LLNL Lab Report CSEWG/USNDP 2006

D.A. Brown, D. McNabb

for the CNP Group

# Computational Nuclear Physics Group Overview

- Main conduit for communication and coordination between LLNL Programs and N Division:
  - Coordinate nuclear data related experiment and theory activities in N Division
  - Perform evaluations in support of LLNL program
  - Collect & disseminate other LLNL evaluations
  - Manage LLNL nuclear data infrastructure
    - Website
    - Processing codes
    - Data access libraries
    - Nuclear data libraries

- Chair Homeland Security Nuclear Data Taskforce

- Effort and funding:
  - 0.5 FTE from USNDP, 8.5 FTE from PDRP & NHI/DNDO

Dissemination

- New Nuclear and Atomic Data System (NADS) features:
  - Translated data
  - Documentation of evaluations
  - Standalone mode can integrate in other systems
- Website redesign: we're evolving from group website to LLNL nuclear data portal
  - Nuclear and Atomic Data Viewer
  - Translated ENDF data
  - Our processing codes and access routines
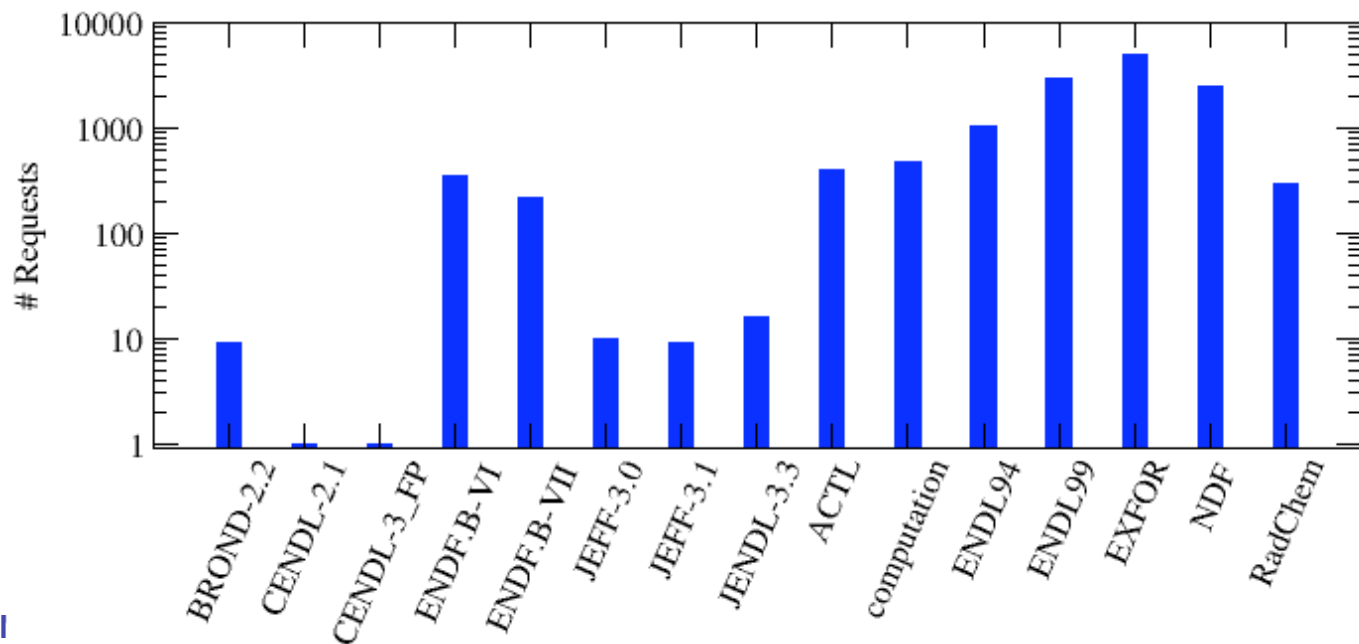 - Various simulation codes

