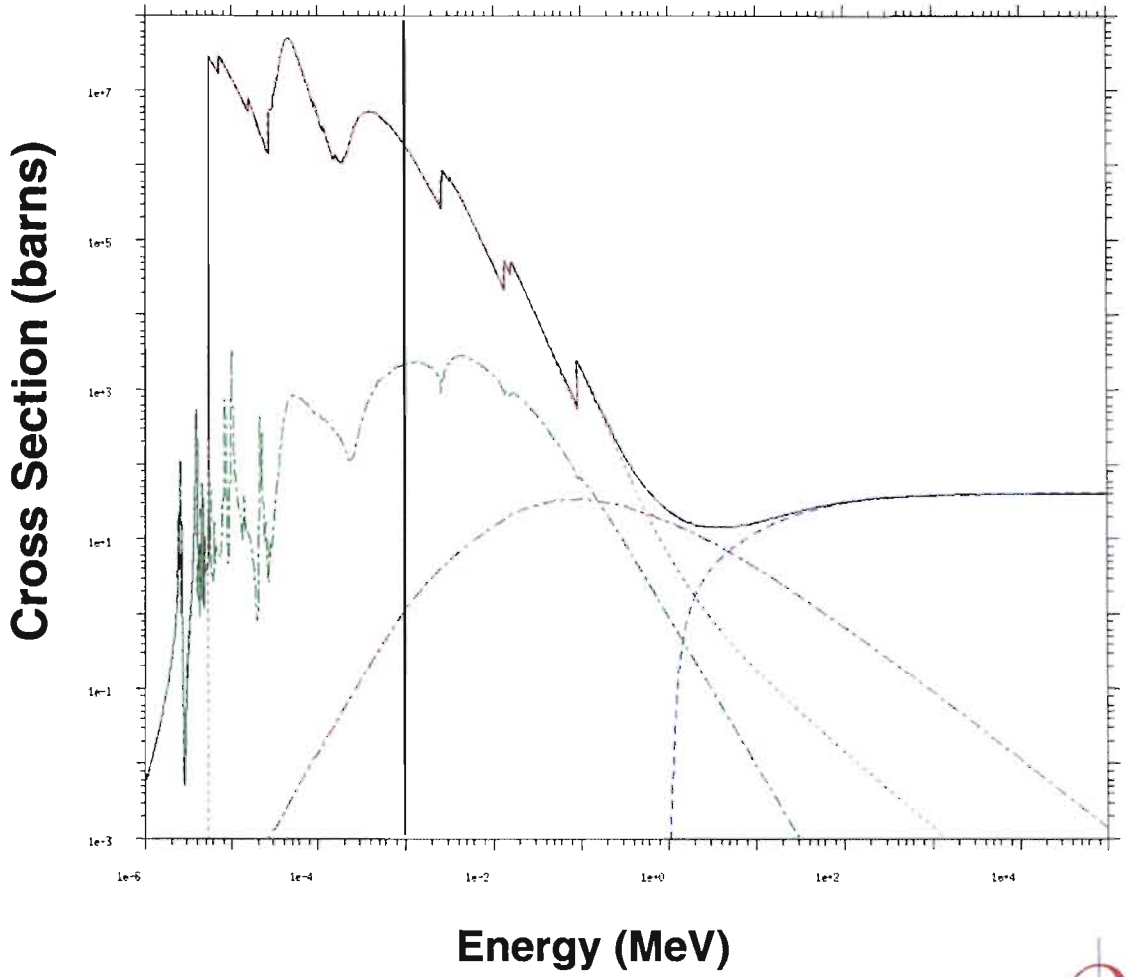
Old Nitrogen Cross Sections



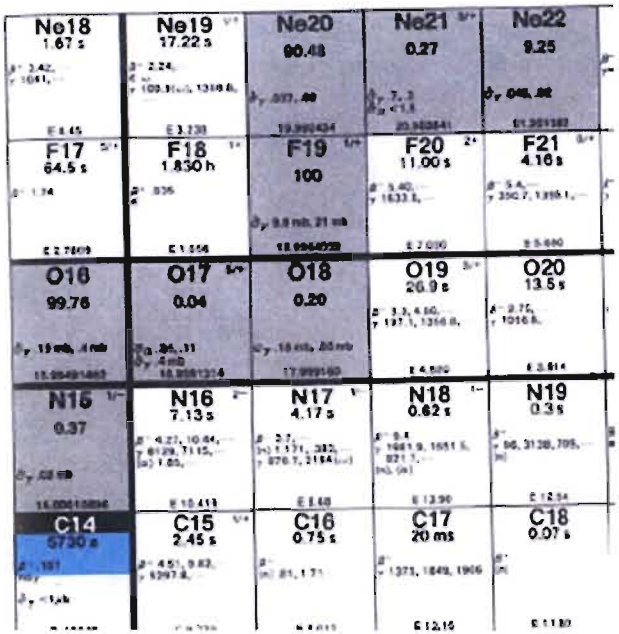
New Nitrogen Cross Sections



Cross Sections for Lead



Beta decay nuclides now in MCNPX – exact generation of neutrons



Z < 20, over 3

Li9	177 msec
Be12	24 msec
B13	17.4 msec
B14	14 msec
C16	.75 sec
C17	20 msec
C18	.07 sec
N17	4.17 sec
N18	0.62 sec

Z < 70, over 10

Co72, Co73, Co 74, Co 75
Ni73, Ni74, Ni75, Ni76, Ni77, Ni78
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Br87	55.9 sec
Br88	16.4 sec
Br89	4.37 sec
Br90	1.9 sec
Br91	0.54 sec
Br92	0.34 sec

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Eu165 (Z=63)

Rest are being worked on

