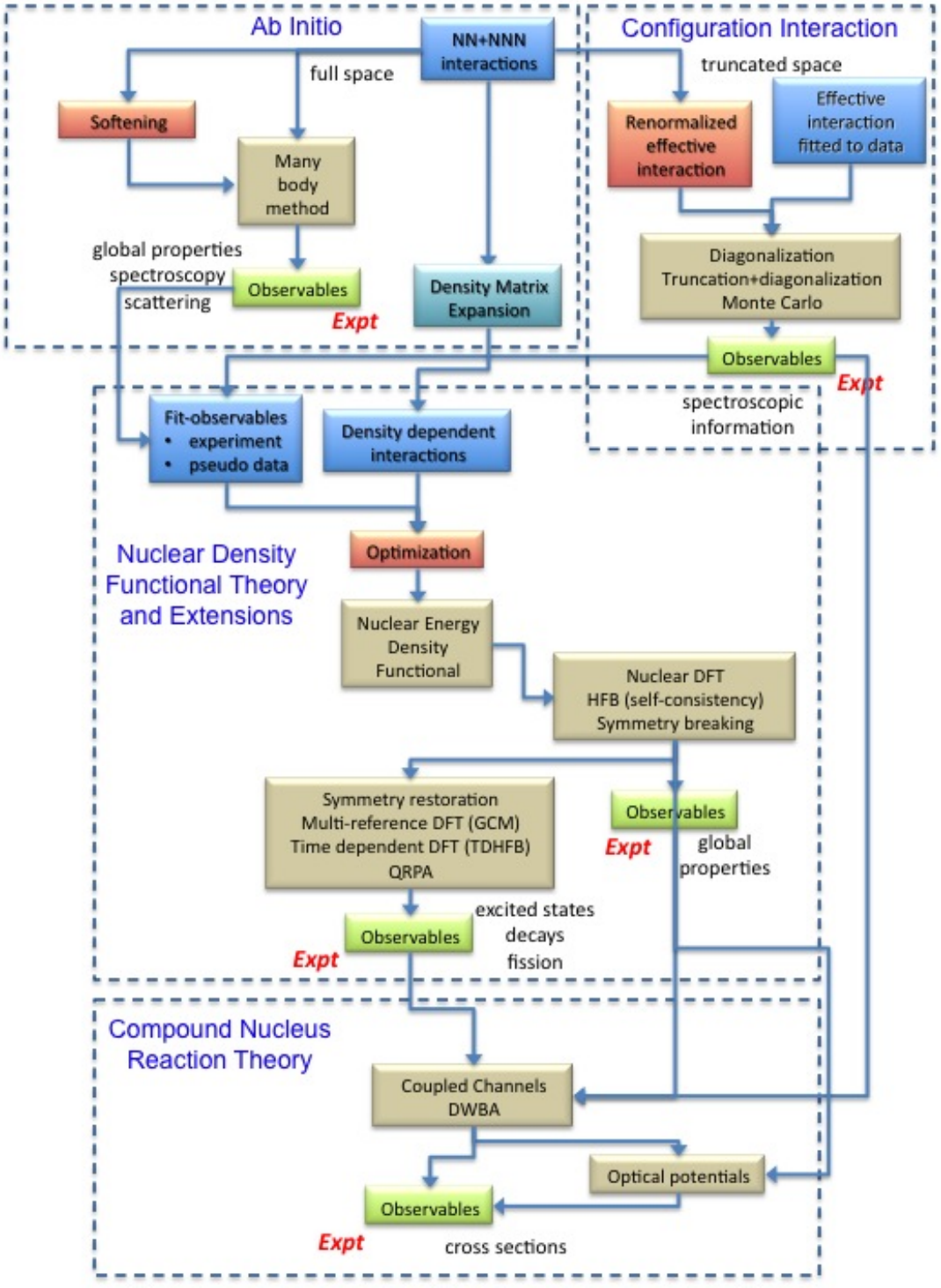

Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)
Symmetry breaking
Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA
Observables
Expt
global properties
Observables
excited states
decays
fission
Expt
Compound Nucleus Reaction Theory
Coupled Channels
DWBA
Optical potentials
Observables
Expt
cross sections