UCRL-PRES-225849

NADS Usage Statistics
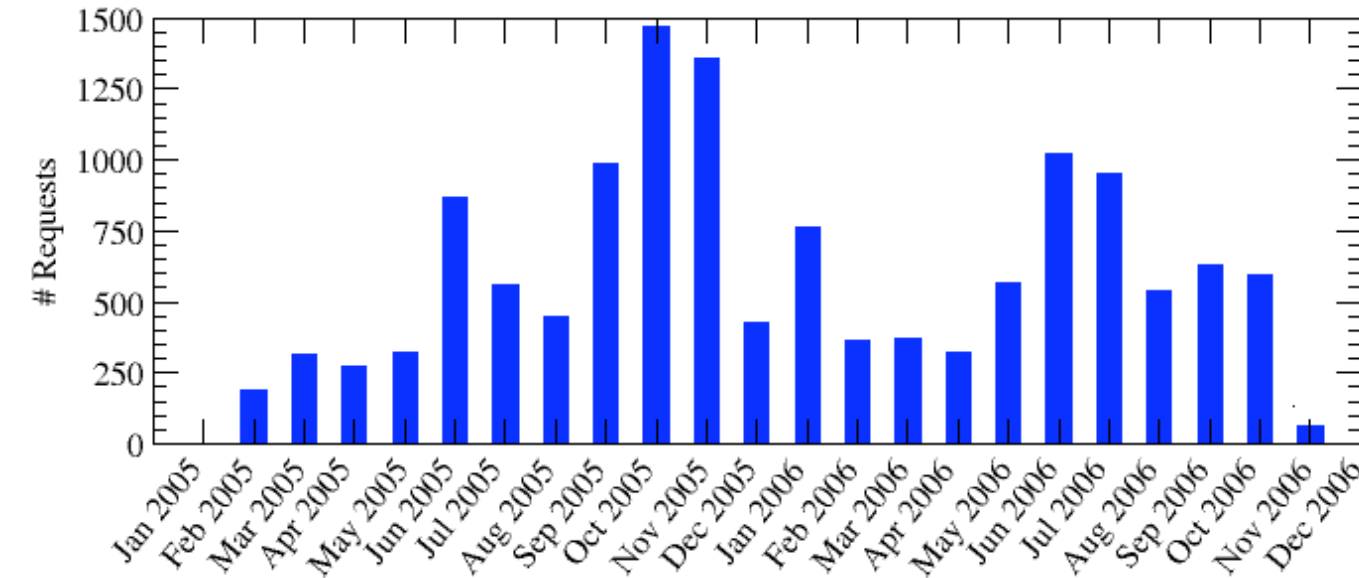
Total data requests: 13416

Total number of sessions: 3107

Average number of data per sessions: 4

Evaluation activity

- ^{74}As, ^{75}As full evaluations (joint PDRP, USNDP funding)

- ^{240}Am full evaluation, in progress (PDRP)

- Post-fission β-delayed γ data for ^{235}U, ^{239}Pu

- 489 partial (cross-section only) evaluations for activation (PDRP funding)

  – Performed by R. Hoffman NTM group, we packaged

- Merging EGAF into ENDF/B-VIIβ3 evaluations, in progress (USNDP funding)

N Division highlights

UCRL-PRES-225849

Translated ENDF data release

- Translated ENDF/B-VIIβ2,β3, ENDF/B-VI, JEFF-3.1, JEFF-3.0, JENDL-3.3, CENDL-2.1, CENDL-3_FP, Maslov into ENDL format

- 8x increase in nuclear data available to LLNL

- Data posted to http://nuclear.llnl.gov/
  - Tarballs
  - Nuclear and Atomic Data System

- Received Physics and Advanced Technology PDRP award

PI: D. Brown
Entire CNP group

UCRL-PRES-225849

New Theory for Nuclear Reactions

Goal: Describe nuclear reactions with light nuclei using fundamental nuclear interactions

- Extension of no-core shell model with resonating group method
  - RGM is in development, currently we renormalize the asymptotic behavior with data
- Thermonuclear reactions
  - d(t,n)α at low temperature
  - ^{7}Be(p,γ)^{8}B, ^{3}He(α,γ)^{7}Be, α(2α,γ)^{12}C
- Neutron-induced reactions
  - ^{6}Li(n,α)t, ^{11}B(n,n'γ)^{11}B
  - ^{10}Be(n,γ)^{11}Be
- Support from ASC, DOE/NP, and SciDAC