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

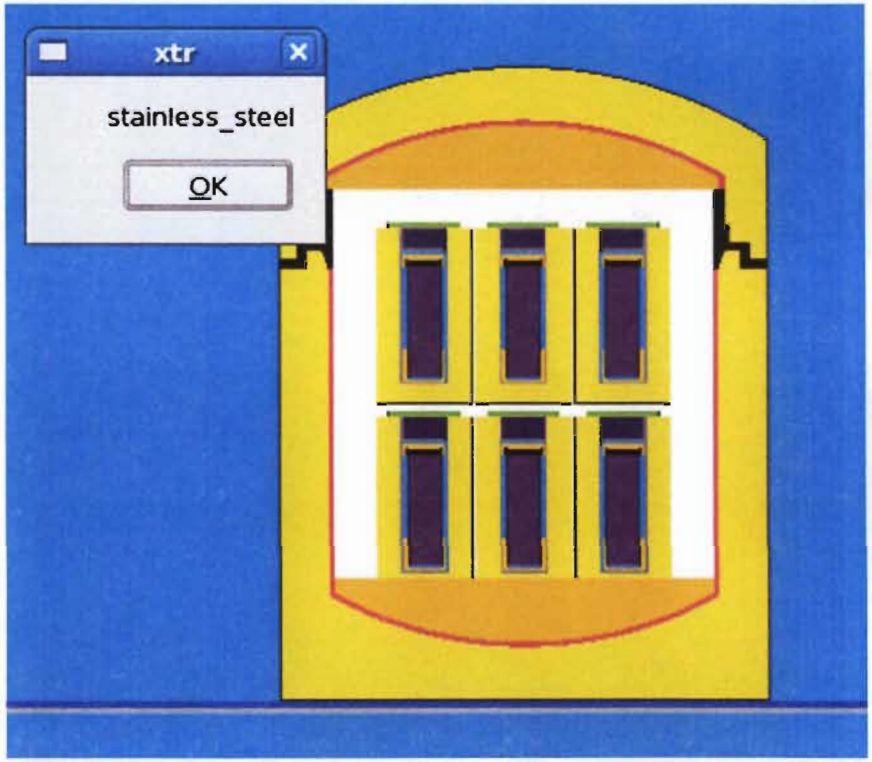
MCNP & MCNPX		TR-X
– Text only input	→	Graphic point and click interaction
– Small geometry changes can lead to large number of input modifications	→	Geometry manipulation simplified with templates
– Data analysis limited – Tallies – Cross Sections – Plotting available only with x-windows	→	Data handling expanded -- OUTP tables parsed & plotted -- Export to Excel format -- Comparison of cross section plots -- Runs natively under Widows, Mac, or Linux/Unix
– Mistakes are common and may be hard to spot	→	Wizards to check for common mistakes
– Running on Clusters confusing	→	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.

