Data and Codes Working Group Summary
Oct. 10, 2012

This Working Group addressed four questions: What is needed to evaluate and transform nuclear / astronomy data and codes reliably and efficiently for use in nuclear astrophysics ? What are the best evaluation procedures and how can they be developed and implemented ? How should information be distributed – formats ? What additional public codes are needed and how should one develop ? The session included five presentations and a (limited) time for open discussion.

In his talk on "Online resources for Nuclear Astrophysics", Michael Smith (ORNL) surveyed some of the very useful datasets, codes, and tools that are available online to assist in nuclear astrophysics research. He described resources at the NNDC, JINA (MSU), Clemson, NACRE, LLNL, North Carolina - STARLIB, MESA and NuGRID, Notre Dame – AZURE, KADONIS, ULB Bruxelles NETGEN, TUNL, LANL, nucastrodata.org, Computational Infrastructure for Nuclear Astrophysics, nuclearmasses.org, and bigbangonline.org. He also described data work that was centered on "cloud computing" services to be a transformative vision for the future of the field. The possibilities include: having a digital assistant who automatically collects relevant masses, level schemes, references; a way for experts to easily upload supplemental information for your evaluations; having all major databases just one mouse click away; having an evaluation template automatically filled out for you; running analysis and application codes without compatibility, updates, backups, or cyber security issues; designing custom views of datasets from a variety of visualization tools; having a "virtual expert" online 24/7 to consult with questions; sharing your large data sets easily with colleagues; easily uploading your evaluation and visually tracking its progress for reviews, revisions, and acceptance; using a pipeline to process your evaluated data for use in simulations codes; running and visualizing these simulations, then sharing the results with colleagues. It would be extremely advantageous to have such services available online and free to use: they would help streamline our work, increase our productivity [do more with less], reduce repetition, and attract students with their novel computing approach. In fact, prototypes of many of these tools are already available, giving our community the chance to make a jump to a cloud-based approach to nuclear data. One example is the existing integration of data collection, processing, visualization, management, and end-user applications that is constructed within the Computational Infrastructure for Nuclear Astrophysics at nucastrodata.org: this is the first virtual “pipeline” of results from the nuclear laboratory to astrophysics codes. Other needs for the future of our field include fostering close ties of researchers and data experts to better serve community, launching a community-wide effort to evaluate reactions of importance to nuclear astrophysics, and creating workshops devoted to evaluation methodologies customized for nuclear astrophysics. Overall, there are very useful resources addressing a variety of nuclear astrophysics activities that are already online, serving to make our data and coding efforts easier. The first efforts in a new approach – Cloud Computing – have the promise to transform the field, and there are surely many exciting developments ahead.

In his presentation on "NNDC Services", Boris Pritychenko (NNDC/BNL) gave a detailed description of the services offered by the National Nuclear Data Center at BNL. Their systems had almost 3 million retrievals in FY2011, and this number has been growing every year. Boris detailed recent work in the Evaluated Nuclear Data File ENDF – for reaction information – and the Evaluated Nuclear Structure Data File ENSDF – for structure information. He also described the Nuclear Science references, the format EXFOR used for cross sections, EMPIRE (see below for more information) and other codes stored in an online repository. He has also used ENDF reaction information to calculate Maxwellian Averaged Cross Sections (MACS) for many neutron-induced reactions important to astrophysics and compared the results with KADONIS and other rate libraries.

In his talk on "Astrophysics Modeling", Brad Meyer (Clemson Univ.) suggested that a transformative strategy for the future would be to develop open source codes that are free and available in a publicly accessible repository. This would be especially useful for training students in nuclear astrophysics techniques. He advocates making codes simple to attract more users, as the number of users is inversely proportional to the code complexity. He described his libnucnet system, online at www.webnucleo.org and at sourceforge.net/p/nucnet-tools/home/Home,that streamlines implementation of new nuclear data and calculations in to network models. It uses JINA REACLIB XML format as the preferred data input. He also advocates exploring the nanoHUB.org model for online communities, and suggests that nuclear physics / astrophysics investigates creating such a hub. The HUBZero is an open source system that enables a wide variety of codes to be put online, controlled with a standardized graphical user interface and visualized with a variety of plotting routines. He also discussed the utility of gateways, they can be extremely useful but also need resources to continue operating. Micropayments and follow-on sponsors are some ways that could provide funding to gateways to sustain them. While such a big hub and/or gateway should not exclude other efforts, they have to be very serious efforts to be taken seriously.