PIs: Erich Ormand, Petr Navratil

Illustration of convergence with model space
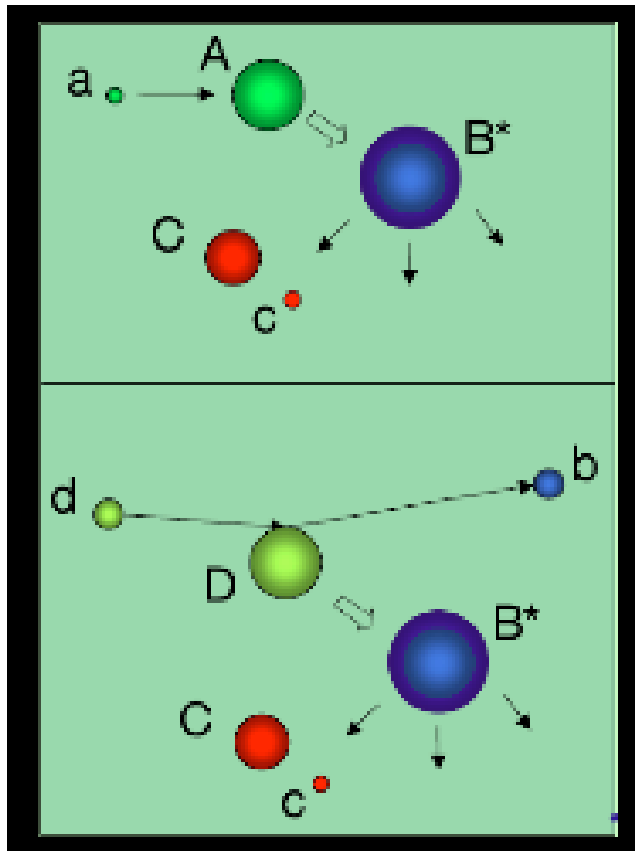S-factors calculated down to zero energy

49
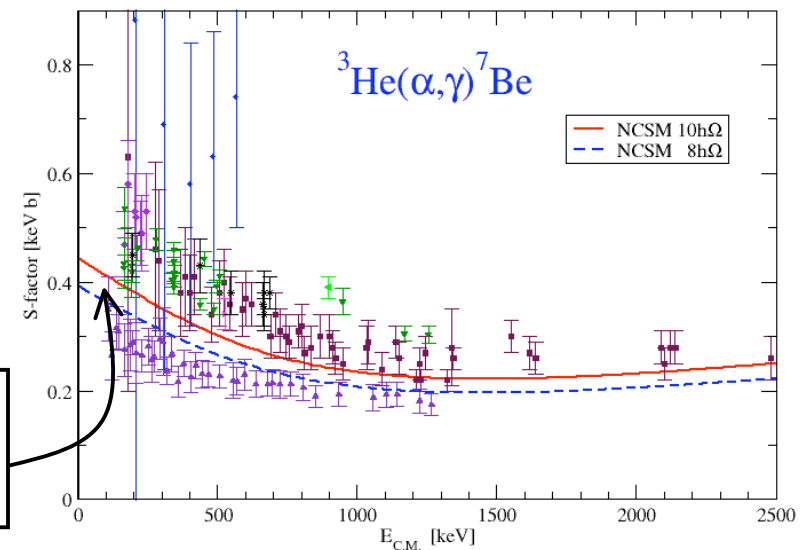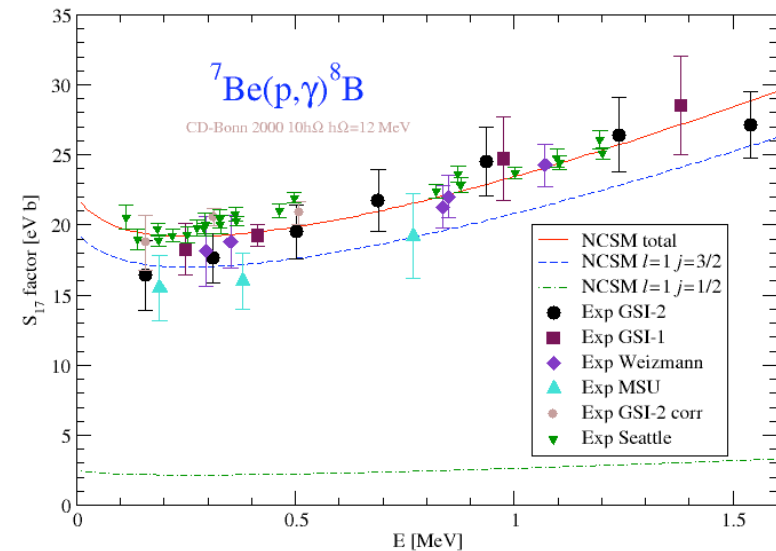
Fission modeling