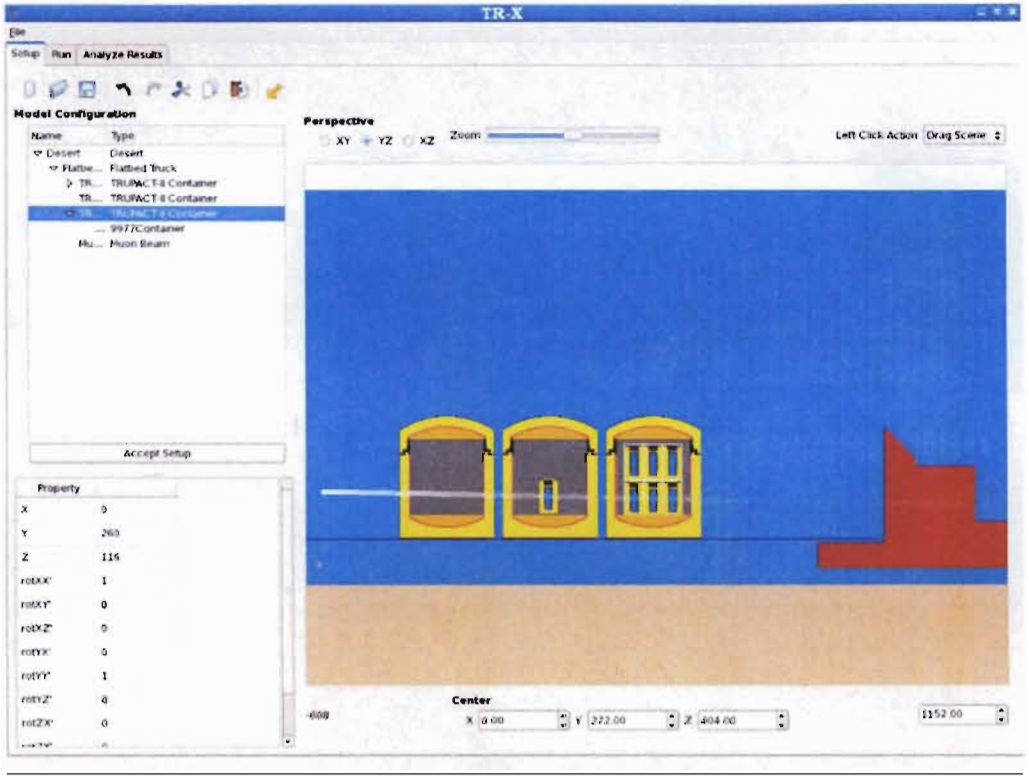
TR-X: Templates

- 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

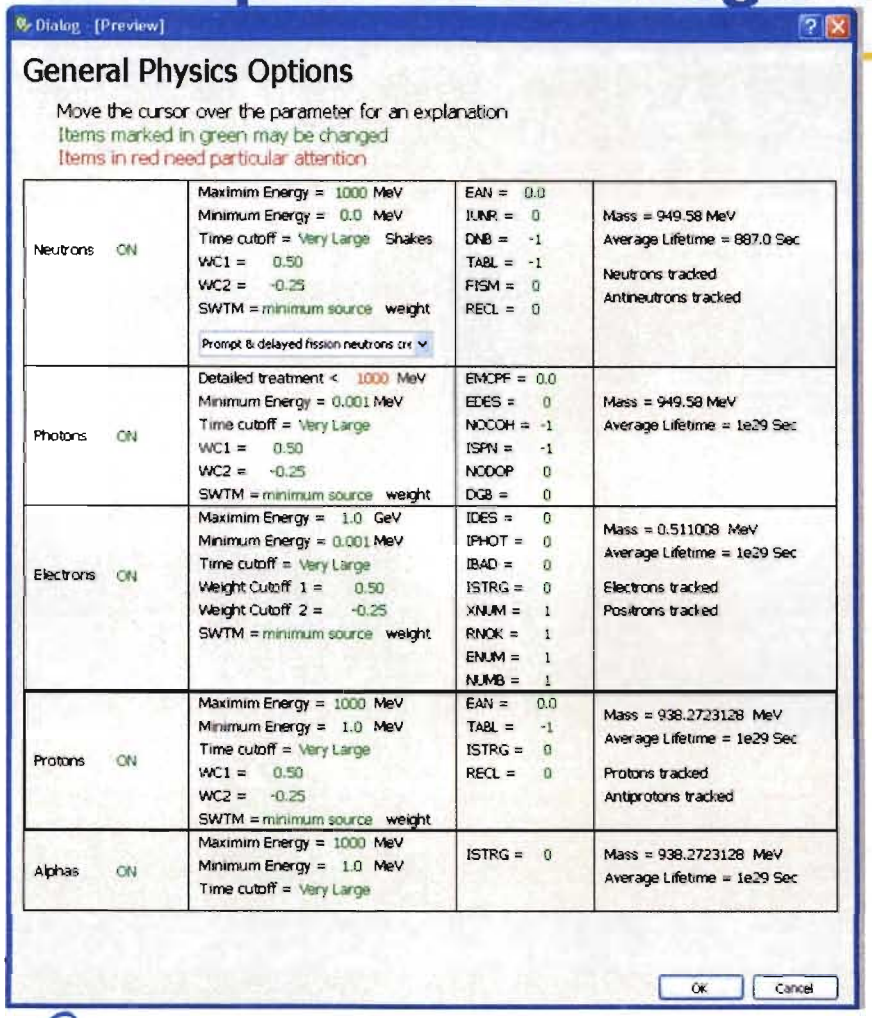
Physics Wizard

- 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



- One example of a Wizard sub-page is the General Physics Options page.
- This page presents users with options form 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

