

Lawrence Livermore National Laboratory

LLNL Report



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Computational Nuclear Physics Overview

- Main conduit for communication and coordination between LLNL Programs and N Section (which is now part of Physics Division):
 - Coordinate nuclear data related experiment and theory activities in N Section
 - Chair Homeland Security Nuclear Data Taskforce
 - Manage LLNL nuclear data infrastructure
 - Website
 - Processing codes
 - Data access libraries
 - Neutron and photon transport routines
 - Manage LLNL nuclear data libraries
 - Perform evaluations in support of LLNL program
 - Collect & disseminate other LLNL evaluations
 - Provide non-LLNL nuclear data libraries to LLNL customers



Workforce

- CNP group is growing
 - Rob Hoffman
 - Moved over from Nuclear Theory and Modeling group
 - Sofia Quaglioni
 - Converted to term position from post-doc from NTM group
 - George Chapline
 - Jim Hall
 - Interviewing post-doc candidates for new data-format project
 - ARRA funding via USNDP
- Jason Pruet is on assignment in Washington
 - Eugene Brooks is acting group leader until he returns
- CNP collaborates with others at LLNL ...
 - Nuclear Theory: Jutta Escher, Petr Navratil, Erich Ormand, Ian Thompson, Walid Younes
 - Nuclear Experiment: Lee Bernstein, Jason Burke, Rick Norman, Ching-Yen Wu
 - Marie-Anne Descalle (former AP division), Brad Sleaford (Engineering), Doug Wright (High Energy)
- and outside LLNL
 - Other labs: LANL, LBNL, INL, TUNL
 - Academic Alliance partners: Yale, Richmond, Rutgers, UC Berkeley



Computational Nuclear Physics is producing many new and revised evaluations for the next ENDF release

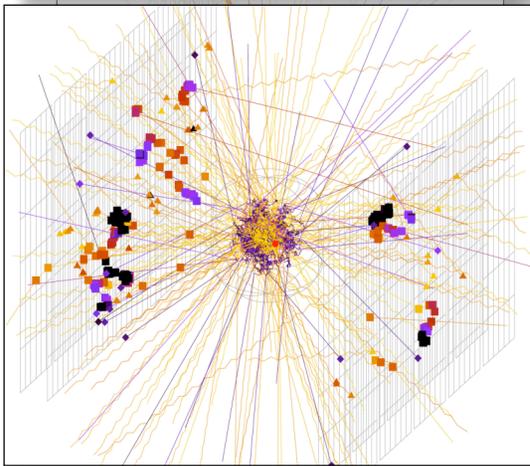
- Actinides
 - Submitting report for recommended JENDL/AC-2008 evaluations (59 minor actinides) for ENDF/B-VII.1
 - Reemerge ^{240}Am resonances for ENDF/B-VII.1
 - ^{239}U evaluation submitted for ENDF/B-VII.1
- Structural materials
 - Submitting for ENDF/B-VII.1: Ta, Re, Zn
- Radio-Chemical evaluations
 - Submitting for ENDF/B-VII.1: As, Kr, Xe



Targeted modeling gaps of high value to DNDO

All three physics models released on external website: <http://nuclear.llnl.gov>

Fission multiplicity



Multiple neutrons and gamma-rays produced from fission

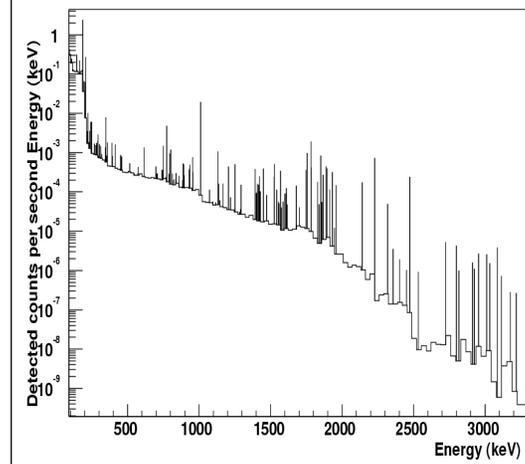
Essential physics for fission-chain detector concept: can detect shielded HEU