- 1st-ever Skyrme-Hartree-Fock calculations in ^{236}U using large-scale RPA calculations

  – RPA restores rotational symmetry of Hamiltonian broken by Hartree-Fock approximation

- Currently writing LLNL Hartree-Fock-Bogoliubov code for finite-range interactions

  – More realistic than commonly used Skyrme = zero-range

  – Emphasis on code speed: will be used in large-scale calculation of fission dynamics
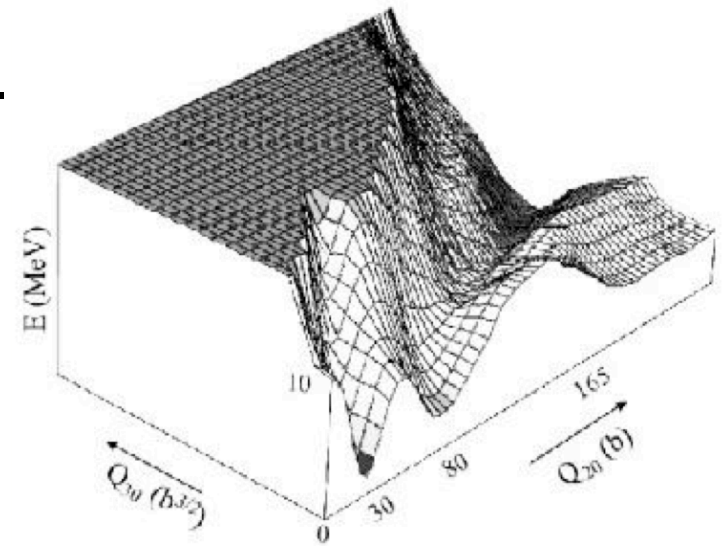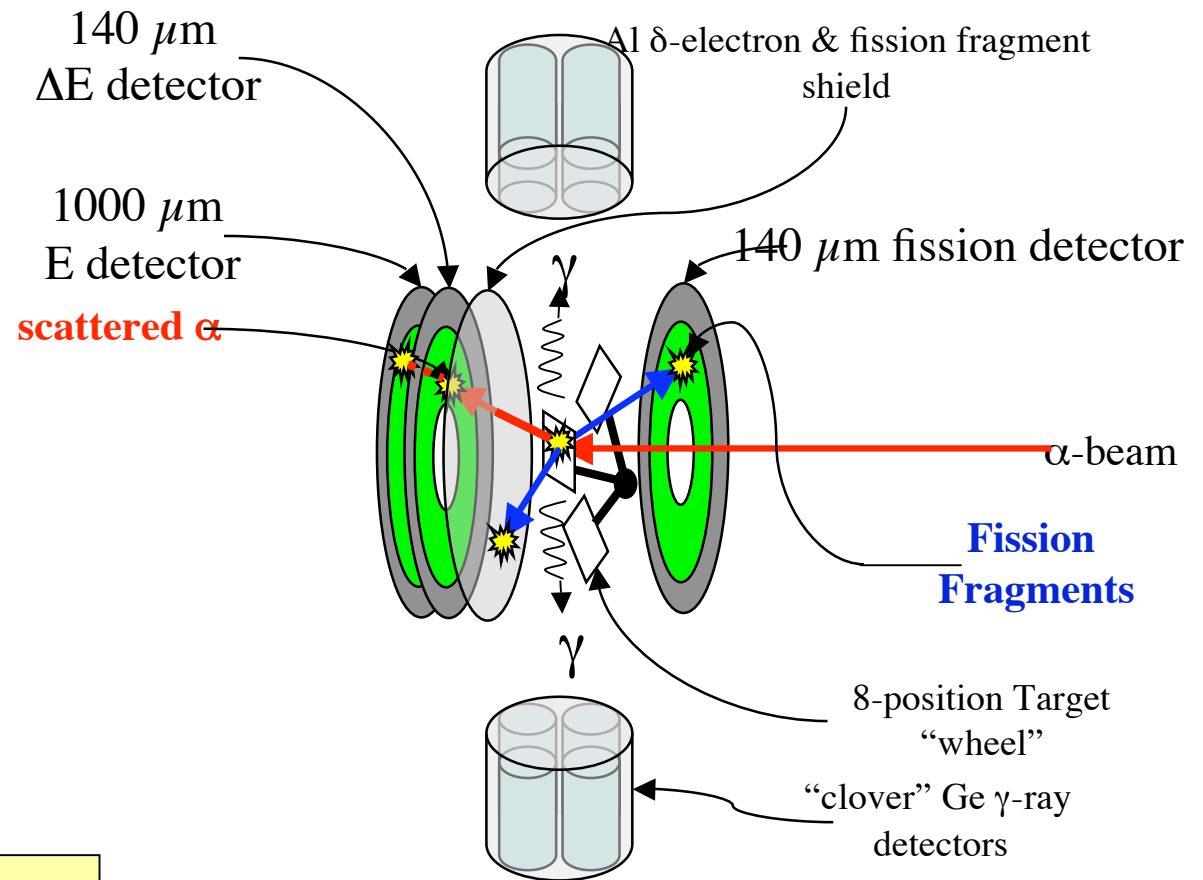

