

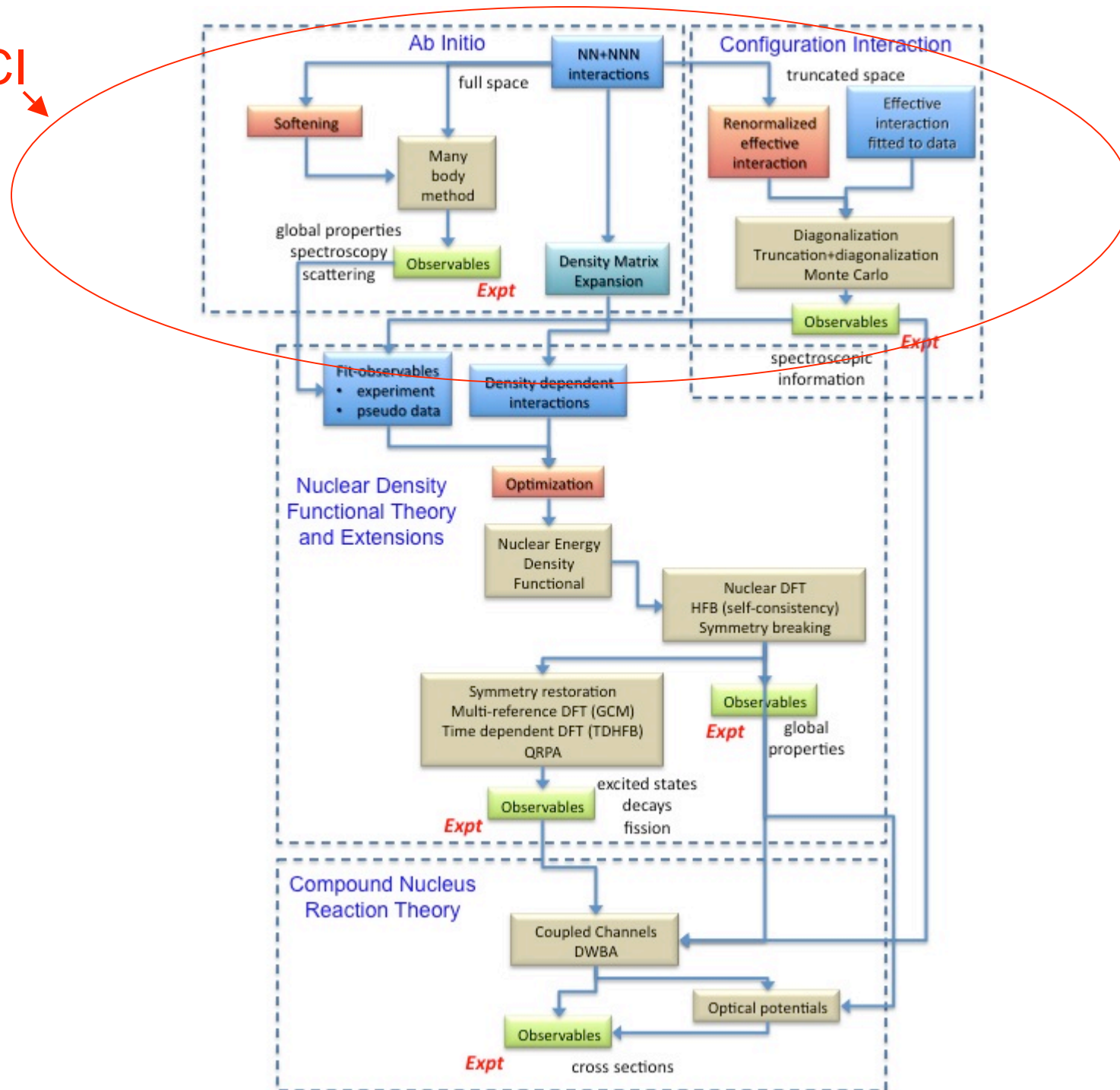
# Leadership Class Configuration Interaction (LCCI) Code Project of SciDAC/UNEDF