DHDO 06-08: \$1.6M

Interface also provided for MCNP, MCNPX, Geant4, COG

Doug Wright (PI), Dave Brown, John Buyer, Chris Hagmann, Tom Gosnell, Jeff Gronberg, Larry Hiller, David Lange, Jerome Verbeke, Ramona Vogt

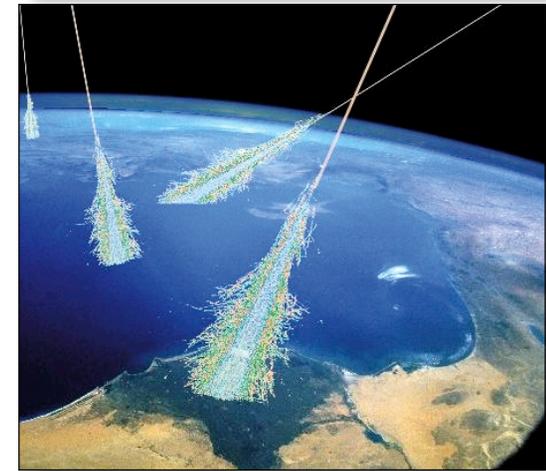
Gamma-ray Emission



Gamma-ray source intensity for aged mixtures of Special Nuclear Material

Source term for SNM in all gamma-ray detection concepts

Cosmic-ray showers

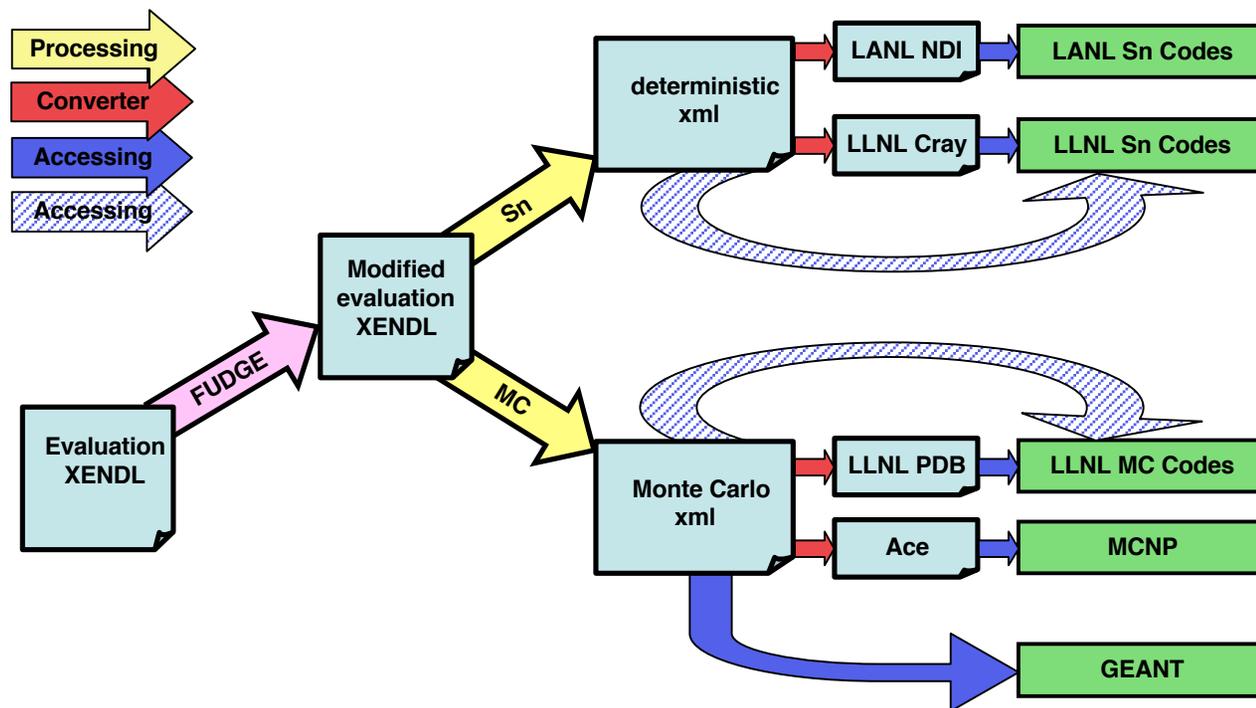


Energetic particles produced in upper atmosphere that reach the ground

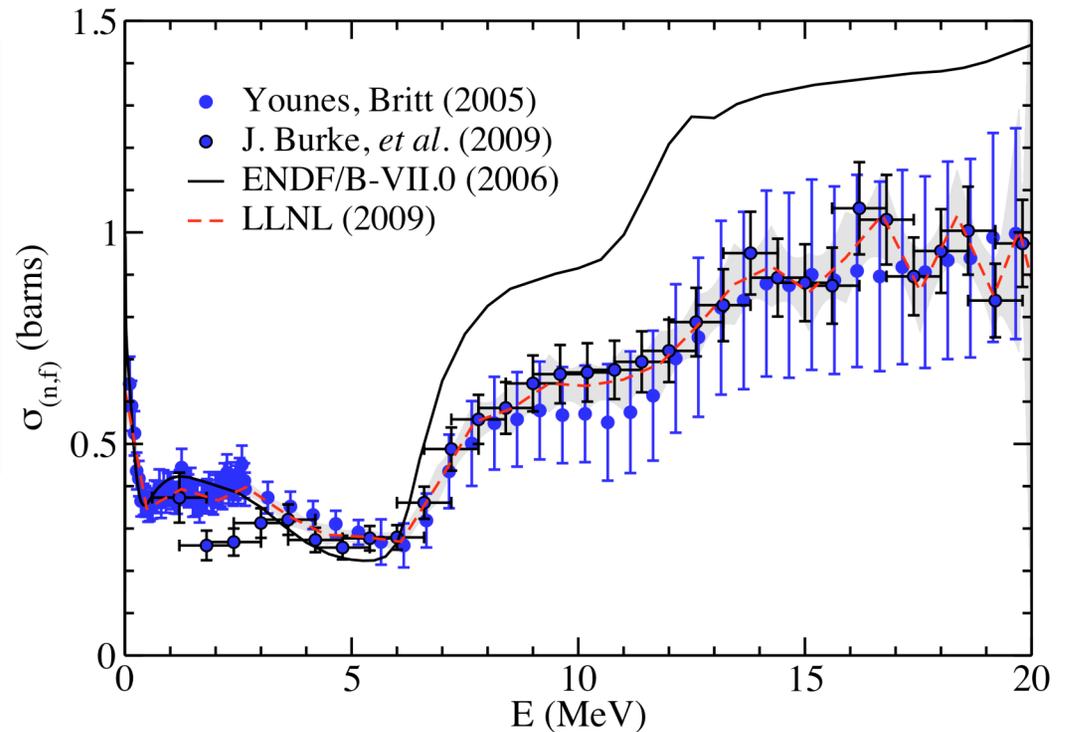
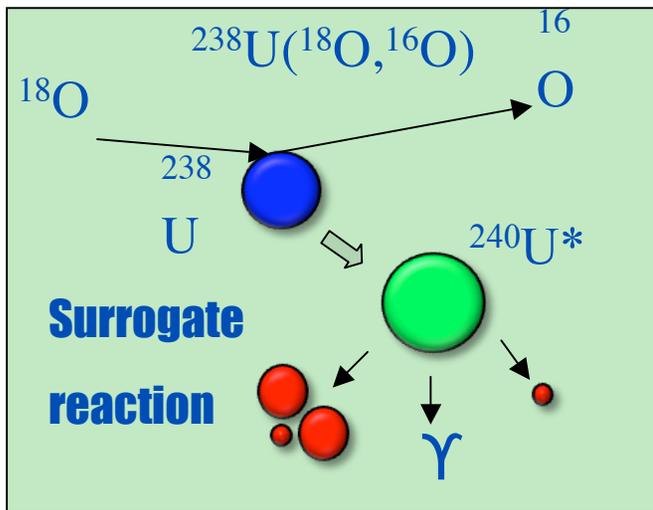
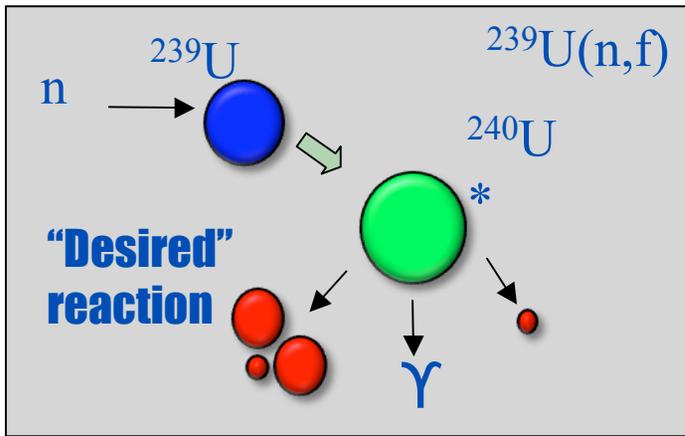
Significant background in neutron detection, especially for maritime cargo applications