PI: Walid Younes

Collaboration w/ Daniel Gogny, BIII

Continued investment in "surrogate" reactions as a way to deduce neutron cross section data
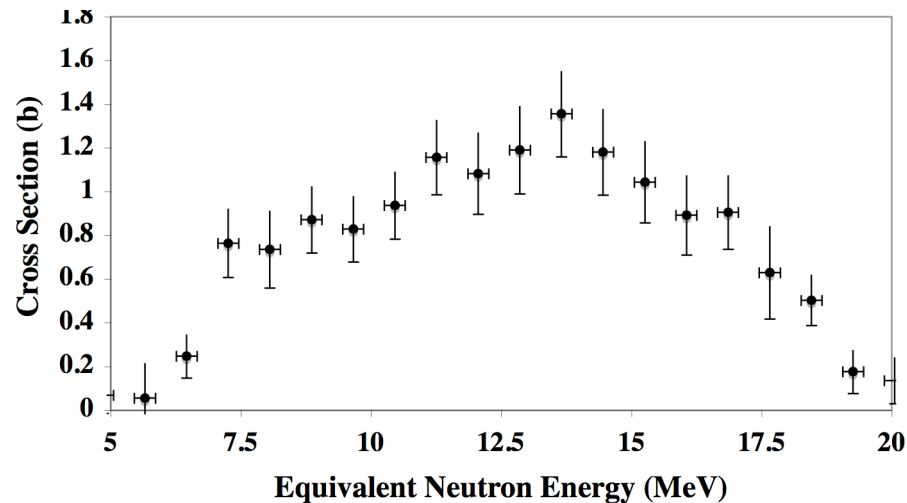