## Introduction

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Version 5 - June 23, 2010

LCCI



## LCCI Project Background

Official LCCI project launch - June 2009

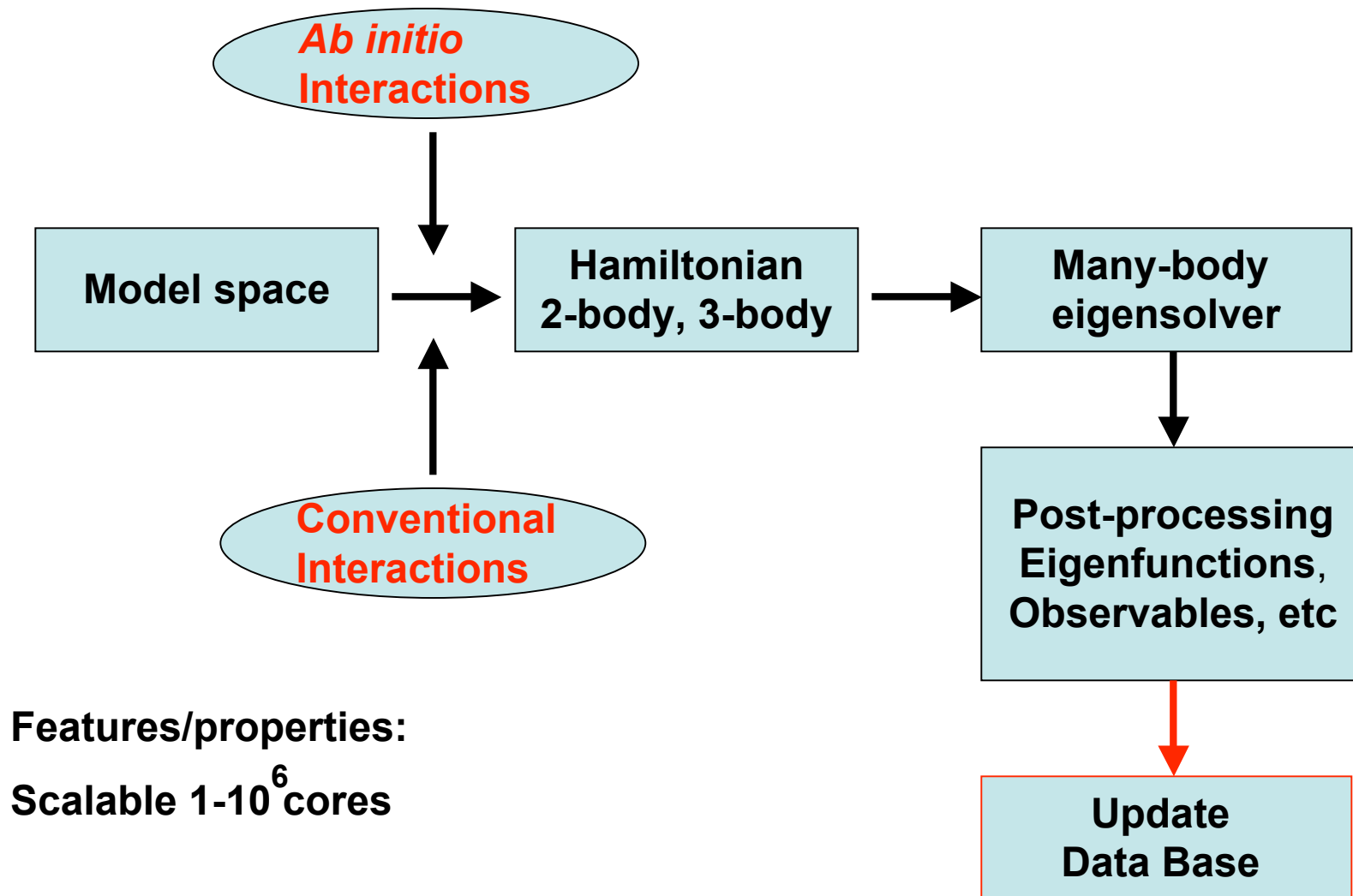
Face-to-face meetings held twice annually - next meeting scheduled for APS DNP Meeting, November 2010

Meetings are open to UNEDF members and invited guests.

Summary of 6 meetings to date and links to the white paper, “CI-Solver Task Force draft planning document”, at [www.unedf.org/users/projects/lcci.php](http://www.unedf.org/users/projects/lcci.php)

[Note UNEDF username and password required]

## LCCI Environment - Overview



Goal: LCCI code should solve, at least, the identified consensus structure problems from “extreme scale” white paper

## LCCI Codes deposited initially on Oct. 2-4, 2009

<u>Codes</u>	<u>Contact</u>	<u>email</u>	<u>Updated</u>	<u>Next update?</u>
BIGSTICK	Plamen Krastev	pkrastev@sciences.sdsu.edu	June 2010	~Oct, 2010
MFDn	Pieter Maris	pmaris@iastate.edu	June 2010	~Oct 2010
NuShellX	Mihai Horoi	horoi@phy.cmich.edu	June 2010	~Oct 2010
trdens	Petr Navratil	navratil1@llnl.gov	April 2010	~Oct 2010
ncsmv2eff	Petr Navratil	navratil1@llnl.gov	March 2010	~Oct 2010

Source codes for each resides in its own subdirectory in NERSC project space:

/project/projectdirs/unedf/lcci

with a README file, one or more scripts, and test cases

## Consensus at Hawaii meeting, October 2009

### Policies and procedures for revisions

Revisions can be deposited at any time with a suitable revision label on the newly created subdirectory