# Year-4 Deliverables (from Year-3 annual report)

- Ab-initio Deliverables
  - Calculate ab initio one-body densities for spherical and deformed nuclei and use them to inform DFT
  - Calculate lowest $2^+$ excitation and $E2$ transition form factor for $^{12}$C with GFMC. Initial work toward Hoyle State
  - Improve Asynchronous Dynamic Load-Balancing for largest computers
  - Calculate $^{14}$C beta decay with MFDn
  - Investigate improved basis states and convergence in CI
  - Study role of NNN forces in medium mass nuclei with CC
  - Develop CC-DFT interface
  - Ab-initio calculations for deformed and superfluid neutron drops in external potentials with comparisons to DFT
- Ab initio Functionals Deliverables
  - Extend DME and validate against ab initio calculations. Initial work toward $^{40}$Ca DME comparisons
  - Further development of $\pi$–DME functionals. Include pairing. Continue development of orbital-based DFT and test vs. DME

# Year-4 Deliverables (from Year-3 annual report)

- DFT Applications Deliverables
  - Develop Skyrme-DFT multiwavelet HFB code based on MADNESS, optimized for petaflop boxes. Implement outgoing boundary conditions for interior and exterior scattering problems in 3D
  - Profile ASLDA DFT solver with pairing
  - Optimize generalized Skyrme functional containing novel long-range terms from DME using the MFQns algorithm and ”Golden Data Standard”. First applications of UNEDF-1
  - Complete first version of parallel HFODD code; improve parallel interface to HFODD
  - Implement the Augmented Lagrangian Method for fission calculations in multidimensional collective spaces

# Year-4 Deliverables (from Year-3 annual report)

- DFT Extensions Deliverables
  - Develop the deformed QRPA code for charge-exchange modes, and use it to study beta decay of nuclei in the r-process
  - Improve the generation of initial conditions for TD-SLDA, and study dilute fermion atomic and nuclear systems
  - Initial work on the Leadership-Class Configuration Interaction code
  - Improve the scalability of the CI codes NuShellX and REDSTICK
  - Improve the scalability of the CI Moments code, and calculate the nuclear level densities for the heavier nuclei in the rp-process path

# Year-4 Deliverables (from Year-3 annual report)

- Reaction Deliverables
  - Investigate reactions in light nuclei using ab initio methods: NCSM with RGM, GFMC, and J-matrix methods. Benchmark n-7Li, n-8He, and n-9Li scattering. Generate two- and three-body transition densities.
  - Fold QRPA transition densities, with exchange terms, for systematic neutron-nucleus scattering.
  - Derive optical potentials using parallel coupled-channel reaction code capable of handling 105 linear equations
  - Use CCh channel wave functions for direct and semi-direct (n,??) capture processes.
  - Consistently include multi-step transfer contributions via deuteron channels and implement and benchmark the two-step method to generate non-local optical potentials.
  - Extend and apply KKM model to scattering with doorway states

# Preparation for UNEDF annual report

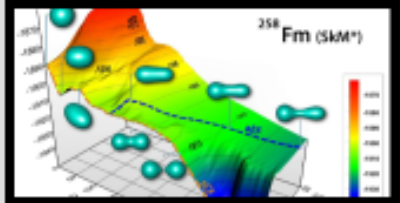
- Needed from the section leaders
  - Progress reports on Year-4 deliverables
  - Year-5 plans and lists of Year-5 project deliverables
- To me by email ASAP (`furnstahl.1@osu.edu`)
  - Papers acknowledging UNEDF (both published and preprints)
  - UNEDF-related talks
  - Check unedf.org for what is missing!
  - UNEDF-related “Good News”
  - Highlights — at least one from every sub-project!
- Guidelines for the continuation progress report