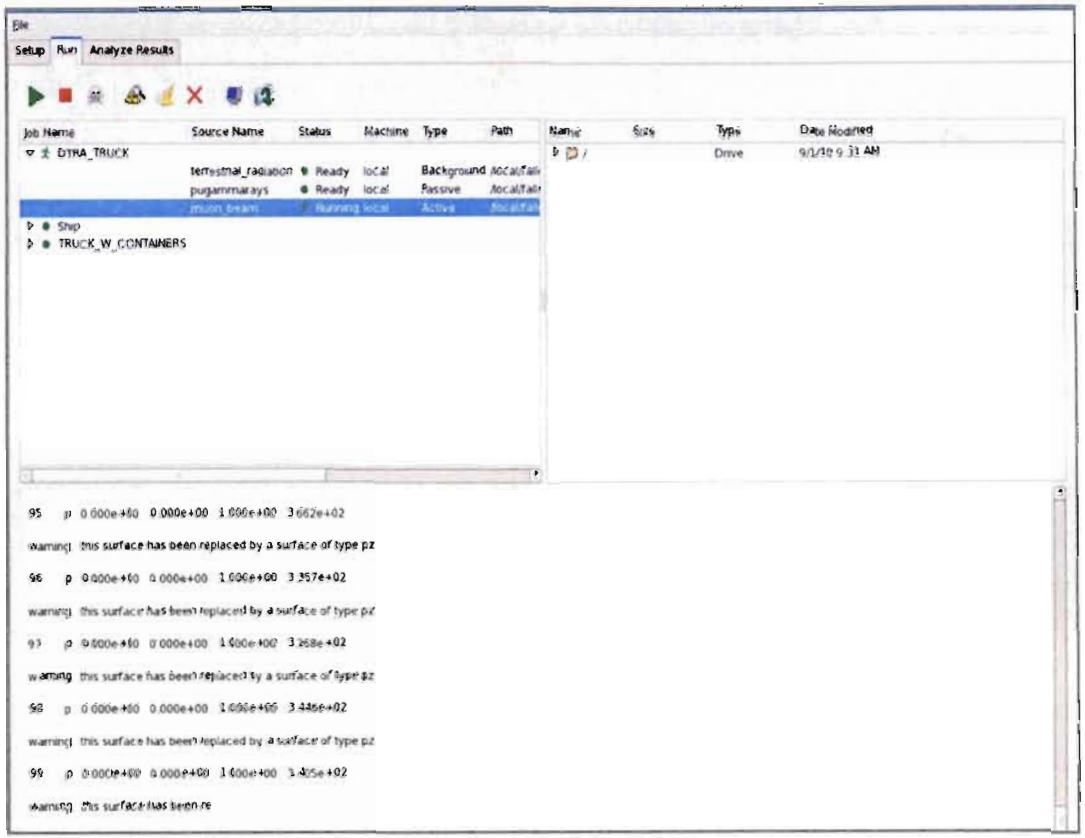
- Tool to gather needed information for running MNCP(X) on a remote machine
  - Machine name and path
  - Credentials to use for login
  - Type of credential verification
  - Number of processors on the machine
  - Submission process used to start jobs
- Does not set up the remote machine, the user must 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