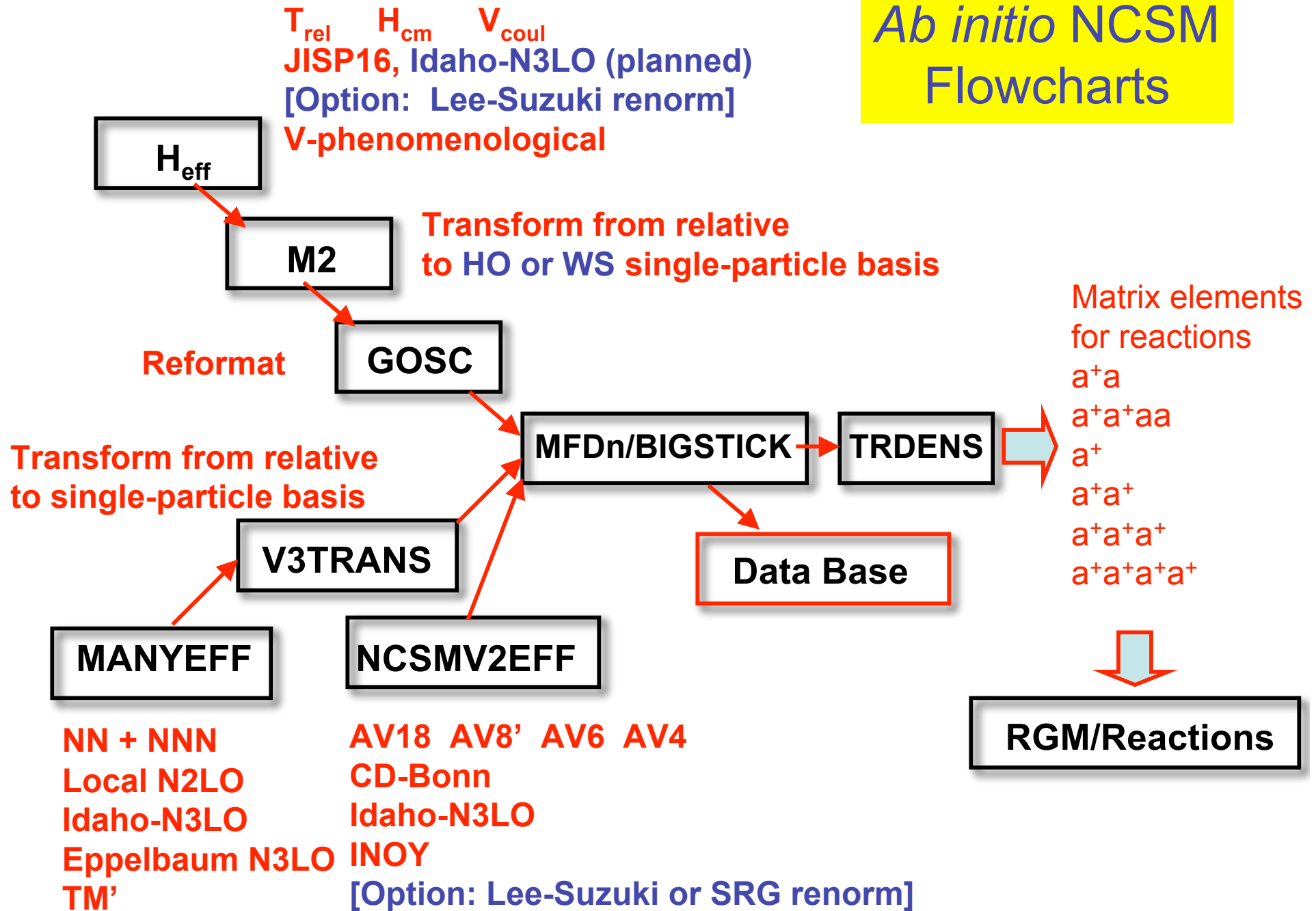
Previous versions should not be deleted from the project space.

Owners of codes need to retain their originals in a safe place as the codes deposited at NERSC in project space are not backed up. The following statements are from the NERSC web pages:

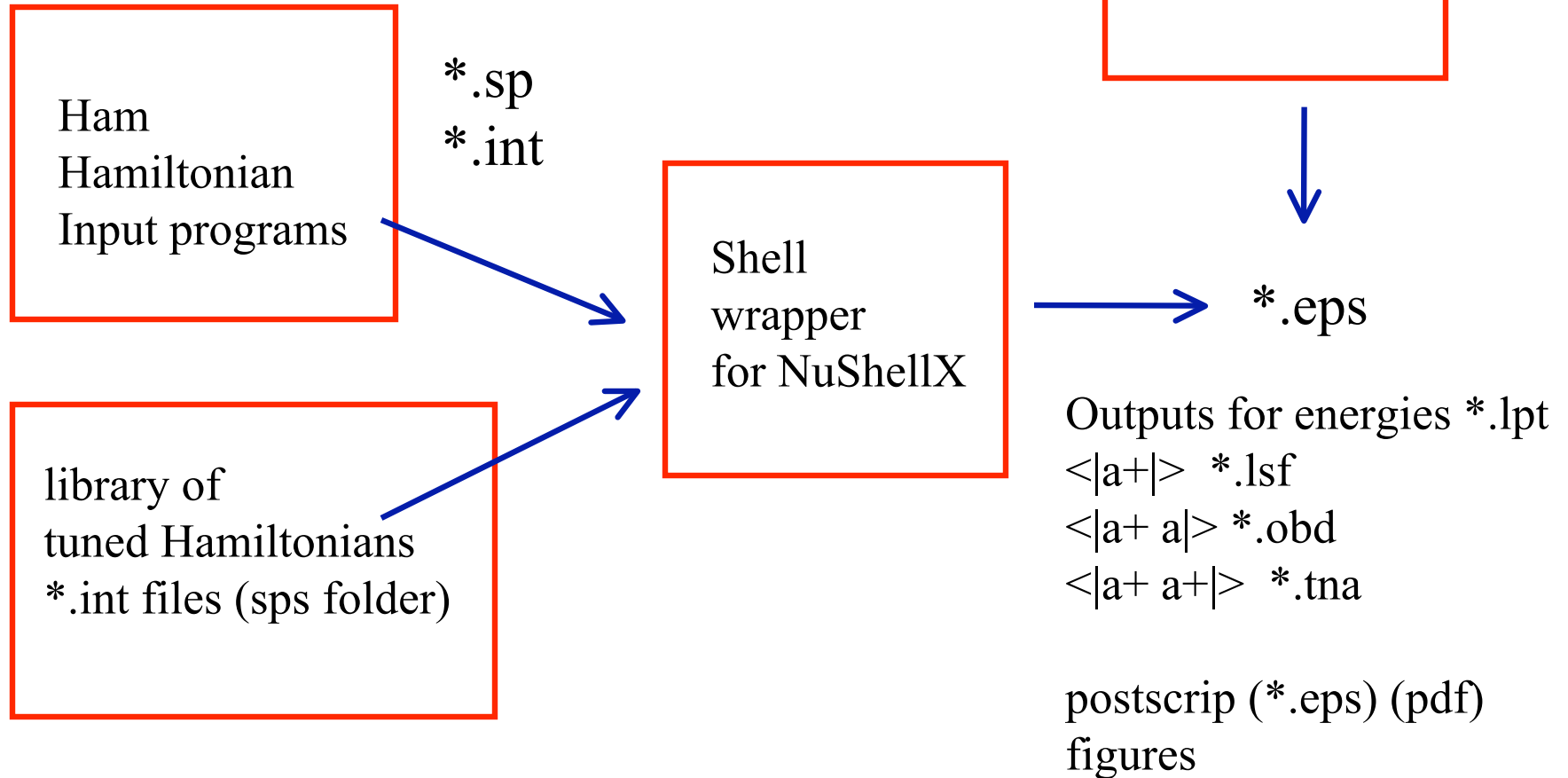
“Files in global homes are not subject to purging. However, they are also not backed up, except for disaster recovery of the entire filesystem. That is, individual files and/or directories can not be restored from the disaster recovery backups.”