# UNEDF SciDAC Collaboration

## Universal Nuclear Energy Density Functional



MTEX




SRG+MFD

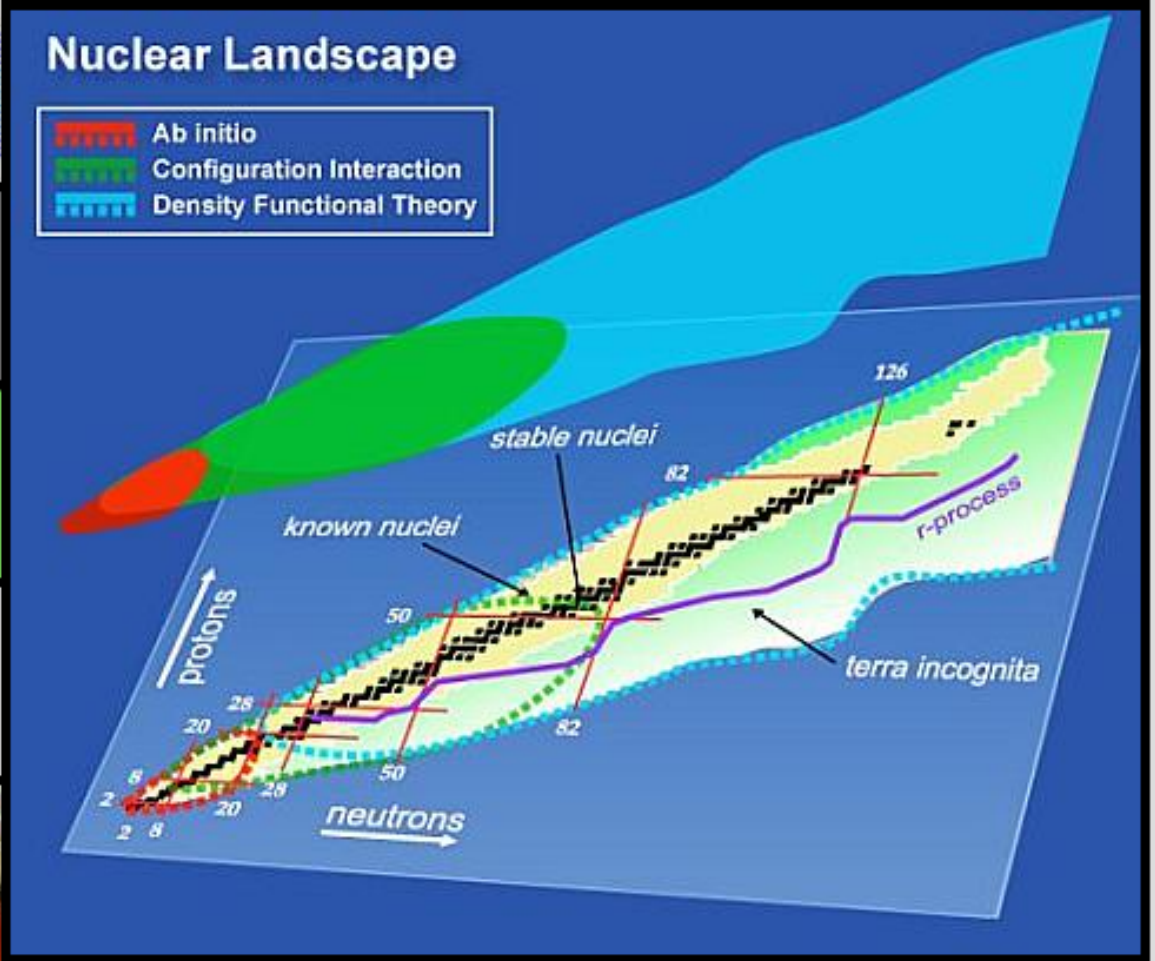
$\lambda$ =4.0 fm$^{-1}$ $\lambda$ =2.0 fm$^{-1}$

$^4$He + n

NCSM/RGM

Jaguar

MADNESS




UNEDF is a collaboration of physicists, computer scientists and applied mathematicians using high-performance computing to explore the nuclear landscape. Point to the buttons at left to highlight computational sub-projects; click for details. Refresh for more.