LLNL leading the way in modernization of nuclear data formats

- Upgrading data formats to data rich XML format
- Received ARRA funding
 - Interviewing post-doc candidates for position



LLNL continues to lead the experimental and theoretical development of the surrogate reaction technique



$$\sigma({}^{239}\text{U}(n,f)) = \frac{N_{p-f}({}^{238}\text{U}({}^{18}\text{O}, {}^{16}\text{O}f))}{N_{p-f}({}^{234}\text{U}({}^{18}\text{O}, {}^{16}\text{O}f))} \times \sigma({}^{235}\text{U}(n,f))$$

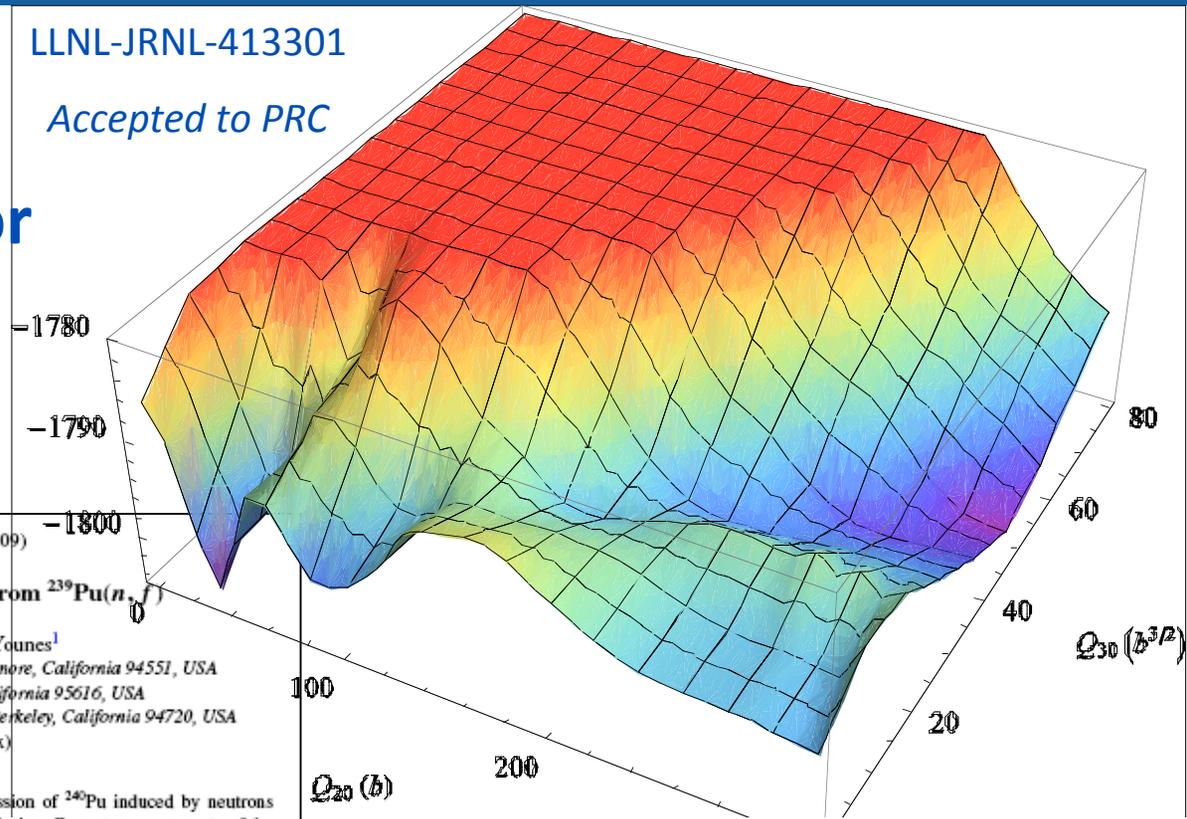
Theoretical effort underway to understand the J^π dependence of the surrogate approach and go beyond Wiesskopf-Ewing Approx.

