The Nuclear Landscape and the Big Questions (NAS report)

- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

Experimental relevance: FRIB, LEPN Facilities, NNSA facilities, JLab, JINA, SNS, …
Nuclear Interactions and Structure:
chiral EFT, light nuclei,

Reactions in light nuclei:
BBN, solar neutrinos,
accelerator neutrinos, NIF, ...

Density functional theory
FRIB, fission, astrophysics

Nucleonic matter:
neutron stars, \( \nu \) opacities
NUCLEI council:
Richard Furnstahl, OSU
Mihai Horoi, CMU
Hai Ah Nam, ORNL
Esmond Ng, LBNL
Sanjay Reddy, UW
James Vary, ISU

NUCLEI team:
Scott Bogner, MSU
Jon Engel, UNC
George Fann, ORNL
Stefano Gandolfi, LANL
Robert Harrison, ORNL
Gaute Hagen, ORNL
Dave Higdon, LANL
Chuck Horowitz, IU
Pieter Maris, ISU
Erich Ormand, LLNL
Thomas Papenbrock, UT
Lucas Platter, ANL
Steven Pieper, ANL
Sofia Quaglioni, LLNL
Nicolas Schunck, LLNL
Masha Sosonkina, Ames, ODU
Stefan Wild, ANL
Robert Wiringa, ANL
Chao Yang, LBNL

Strong collaboration between physicists and applied mathematicians computer scientists
Ab initio description of $^{12}$C

GFMS (Pieper et al.)

The ADLB (Asynchronous Dynamic Load-Balancing) library & GFMC. GFMC energy 93.5(6) MeV; expt. 92.16 MeV. GFMC pp radius 2.35 fm; expt. 2.33 fm.

Asymptotic Normalizations

Nollett and Wiringa, 2012
Making a simple programming model scalable: The Asynchronous Dynamic Load Balancing Library

**Objectives**
- Enable large-scale computations at high efficiency
- Simplify programming model
- Scale to leadership class machines

**Impact**
- Demonstrate capabilities of simple programming models at petascale and beyond
- Show path forward with hybrid programming models in library implementation

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**Improved Efficiency (compute time/wall time) with more nodes**

Efficiency = compute_time/wall_time – 6 Oct 2009

- ADLB
- ADLB+OMP
- 12C ADLB+GFMC

Number of nodes (4 OMP processes per node)

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**OpenMP scaling on BG/Q nodes**

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See poster by Hai Ah Nam

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**SCIDAC-3 NUCLEI Project**

Larger Computers (BG/Q)
Fault Tolerance
Performance Analysis
MPI-3 features
Anomalous Long Lifetime of Carbon-14


NUCLEI project: large-scale diagonalization (Chao Yang poster)

- Physics Requirement: Larger Model Spaces
- Reduce memory requirements: regenerating Hamiltonian flash-memory non-volatile disk
- Will also leverage work with FASTMath Institute to improve numerical quality of solvers.
- The MADNESS team will export a prototyped scalable dense eigensolvers from MADNESS with an open interface for other applications in the NUCLEI project.
Nuclear reactions

Ab initio theory reduces uncertainty due to conflicting data

Data deviate from NCSM/RGM results at low energy due to lab. electron-screening

NCSM/RGM is pioneering ab initio calculations of light-nuclei fusion reaction with NN interaction. Here, $^3$He($d,p$) $^4$He S-factor.


Larger Nuclei: Coupled-cluster method

Coupling Ab-Initio Approaches to Density Functional Theory

Neutron drip line and R-process nucleosynthesis
Optimization Plans in NUCLEI
Stefan Wild / SUPER

New Optimization Capabilities

- State-of-the art mathematical/numerical optimizations of next-generation EDFs (with LLNL, ORNL, Tennessee)
- Optimization of basis states and non-perturbative coupling constants arising in chiral Hamiltonians (with ISU)
- Enable nucleus lifetime computations with collective action minimizations (with LLNL, others)
- Exploit additional parallelism at the simulation-optimization interface
- Extend POUNDERS to address missing states and available sensitivity information
- Incorporate uncertainties and QUEST technologies

Coupling NUCLEI Subgroups

- Incorporate new observables from various NUCLEI subgroups
  - giant resonance data,
  - binding energy of neutron droplets in a trap,
  - ...

Deploy code optimization tools

- Introduce performance, energy, and resilience tools developed by the SUPER SciDAC Institute for use in NUCLEI codes
- Deliver representative NUCLEI computational kernels to SUPER
How many protons and neutrons can be bound in a nucleus?