## Good News

UNEDF project on rare-earth nuclear excitations awarded 10 million processor hours

UNEDF members Jonathan Engel and Jun Terasaki of the University of North Carolina have been awarded 10M cpu hours on the ORNL supercomputer Kraken for the project *Systematics of Nuclear Surface Vibrations in Deformed Nuclei*. The award is from the NSF-funded TeraGrid program, which provides leadership class resources at eleven partner sites for open scientific discovery.

UNEDF F-17 halo work featured in Science Daily

Ab initio coupled-cluster calculations of Fluorine-17 by UNEDF-members Gaute Hagen and Thomas Papenbrock of Oak Ridge National Lab and the University of Tennessee, together with Morten Hjorth-Jensen of the University of Oslo, pin down details of the proton-halo state.

UNEDF sub-project featured in SciDAC Review

Rusty Lusk and Steve Pieper describe the Asynchronous Dynamic Load Balancing (ADLB) library for high-performance computing and its application to Green's Function Monte Carlo (GFMC) calculations of nuclei.

UNEDF collaborators Steve Pieper and Bob Wiringa awarded APS Bonner Prize

The Tom W. Bonner Prize is the highest award for research given by the APS Division of Nuclear Physics. Full details on the award to Steve and Bob are available.

DOE awards 40 million processor hours for computational nuclear structure

For the third straight year, the DOE INCITE program awarded a large number of hours for UNEDF computational nuclear physics projects. More details are available.