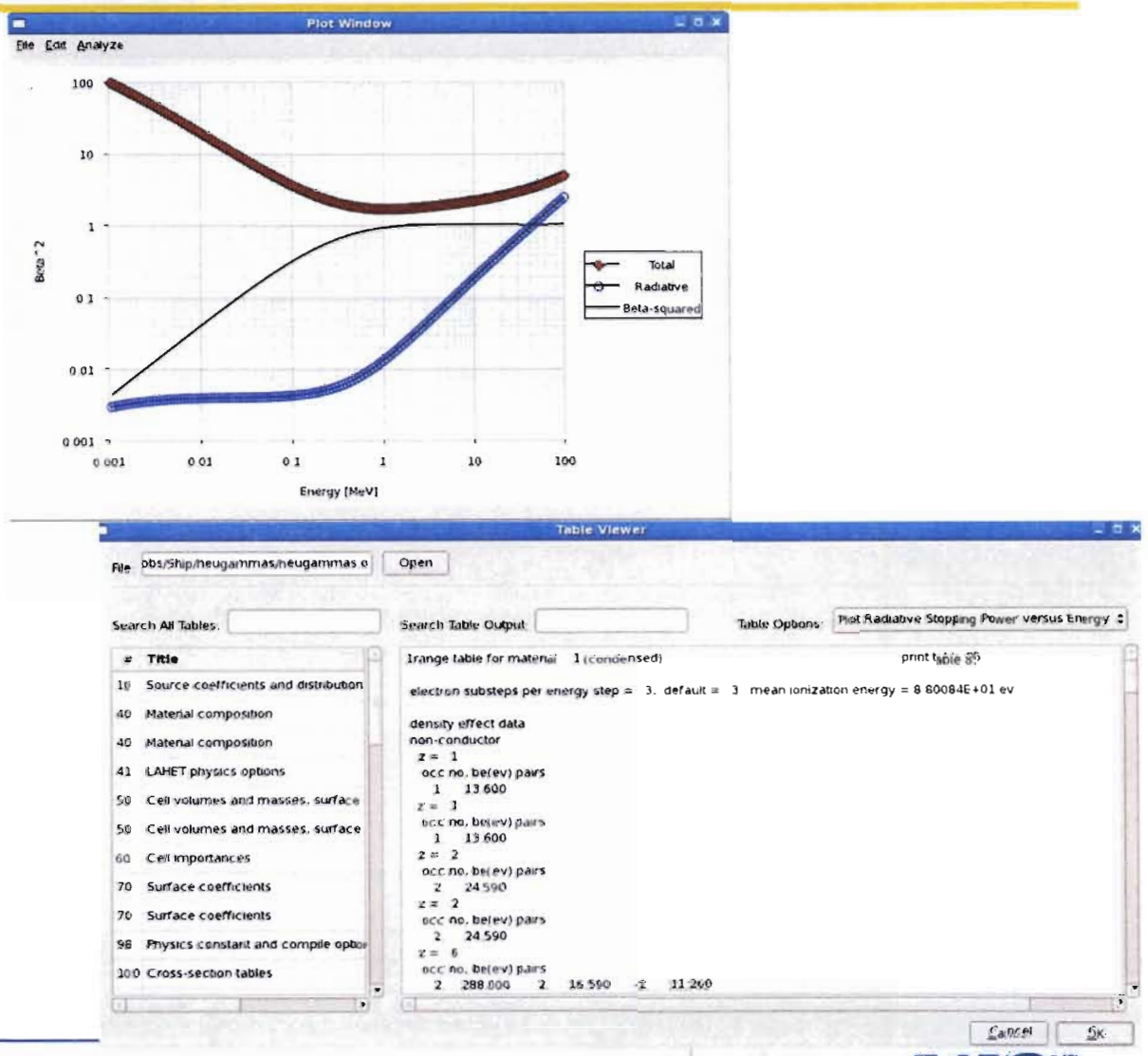
TR-X Page 2: Scenario Execution

- 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.



TR-X: Analysis – Page 3

- New tools are available for visualizing OUTP file data produced by a run.
- Tool 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.



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Conclusions

Questions?

TR-X development is sponsored by DTRA.