Skyrme-DFT: $6,900 \pm 500_{\text{syst}}$

Erler et al., Nature 486, 509 (2012)

http://www.livescience.com/21214-atomic-nuclei-variations-estimate.html
http://www.sciencedaily.com/releases/2012/06/120627142518.htm
LACM, Fission: the ultimate challenge
(see Jordan McDonnell poster)

Optimized Functionals

Large-scale DFT

Collective dynamics

Confrontation with experiment; predictions

Numerical Techniques

PRC 78, 014318 (2008)

PRC 84, 054321 (2011)

PRC 80, 014309 (2009)

PRC 85, 024304 (2012)

PRC 80, 014309 (2009)

$^{240}\text{Pu}$

$^{252}\text{Fm}$

$^{256}\text{Fm}$
Quest for understanding the neutron-rich matter on Earth and in the Cosmos

RNB
Facilities/
NuN topical collaboration

Nuclear matter equation of state

Nuclear observables

Astronomical observables

Microphysics (transport, ...)

Nuclear interactions

Many body theory

Neutron star crust


Equation of State and Neutron Stars

Equation of State

Mass/Radius
Connections to Other Fields: Cold Atoms

Vortex Dynamics

Bulgac et al., Science, 332, 1288 (2011)

http://www.physicstoday.org/resource/1/phtoad/v64/i8/p19_s1

Equation of State

Exotic pairing phases


Lee-Yang

Carlson, Gandolfi, Gezerlis, PTEP (2012)
NUCLEI: some Computational Challenges

- Efficient usage of heterogeneous machines (GPUs)
- Reducing communications (topology awareness)
- Load Balancing at the Largest Scale Computers
- Matching Across Physical Scales (UQ)
Outlook:

Have developed effective collaborations between math/CS and physics. Excellent team of applied mathematicians, computer scientists, and physicists.

Look forward to working with Institutes: FASTMath, SUPER, QUEST

Exciting science: nuclear science and applications
astrophysics
neutrino physics
BACKUP SLIDES
How many neutrons, protons can get along? Maybe 7,000

New study comes closer than ever to finding answer by estimating number of variations that can exist in an atom.

Scientists have long wondered whether there is a limit to the number of protons and neutrons that can be clustered together to form the nucleus of an atom. A new study comes closer than ever to finding the answer by estimating the total number of nuclear variations that can exist.

The periodic table of elements includes 118 known species of atoms, and each of those exists (either naturally or synthetically) in several different arrangements — with different numbers of neutrons, giving rise to a total of about 3,000 different atomic nuclei. As technology has

Pounding out atomic nuclei

Scientists have long wondered whether there is a limit to the number of protons and neutrons — that can be clustered together to form the nucleus of an atom. A new study comes closer than ever to finding the answer by estimating the total number of nuclear variations that can exist.

The periodic table of elements includes 118 known species of atoms, and each of those exists (either naturally or synthetically) in several different arrangements — with different numbers of neutrons, giving rise to a total of about 3,000 different atomic nuclei. As technology has

Science News

Physicists Pin Down Proton-Halo State

ScienceDaily (May 27, 2010) — A halo may be difficult to acquire in terms of virtue, but it can also be tough to calculate in terms of physics. Thomas Papenbrock, associate professor of physics and astronomy at the University of Tennessee, Knoxville, and his colleagues Gaute Hagen from Oak Ridge National Laboratory and Morten Hjorth-Jensen from the University of Oslo have managed to do just that, however, and report their findings in Physical Review Letters.

Quantum quirk makes carbon dating possible

RADIOCARBON dating relies on carbon-14 to decode an object's age, but the isotope has steadfastly refused to divulge the key to its own unusual longevity. The answer, it seems, lies in the bizarre rules of quantum physics.

Carbon-14 decays with a half-life of 5730 years, so it is often used to date objects up to about 60,000 years old (anything older would have negligible amounts of the stuff).

But most other atoms that decay in the same way - by converting one of their neutrons into a proton - disappear in less than a day. So what's different about carbon-14?

The nucleus of the carbon-14 isotope has six protons and eight neutrons. When it decays, one of the neutrons turns into a proton, and also releases an electron and a neutrino. The result is a nitrogen-14 nucleus with seven protons and seven neutrons.
Nuclear Reactions

Desired Trajectory
Flat Trajectory
Flat-Flat Trajectory

Microscopic Theory of Fission
Neutrinos as Nuclear Physics Laboratories

Physics of Extreme Neutron-Rich Nuclei and Neutron Stars

Desired Trajectory
Flat Trajectory
Flat-Flat Trajectory
Junior Scientists in UNEDF

POST-DOCTORAL ASSOCIATES (2010)