## Announcements (see also **Meetings** and **Job Postings** and **News Archive**)

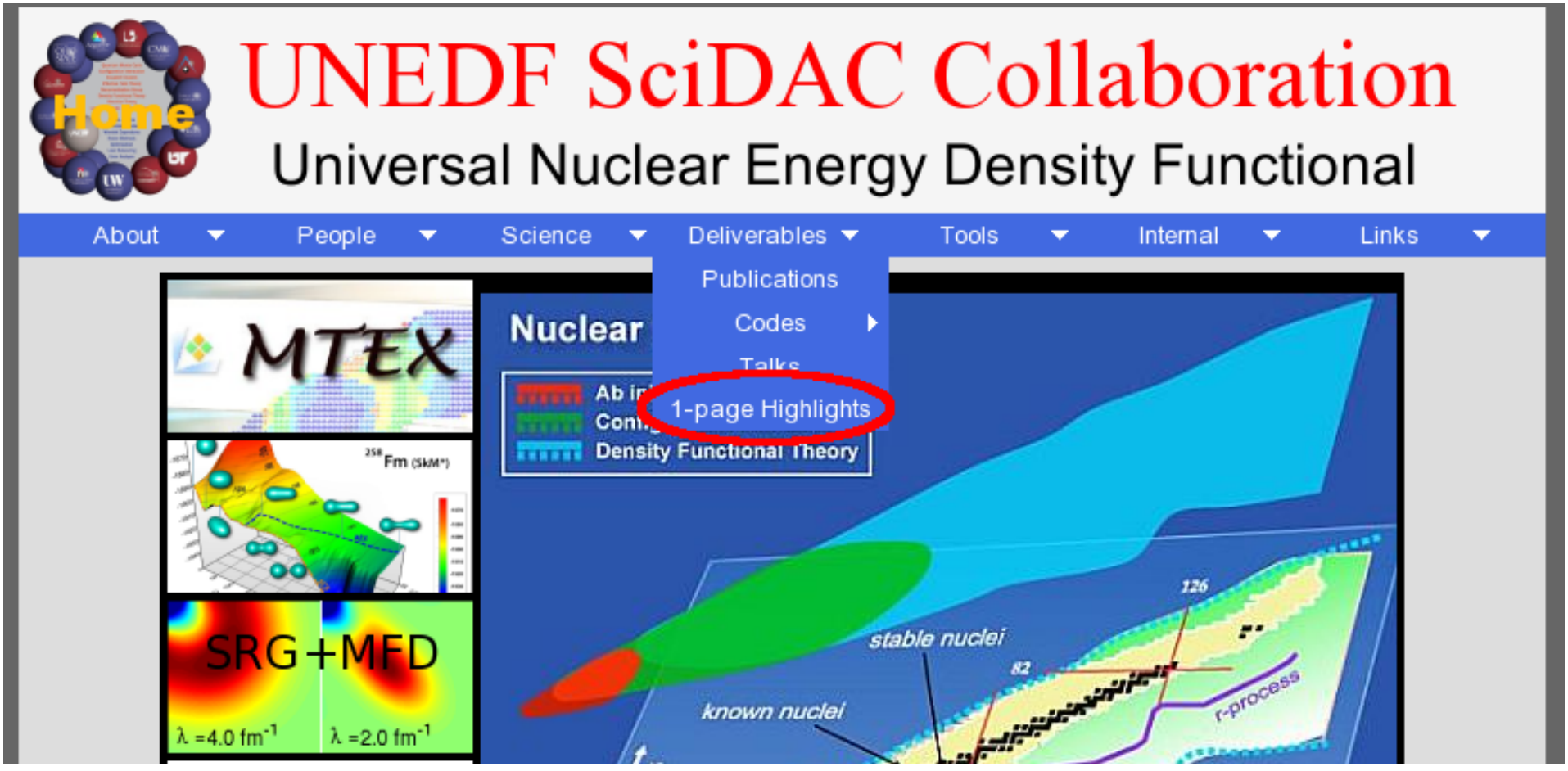
Annual UNEDF Collaboration Meeting, MSU (website)

June 21-25, 2010

SciDAC 2010 meeting, Chattanooga, Tennessee

July 11-15, 2010

# Highlights of research on unedf.org




- One-slide summaries targeted for broad audience
- Notes with details and references
- Look under Internal→One-Pagers for guidelines


# UNEDF SciDAC Collaboration

## Universal Nuclear Energy Density Functional



## UNEDF One-Page Highlights

On this page are links to one-slide summaries of UNEDF-related research accomplishments, plus notes giving contacts and references along with brief explanations of the technical details. All are in pdf format. See also the "UNEDF Highlights" page.

- NEW Nuclear excitement [notes]
- NEW Proton halo in fluorine-17 as a fragile 17-body quantum state [notes]
- UNEDF-TOPS eigensolver collaboration: Breakthrough nuclear science [notes]
- Microscopic description of nuclear fission [notes]
- Building medium-mass atomic nuclei from scratch: coupled cluster [notes]
- Computing masses of atomic nuclei [notes]
- Discovering the secrets buried in theories [notes]
- The uNclear Nuclear Pairing [notes]
- For atomic nuclei, three's a crowd: Enabling microscopic calculations of nuclei [notes]
- Building the UNEDF from the ground up [notes]
- Towards improved cross sections on medium and heavy unstable nuclides [notes]
- High-performance code for nuclear level density [notes]
- Predictions for Proton-Dripping Fluorine-14 [notes]
- Ab initio no-core shell model (NCSM) and resonating-group method (RGM)