Following slides portray code interoperability and current flowcharts

# Ab initio NCSM Flowcharts



\*.sp model space files  
\*.int Hamiltonian files





New and planned additions to this “LCCI Introduction” ppt file:

One slide per major code directing to README file for additional details -

\* \* \* \* \* See following slides \* \* \* \* \*

We plan to expand to one slide per “upstream code” directing to README file or code’s author for further info.

Upstream codes

Heff, M2, GOSC

MANYEFF, V3TRANS, NCSMV2EFF\*

Contact person

James Vary (jvary@iastate.edu)

Petr Navratil (navratil1@llnl.gov)

\*Note that an initial version of NCSMV2EFF is available at  
/project/projectdirs/unedf/lcci/ncsmv2eff

\* \* \* \* \*

Following the code-specific slides, we include the consensus goals from the nuclear physics extreme scale computing workshop report available at:

<http://extremecomputing.labworks.org/nuclearphysics/report.stm>

These physics goals serve as guides for the LCCI project development

# Bigstick – a configuration-interaction code:

W. E. Ormand, LLNL; C. W. Johnson, SDSU; P. G. Krastev, SDSU

- **Purpose:** Solve the general many-fermion problem.
- **Method:** Lanczos algorithm to find low-lying eigensolutions of large Hamiltonian matrix; on-the-fly matrix-vector multiply using factorization.
- **Input:** General single-fermion basis, assuming good angular momentum  $j$ .
  - User-friendly interactive input.
  - Two “species” of particles, e.g. proton/neutron (half-integer  $j$ ) or spin up/down (integer  $j$ ); allows general radial wavefunctions.
  - Flexible truncation of many-body basis covering many common choices.
  - General two-body interactions, assuming only rotational invariance, read in as files of precomputed matrix elements; can read in different formats and multiple files.
  - Can assume or break isospin symmetry.
  - General three-body interactions (in progress)
- **Output:** Produces output wavefunctions compatible with TRDENS.
  - Option to automatically compute one-body transition densities without further post-processing (in progress).
- **Implementation:** M-scheme many-body basis; states of good  $J$  automatically recovered.
  - Works well both on serial machines and with MPI parallelization.
  - Hybrid MPI/OpenMP parallelization (in progress).

For more info see README file at:  
</project/projectdirs/unedf/lcci/BIGSTICK>

# NuShellX – a configuration-interaction code:

B. A. Brown, E. McDonald, M. Horoi, W. D. M. Rae

- **Purpose:** Solve the general many-fermion problem.
- **Method:** Lanczos algorithm to find low-lying eigensolutions of large Hamiltonian matrix; on-the-fly matrix-vector multiply.
- **Input:** General single-fermion basis, assuming good angular momentum  $j$ .
  - User-friendly interactive input.
  - Two “species” of particles, e.g. proton/neutron
  - Flexible truncation of many-body basis covering many common choices.
  - General two-body interactions, assuming only rotational invariance, read in as files of precomputed matrix elements; can read in different formats and multiple files.
  - Can assume or break isospin symmetry.
- **Output:** Produces wavefunctions, spectroscopic factors, one-body transition densities
- **Implementation:** J-scheme many-body basis.
  - Works well both on serial machines and with OpenMP parallelization.
  - Hybrid MPI/OpenMP parallelization (in progress).
  - Wrapper codes for Table of Isotopes and Hamiltonians