140 μm ΔE detector

Al δ-electron & fission fragment shield

1000 μm E detector

scattered α

140 μm fission detector

γ

α-beam

Fission Fragments
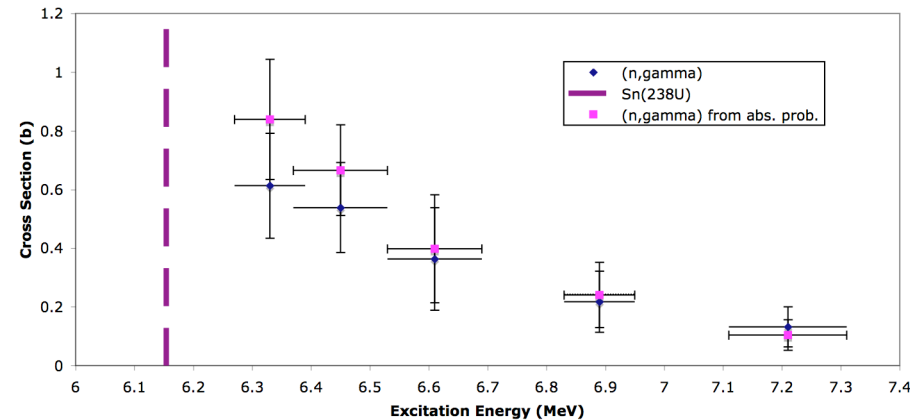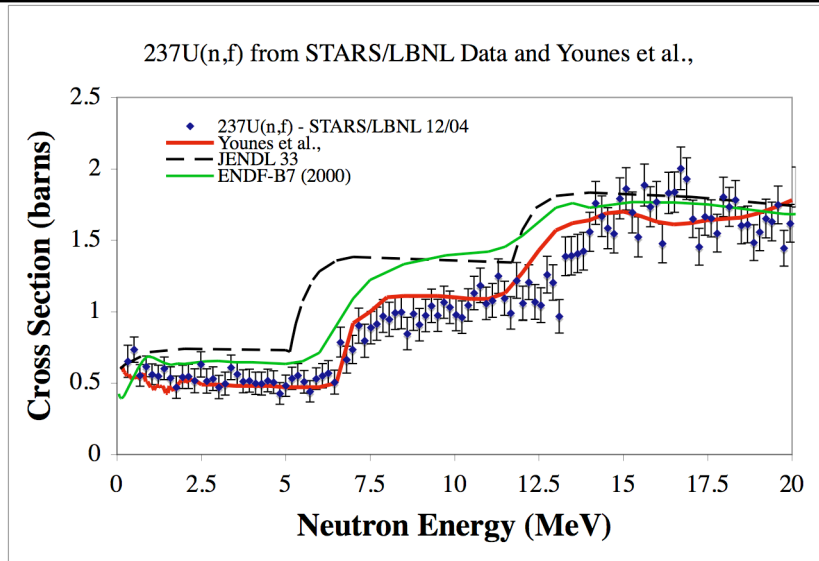
γ

8-position Target "wheel"

"clover" Ge γ-ray detectors

PI: Lee Bernstein
Collaboration between LLNL, Yale, LBNL

Silicon Telescope Array for Reaction Studies (STARS)

Surrogate reaction results

237U(n,f) from STARS/LBNL Data and Younes et al.,

- 237U(n,f) - STARS/LBNL 12/04
- Younes et al.,
- JENDL 33
- ENDF-B7 (2000)

Cross Section (barns) vs Neutron Energy (MeV)

- (n,gamma)
- Sn(238U)
- (n,gamma) from abs. prob.

Cross Section (b) vs Excitation Energy (MeV)

Cross Section (b) vs Equivalent Neutron Energy (MeV)

First-ever deduction of $^{237}U(n,2n)$ and $^{237}U(n,\gamma)$ ($t_{1/2}$=6.75 days)

Things to watch for next year

- Developing subset of XML nuclear data format for deterministic and Monte-Carlo data (B. Beck, M. White (LANL))

- 2007 Release of ENDL library in legacy ENDL and new XML format (D. Brown)

- Continued development of nuclear data infrastructure for use of new XML formatted data

- New http://nuclear.llnl.gov/ nuclear data portal

- New software quality assurance mandates from ASC program