# For all speakers: Points to emphasize

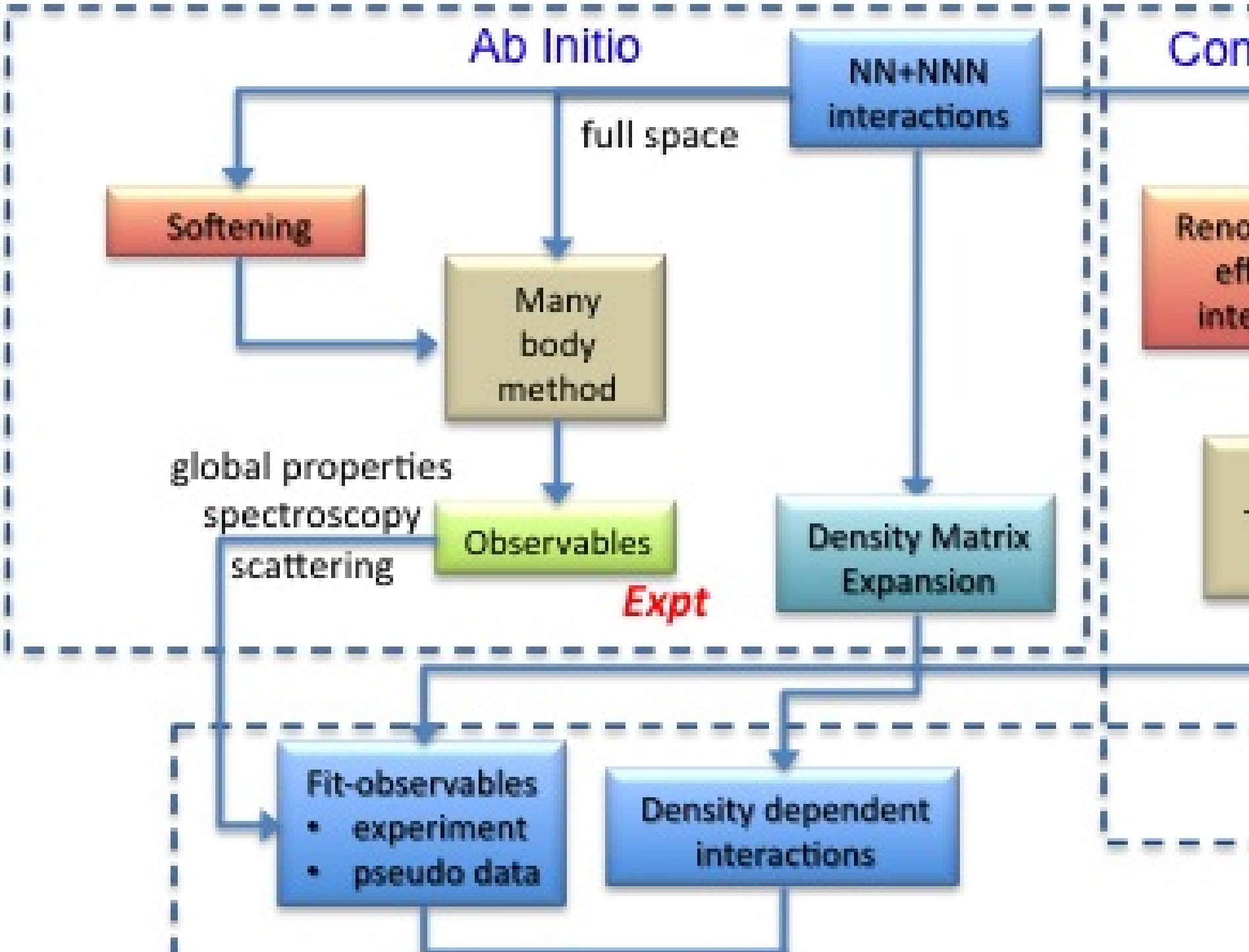
- What are the main accomplishments since the last meeting? Is your Year-4 plan well on track? If not, why?
- What are the aspects of your science that require high-performance computing?