In his talk on "Evaluations", Richard Cyburt discussed four types of data – raw data, evaluated data, input for nuclear astrophysics codes (processed data), and output of nuclear astrophysics codes. He then surveyed some of the resources available in each category and the transformations required, including evaluations, processing, and formatting. For example, the R-matrix code AZURE online at Notre Dame can be used for fitting experimental data and extracting parameters needed for astrophysics calculations, and the STARLIB system performs Monte Carlo calculations to determine the uncertainties of reaction rates based on the uncertainties of nuclear resonances. He also discussed the nuclide database NUCDATALIB that, when combined with his JINA REACLIB reaction rate library, form JINALIB. He has plans to expand JINALIB to include weak rates and validation efforts. He summarized some of the needs and challenges of evaluation work as follows. Data Evaluation requires access to data through literature searches and data repositories. We need to consider what data is acceptable for analysis, as well as determine the uncertainties of the datasets. There are a number of online analysis tools, and we should determine which additional ones are needed for our research. It would be advantageous to set standards for evaluation work – and determine

if these can be community wide. Collaborations need to be encouraged and strengthened. Alternate formats may be necessary to satisfy some users. Finally, having a vision of pulling all these components together would be advantageous.

Annalia Palumbo (NNDC/BNL) spoke on "The Empire Code". EMPIRE is a freely available nuclear reaction model code that can be used for a wide variety of calculations, including those important for nuclear astrophysics. Its capabilities include coupled channel calculations in the inelastic channel, six models of the gamma strength function, and an advanced fission treatment that utilizes the optical model for fission. Various options include multi-modal fission, barriers that can be described as a function of the quadrupole deformation (parameterized by smoothly-joined parabolas or described numerically), and the option of EGSM or HFB level densities at the saddles. Default input parameters are taken from the RIPL-3 database. The calculations of empire compare favorably to other codes such as CIGAR and NON-SMOKER.

Andrew Steiner (Univ. Washington / Institute Nuclear Theory) commented on a new type of data interface, RESTful API, that could be advantageous for cloud-based applications. They are already in use in a number of federal agencies to share scientific data.

A summary of the working group presentations and discussion was given by Michael Smith in the Plenary Session on Oct. 10, 2012. The main purpose here was to pull the presented information together to address the four questions put to the Working Group by the Town Meeting Organizers. The summary follows:

There are many fantastic resources to help nuclear astrophysics research that are already online. Some of these were created by researchers, some by data scientists, while others were created in collaborative efforts. **In order to evaluate and transform nuclear / astronomy data and codes reliably and efficiently for future use in nuclear astrophysics, there are a number of important approaches to pursue**: putting codes online in a "cloud computing" approach; codes should be open source; a community-wide effort is needed to evaluate important reactions; robust database utilization with GUIs customized for different users should be emphasized; and researchers should reach out to the astrophysics modeling community to provide them with needed input as well and to the nuclear data community for their expertise in evaluations. **The best evaluation procedures and ways to develop and implement them include:** quantifying reaction rate uncertainties based on resonance uncertainties; reaching out to the nuclear data community for evaluation procedures [codes, covariances…]; develop online guides for evaluations to streamline and standardize work; and host workshops on evaluation methodology tailored for nuclear astrophysics. **Regarding how information should be distributed**: no single format will work for all the diverse phenomena in nuclear astrophysics; robust database storage with custom graphical user interfaces are an excellent solution for many cases; the XML format being explored; the JINA REACLIB system is receiving community input (rates) and should be continued; multiple distribution sites are currently quite effective in satisfying diverse user needs; and it would be interesting to explore a unifying HUB approach (nanoHub.org) for nuclear astrophysics. Finally, **regarding what additional public codes are needed and how**

they should be developed: public codes are needed in every area – stellar models, nuclear structure and reactions, observation processing, nucleosynthesis; it may be very beneficial to develop (when possible) these as open source, free (modifiable) software available in a publicly accessible repository; and getting codes online "in the cloud" could be collaborative effort of research and data communities.