For more info see README file at:  
</project/projectdirs/unedf/lcci/nushellx>

# MFDn - Many Fermion Dynamics - nuclear

## A configuration interaction code

- General-purpose and portable many-fermion code; solves very large matrix Hamiltonian in a Slater determinant basis
- Uses general single-fermion basis, assuming good angular momentum  $j$ .
- One or two “species” of particles, e.g. proton/neutron (half-integer  $j$ ); allows general radial wavefunctions
- Flexible truncation of many-body basis covering several common choices.
- General two-body and three-body interactions, assuming only rotational invariance; read in as files of precomputed matrix elements; can read in different formats; reads in and independently scales multiple interaction files
- Option to run with an external field
- M-scheme many-body basis; states of good  $J$  automatically recovered.
- Lanczos eigensolver using full many-body matrix stored in core.
- Works both on serial machines and with MPI/OpenMP parallelization
- Produces output wavefunctions compatible with TRDENS
- Option to automatically compute one-body transition densities without further post-processing
- Options to evaluate various suites of observables
- Total J version (in progress)

For more info see README file at:  
</project/projectdirs/unedf/lcci/MFDn>

# TRDENS basic features

- **Purpose:** Calculate matrix elements of combinations of creation and annihilation operators
  - Currently coded:  $\langle a^+a \rangle, \langle a^+a^+aa \rangle, \langle a^+ \rangle, \langle a \rangle, \langle a^+a^+ \rangle, \langle aa \rangle, \langle a^+a^+a^+ \rangle, \langle aaa \rangle, \langle a^+a^+a^+a^+ \rangle, \langle aaaa \rangle, \langle a^+a^+a \rangle \dots$
- Initial and final eigenstates from the same nucleus or from different nuclei
  - Eigenstates declared as pointers: For the same nucleus  $|f\rangle \Rightarrow |i\rangle$
  - Currently eigenstates generated by the following codes can be input
    - “Arizona” MFD
    - NCSD (No-Core in Slater Determinant basis)
      - calculates on the fly with hashing search
    - Antoine
    - Robert Roth’s Importance-Truncated NCSM code
    - MFDn - v13
    - Bigstick
- **Output**
  - ASCII file with the densities
  - Observables such as B(E2), B(M1), B(GT), translationally-invariant densities, form factors, mean values of H, T, Coulomb...

For more info see README file at:  
</project/projectdirs/unedf/lcci/trdens>



## Overview of Iowa State “upstream” codes

Further information: James Vary (jvary@iastate.edu)

### Heff

Generates two-body matrix elements of an interaction in the relative coordinate harmonic oscillator basis. Includes capability to unitarily transform from one harmonic oscillator basis to another. Contains the option to perform the Lee-Suzuki renormalization transformation.

### M2

Transforms two-body matrix elements from the relative coordinate harmonic oscillator basis to the harmonic oscillator single particle basis (Talmi-Moshinsky Transformation). Also contains the option to transform to the Woods-Saxon single particle basis by a finite expansion in an underlying harmonic oscillator basis. Options include capability of generating  $T_{rel}$ ,  $V_{coul}$ , etc matrix elements in the chosen single particle basis. Option to generate Minnesota and other interactions.

### GOSC

Transforms output files from M2 (matrix elements grouped by [J,T,Parity]) to one of the input formats used by MFDn (e.g. matrix elements grouped by [a,b,c,d]). The output format of GOSC is specified by the parameter “IPOTENTIAL” within the code.