LLNL efforts have resulted in new theoretical understanding of fission

Energy surface for Pu-240 fission

LLNL-JRNL-413301

Accepted to PRC



PHYSICAL REVIEW C 00, 004600 (2009)

Event-by-event study of prompt neutrons from $^{239}\text{Pu}(n, f)$

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Employing a recently developed Monte Carlo model, we study the fission of ^{240}Pu induced by neutrons with energies from thermal to just below the threshold for second-chance fission. Current measurements of the mean number of prompt neutrons emitted in fission, together with less accurate measurements of the neutron energy spectra, place remarkably fine constraints on predictions of microscopic calculations. In particular, the total excitation energy of the nascent fragments must be specified to within 1 MeV to avoid disagreement with measurements of the mean neutron multiplicity. The combination of the Monte Carlo fission model with a statistical likelihood analysis also presents a powerful tool for the evaluation of fission neutron data. Of particular importance is the the fission spectrum, which plays a key role in determining reactor criticality. We show that our approach can be used to develop an estimate of the fission spectrum with uncertainties several times smaller than current experimental uncertainties for outgoing neutron energies of less than 2 MeV.

LLNL-JRNL-415141

PRC 80, 044611 (2009)



Ab initio no-core shell model (NCSM) & resonating-group method (RGM)

Leading the way for new evaluations for thermonuclear reactions

- NCSM/RGM – dynamic (& static) properties**

- *Ab initio* calculations for reactions and clustering in nuclei
- Expansions on channels of nucleon clusters and their relative motion

$$H\Psi^{(A)} = E\Psi^{(A)} \quad \begin{matrix} \vec{r}_{A-a,a} \\ (A-a) \quad (a) \end{matrix}$$

$$\sum_{\nu} \int d\vec{r} \left[\mathcal{H}_{\mu\nu}^{(A-a,a)}(\vec{r}', \vec{r}) - E\mathcal{N}_{\mu\nu}^{(A-a,a)}(\vec{r}', \vec{r}) \right] \phi_{\nu}(\vec{r}) = 0$$

$\left\langle \begin{matrix} (A-a) & (a) \\ \vec{r}' & \vec{r} \end{matrix} \left| \hat{A} H \hat{A} \right| \begin{matrix} (a) & (A-a) \\ \vec{r} & \vec{r}' \end{matrix} \right\rangle$

Hamiltonian kernel

$\left\langle \begin{matrix} (A-a) & (a) \\ \vec{r}' & \vec{r} \end{matrix} \left| \hat{A}^2 \right| \begin{matrix} (a) & (A-a) \\ \vec{r} & \vec{r}' \end{matrix} \right\rangle$

Norm kernel

