

8 Outside Users

8.1 Studies of the low energy fission of the actinides using surrogate reactions

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The nuclear fission process is both technologically important and because of its complexity, difficult to model with certainty. Among the measurable quantities in fission of technological importance are the prompt neutron spectra and multiplicities. The variation of these quantities with fragment mass division, nuclear excitation energy E^* , nuclear composition (Z,A) and the fragment kinetic energy release offers insight into the partition of energy during the large scale collective motion of the scission process.¹ While the neutron multiplicities and spectra of some of the major actinides of interest to nuclear technology have been well-characterized, there is a paucity of data on the minor actinides. Accordingly we are engaged in an effort to characterize the fission properties of several minor actinides. Since we are generally interested in neutron emission from these nuclei, we are using reactions (surrogate reactions) other than neutron capture to induce fission.

In our first experiments at the CENPA, we formed the fissioning nuclei, ^{237}U , ^{238}U , ^{239}U , ^{236}Np , ^{237}Np , ^{238}Np , ^{240}Np and ^{239}Pu using surrogate reactions like (d,pf), (d,d'f), etc. We attempted to measure the fission cross section, mass-yield distributions, fission neutron multiplicities, and fission neutron spectra as a function of the excitation energy of these nuclei.

Our experimental setup is shown in Fig. 8.1-1. The incident deuteron beam strikes a thin ($\approx 0.5 \text{ mg/cm}^2$) target of ^{238}U or ^{237}Np and emitted charged particles are detected in a three element counter telescope at 90° with respect to the incident beam. Fission fragments are detected by either Si strip detectors or arrays of individual surface barrier detectors. The time of flight and multiplicity of any coincident neutrons is measured using a series of BC501A liquid scintillators. By gating on the energy and (Z,A) of the emitted charged particles, excitation functions are deduced.

Our first run occurred in January-February, 2006. Data analysis is in progress.

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¹R. Vandenbosch and J. R. Huizenga, *Nuclear Fission*, Academic, New York, NY (1973).

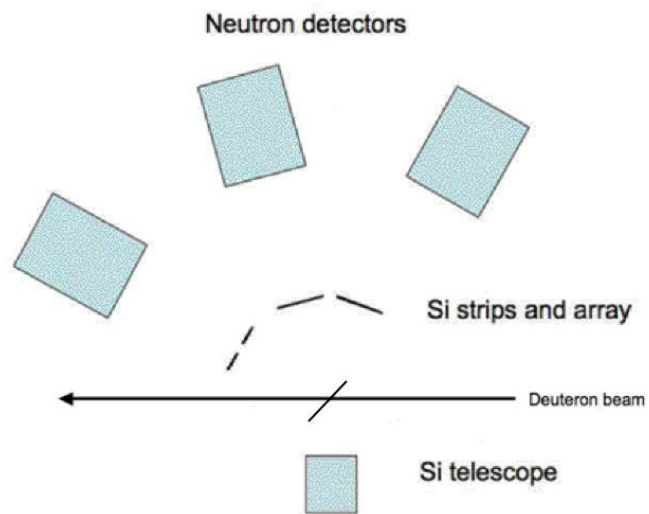


Figure 8.1-1. Schematic diagram of the experimental setup. An additional neutron detector is located out of the reaction plane above the target.

8.2 Department of Astronomy Beowulf cluster*

E. Agol,[†] V. P. Debattista,[†] C. J. Hogan,[†] N. A. Kaib,[†] T. R. Quinn,[†] R. Roskar,[†] J. H. Steffen[‡] and K. Zurek[‡]

The 64-processor Beowulf cluster (metate) located at CENPA has been used by T. Quinn and collaborators in the Astronomy and Physics departments for both cosmological and planetary applications.

On the cosmological side Physics graduate student, K. Zurek, in collaboration with C. Hogan and T. Quinn has been calculating the generation of cosmic structure via a late phase transition of an axion field. These structures could be of interest for microlensing experiments, but numerical simulations of their non-linear collapse are needed to make predictions of their lensing properties.

Astronomy graduate student, R. Roskar, in collaboration with postdoc, V. Debattista, and T. Quinn, is simulating the evolution of the disks of spiral galaxies in the presence of bar instabilities. They are trying to understand the origin of breaks in the usual exponential disk structure.

Physics graduate student, J. Steffen, in collaboration with E. Agol, has been doing planetary orbit integrations in order to identify or constrain the secondary planets in known, transiting systems using a novel timing technique.¹

Astronomy graduate student, N. Kaib, in collaboration with T. Quinn, is modelling the formation of the Oort Cloud in a realistic star formation environment. This work investigates the effect that the Sun's birthplace has had on the evolution and structure of the Oort Cloud.²

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¹E. Agol, J. H. Steffen, *et al.*, MNRAS 359 567, (2005); and J. H. Steffen and E. Agol, MNRAS 364 96L, (2005).

²Kaib, N. & Quinn, T., 2006; *The Effect of the Sun's Early Environment on Oort Cloud Formation and Comet Showers*, [Abstract]; AbSciCon 2006, Washington, DC. Internat. J. Astrobiology, Supplement 1 (2006).

8.3 Molecular dynamics of proteins and peptides*

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The Department of Medicinal Chemistry shares the CENPA co-located Beowulf Cluster “metate”.

Dr. Valerie Daggett’s lab in the Department of Medicinal Chemistry has been using the cluster to work on methods development projects and production work treating protein structure and dynamics. We use all-atom molecular dynamics (MD) simulations to calculate the dynamics of protein motion. This allows us to investigate a wide range of biological problems, including prion diseases (e.g., Mad Cow Disease), the protein folding problem, and the movement of a protein in its normal solvated biological environment. MD is especially useful where experimental probes of dynamics do not have the time resolution to describe rapidly occurring events.

Specific work:

- Replicate Exchange Molecular Dynamics (REMD) is a newer molecular dynamics method that purportedly improves sampling in MD simulations. George White, a recently graduated Ph.D. from the Biomolecular Structure and Design (BMSD) program, worked on the testing and development of REMD. The stability of the metate cluster made it practical for George to parallelize this method over many nodes.

- Peptides: Daigo Inoyama was an undergraduate student who has subsequently gone on to medical school. He used the cluster to simulate small peptides. In this case these were chains of five amino acids, rather than the chains of greater than fifty amino acids that generally form folded proteins. Because of their short chain length, short peptides remain dynamic and do not form the relatively rigid three dimensional fold of most proteins of fifty amino acids or more.

- Prion Protein: The prion protein is the pathological and infectious agent in a variety of neurological diseases including Bovine Spongiform Encephalopathy (BSE, a.k.a Mad Cow Disease) and Creutzfeld-Jakob Disease (CJD). The protein has benign and infectious forms, and they differ only in their fold or conformation. They are chemically identical. Alex Scouras, a Biochemistry graduate student in our lab, used the metate cluster to observe structural changes starting from the benign form of the prion protein.

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