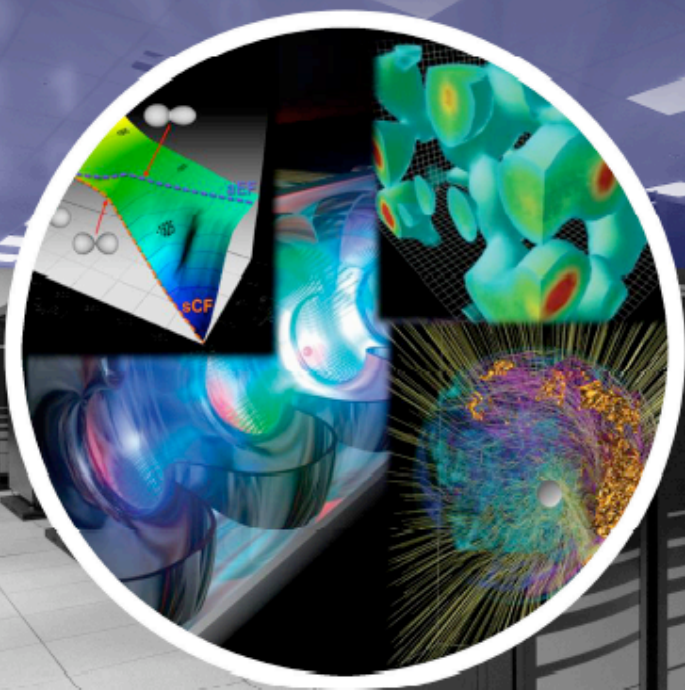


<http://extremecomputing.labworks.org/nuclearphysics/report.stm>

# Scientific Grand Challenges

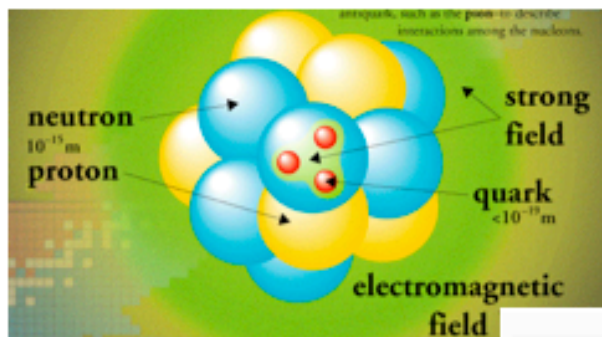
FOREFRONT QUESTIONS IN NUCLEAR SCIENCE AND  
THE ROLE OF COMPUTING AT THE EXTREME SCALE

January 26-28, 2009 • Washington, D.C.



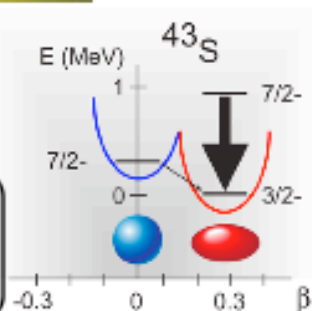
U.S. DEPARTMENT OF  
**ENERGY**

Sponsored by the Office of Nuclear Physics and the Office of Advanced Scientific Computing Research



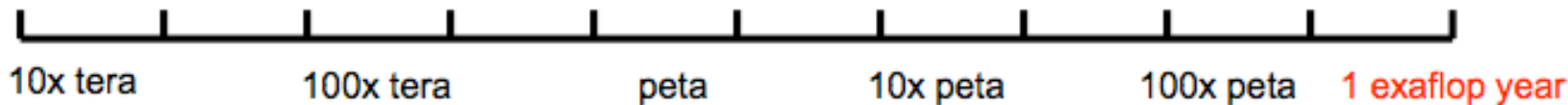
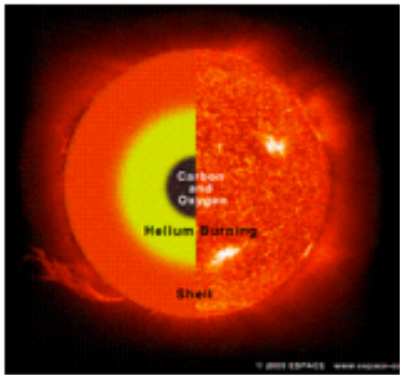
$^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$   
 $^{132}\text{Sn}$  structure