Christopher Calderon, LBNL (staff, Numerica co.)
Joaquin Drut (Professor, UNC)
Stefano Gandolfi, LANL (staff, LANL)
Kai Hebeler, OSU (TRIUMF)
Heiko Hergert, MSU (OSU)
Jason Holt, UTK/ORNL
Eric Jurgenson, LLNL (staff, LLNL)
Markus Kortelainen, UTK (U. Jyväskylä)
Plamen Krastev, UCSD (research, Harvard)
Pieter Maris, ISU (Research Prof. ISU)
Eric McDonald, MSU (staff scientist, MSU)
Gustavo Nobre, LLNL (BNL, NNDC)
Junchen Pei, UTK (Prof., Pekin U.)
Nicolas Schunck UTK (staff, LLNL)
Roman Senkov, CMU
Ionel Stetcu, UW (staff, LANL)
Jun Terasaki, UNC (staff, U. Tsukuba)
Stefan Wild, ANL (staff, ANL)

Effect of UNEDF on workforce
Year-1: 9 students, 17 postdocs;
Year-2: 12 and 12;
Year-3: 10 and 18;
Year-4: 11 and 19

2010: Early Career Award
2010: Math/CS Staff ANL
2010: Staff LLNL
2012: Faculty Guelph
2012: Harvard Research Computing

Relevant instruction (workshops, courses) is crucial for the future of the field
Energy density functional (EDF) predictions rely on large-scale computer simulations that must be calibrated to experimental data.

- **TAO 2.0’s POUNDERS** developed for UNEDF to exploit the mathematical structure of this calibration problem.
- Substantial computational savings over alternative algorithms enables fitting of complex EDFs.

Previous optimizations required too many evaluations to obtain desirable features exhibited by UNEDF0, UNEDF1, …

Derivative-free sensitivity analysis procedure developed for UNEDF exposes correlations and constraining data in 1 minute using 20k cores.

Optimal Derivatives of Noisy Numerical Simulations

**Computational Noise**
In all computations of DOE interest containing:
- adaptivity,
- discretizations
- iterative methods
- petaflops,
- roundoff errors

Includes *deterministic* computations

**Noise Impacts in UNEDF & Beyond**
- Uncertainty in computed outputs
- Unstable derivative estimates for sensitivity analysis
- Can be unrelated to/overwhelm truncation error
- Blurs relationship between tolerance values and stability

**Tools & Techniques**
- *ECNoise* provides reliable estimates of stochastic and deterministic noise in few simulations
- Nonintrusive **stability bounds for extreme scale simulations**, can instruct precision levels/tolerances for subroutines
- Optimal difference parameters calculated without computationally expensive parameter sweeps

"Optimal step was obtained with only two simulation evaluations. Classical approach (circles): result of a sweep across 100 difference parameters, each point requiring a new simulation."

"Estimating Derivatives of Noisy Simulations,” Moré & Wild, ACM TOMS’12
Making a simple programming model scalable: The Asynchronous Dynamic Load Balancing Library

**Objectives**
- Enable Green’s Function Monte Carlo calculations for $^{12}$C on full BG/P as part of UNEDF project
- Simplify programming model
- Scale to leadership class machines

**Impact**
- Demonstrate capabilities of simple programming models at petascale and beyond
- Show path forward with hybrid programming models in library implementation

**Progress**
- Initial load balancing was of CPU cycles
- Next it became necessary to balance memory utilization as well
- Finally ADLB acquired the capability to balance message flow
MFDn: Total-J Progress

- **M-scheme approach**: works directly on the Hamiltonian, extracts all low energy states
- **J-scheme approach**: alternative to find a large number of low energy states for a prescribed total angular momentum (J) value
- **Targeted applications**: investigation of nuclear level densities, evaluation of scattering amplitudes
- **Total-J code**: implementation of the J-scheme approach in Fortran, MPI
- **CS Challenges in Total-J**: Three distinct phases, each with very different computing and storage characteristics

**Phase 1: Construction of the J-basis**
Implemented a multi-level greedy load balancing algorithm

**Phase 2: Invariant Subspace Projection**
In-core implementation to reduce I/O overheads in the out-of-core version

**Application:**
Predicting the Nuclear Level Density of $^6\text{Li}$
(PRELIMINARY)

$^6\text{Li}, N_{\text{max}} = 14, J=3$
dimension of $H \sim 1.7 \times 10^8$
10x speed-up, default striping
4x speed-up, optimal striping
M-scheme: Performance Improvements

Weak Scaling

Strong Scaling for $^{10}$B, $N_{\text{max}} = 8$

ver1: SC’08 paper (beginning of SciDAC2)

ver6: current release (end of SciDAC2)

Speed-up for $^{10}$B
$N_{\text{max}} = 6, 7, 8, 9, 10$

Time (in seconds)

Better
One Demonstration of NP – ASCR Coupling:
Over 20 joint publications resulting from UNEDF

- "..."