*Ab initio* structure  
 in light nuclei

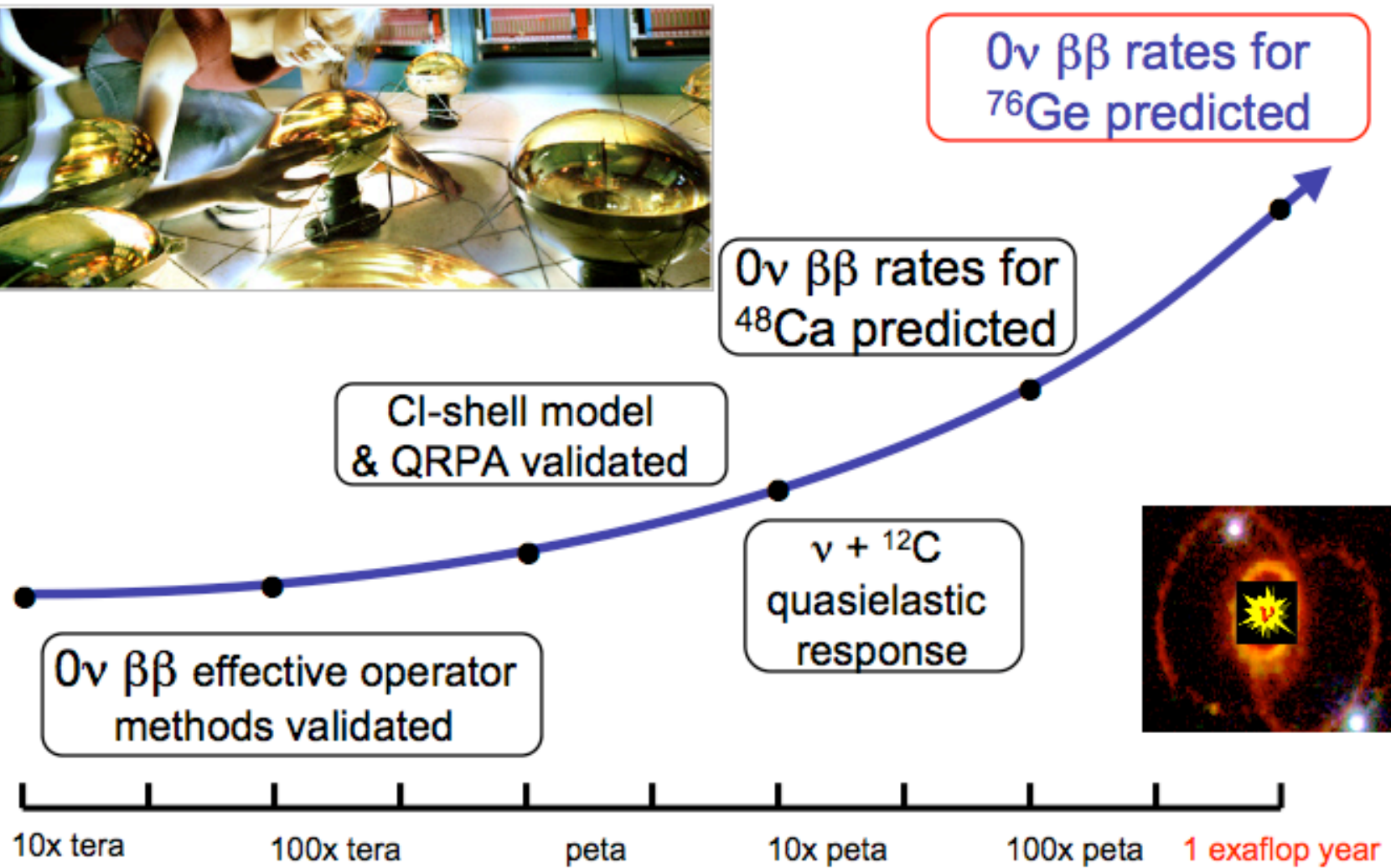


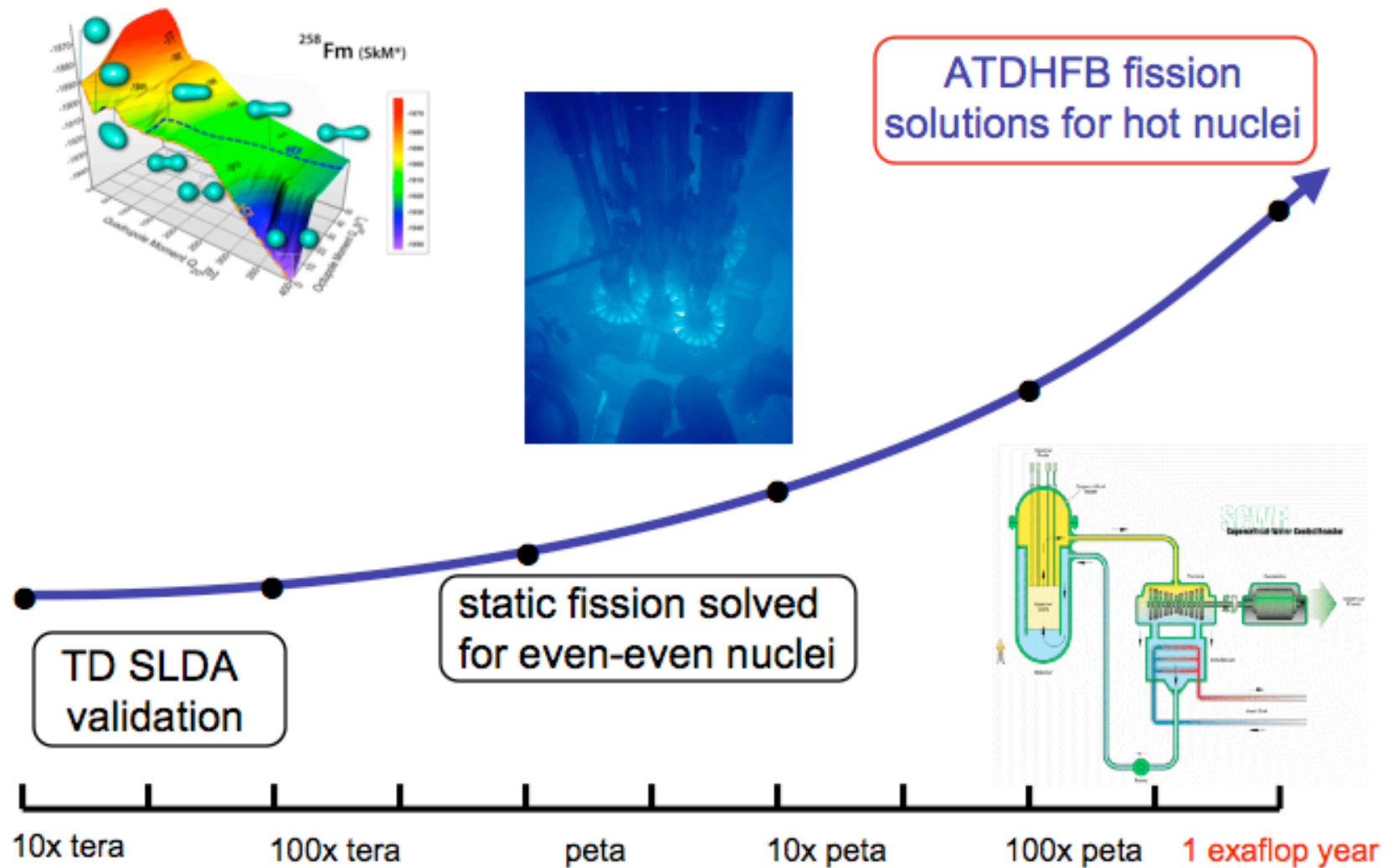
$^{78}\text{Ni}$  structure

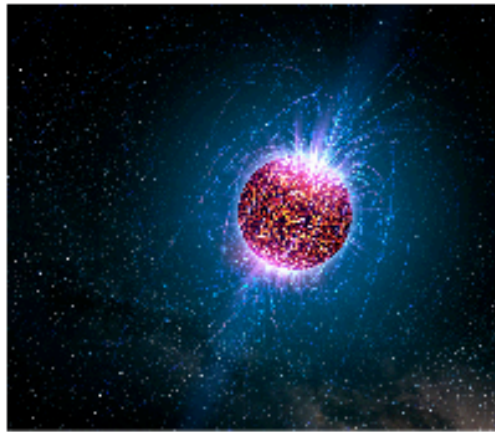
$^8\text{Be}(\alpha, \gamma)^{12}\text{C}$



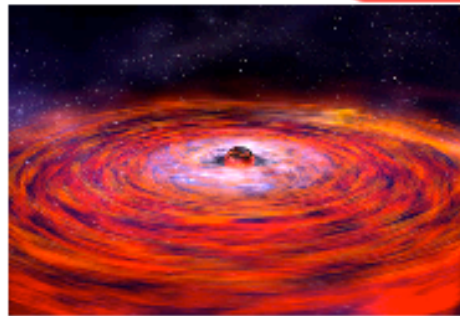






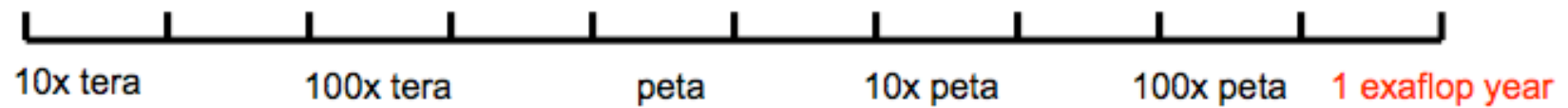
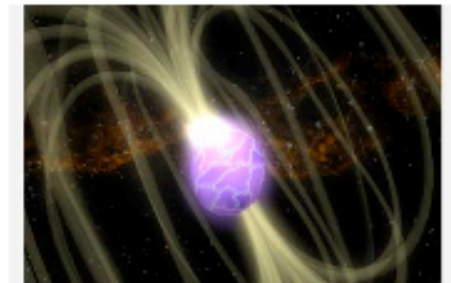


Dynamic/transport properties  
of neutron star crust solved



Static properties  
of neutron star crust solved

Predict shell structure  
of extreme nuclei



## Policy statement on LCCI data release

Adopted at LCCI-2010, March 13, 2010

Nuclear structure spectra, wavefunctions and quantities derived from them, such as one-body density matrices, often represent substantial investments of resources.

Once a group has completed a publication based on their nuclear structure wavefunctions, one-body densities, etc., they are strongly encouraged to deposit those data, with suitable provenance information in the LCCI database.

Suitable provenance information includes identifying codes, input data, scripts, compilers, hardware, etc. employed, as well as relevant publications, so that an expert researcher could reproduce the data.

## Policy statement on LCCI data access

Adopted at LCCI-2010, March 13, 2010

Nuclear structure spectra, wavefunctions and quantities derived from them, such as one-body density matrices, often represent substantial investments of resources.

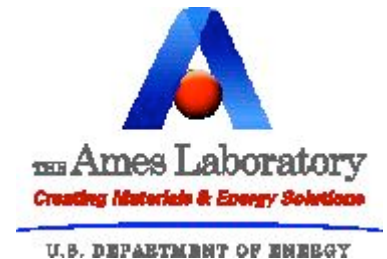
Data deposited in the LCCI data base are available to all users of the system (currently NERSC). Access is granted by the group generating that data with the understanding that users will cite the relevant publications presenting the science and technology underpinning that data and will cite the LCCI database.

# ***A Database Management System for LCCI***

***Ritu Mundhe, Fang Liu, Masha Sosonkina  
Ames Laboratory***

***Miles V. Aronnax, Iowa State***

See introduction in separate file:  
Database\_Mgmt\_System\_v1.pdf



## LCCI Wrapper

Goal: Single LCCI wrapper to access all LCCI resources

Initial working wrappers - Bigstick, MFDn, NuShellX

Note: “Hands On” session following Brad Sherrill’s talk

LCCI python wrapper development stages

Intermediate - Bigstick/MFDn (Year 4)

Final - Bigstick/MFDn/NuShellX (Year 5)

MFDn: - sets up a run for Franklin or Hopper using an available  
2- or 3-body interaction files

- Python script generates a batchscript to be submitted to batch queue
- successful run produces output suitable for inclusion in LCCI database

Bigstick: - menu driven input already, user friendly

- template input files available
- template batchscript for submission to batch queue available

## LCCI Year 4 roadmap

First 4 bullets are periodically updated

- LCCI codes/scripts delivered to UNEDF & updated
- Design/Prototype Data Base Management System (DBMS)
- Design/Prototype unified wrapper - MFDn/Bigstick versions
- Developed NuShellX wrapper
- Hands-On LCCI tutorials - after Brad Sherrill's talk

## LCCI Year 5 roadmap

- Complete a unified LCCI wrapper (ISU/MSU/SDSU)
- Complete LCCI Data Base Management System (DBMS)
- Final versions of UNEDF LCCI codes/scripts delivered to UNEDF