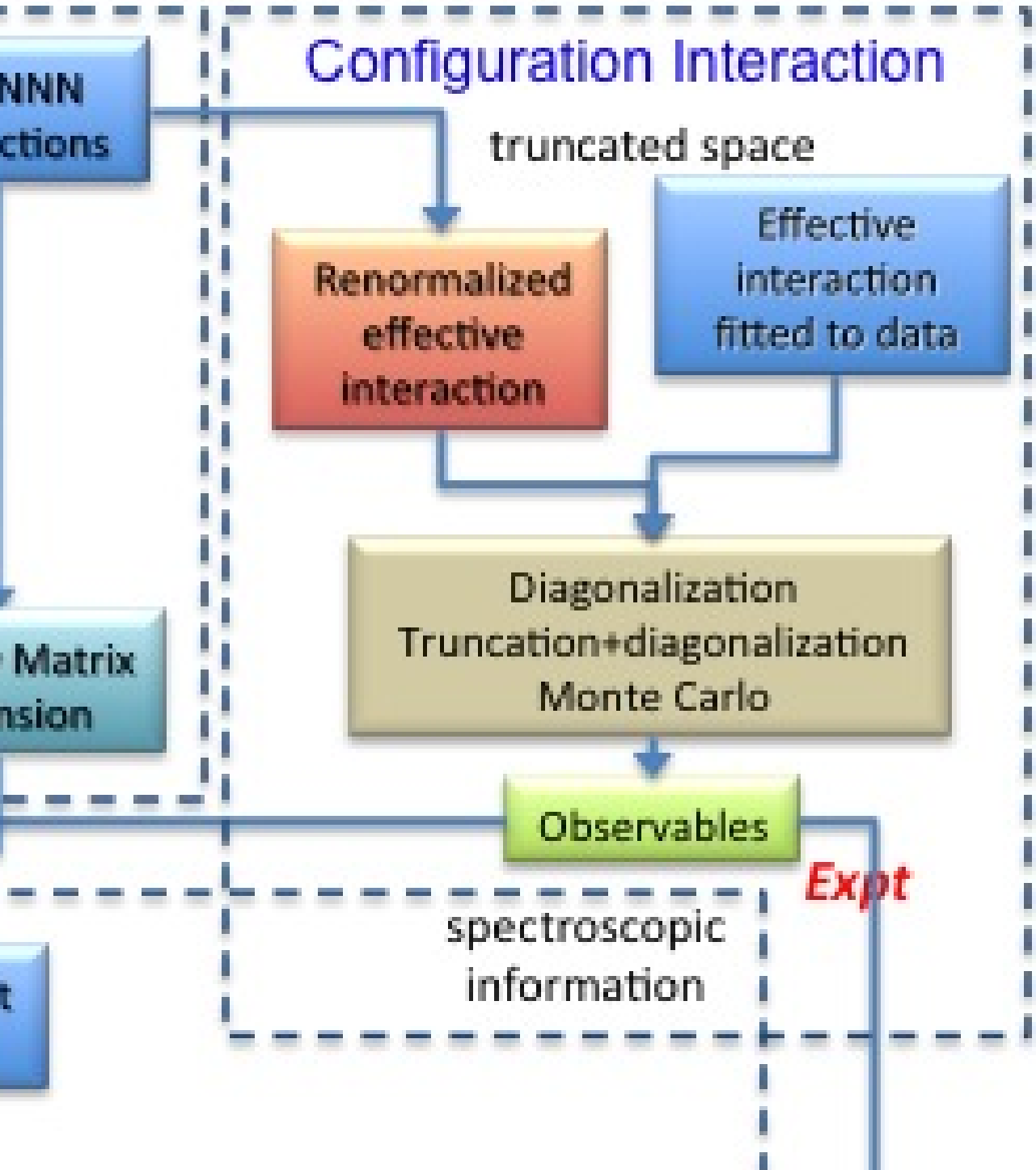
  OR

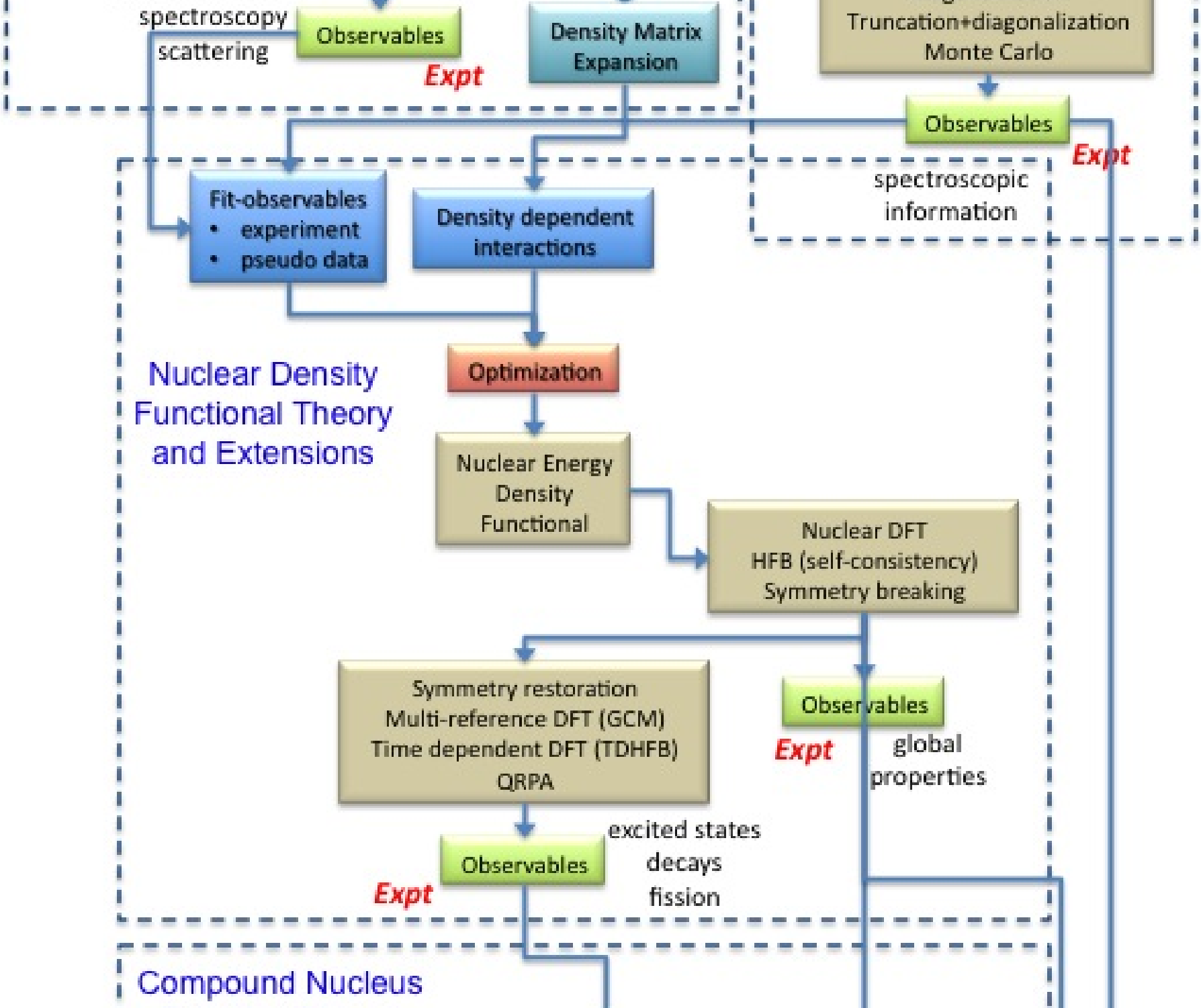
  What problems in high performance computing are you working on in general?
- What are the major computational issues? Are there any questions you would like to bring to the attention of our CS/AM collaborators?

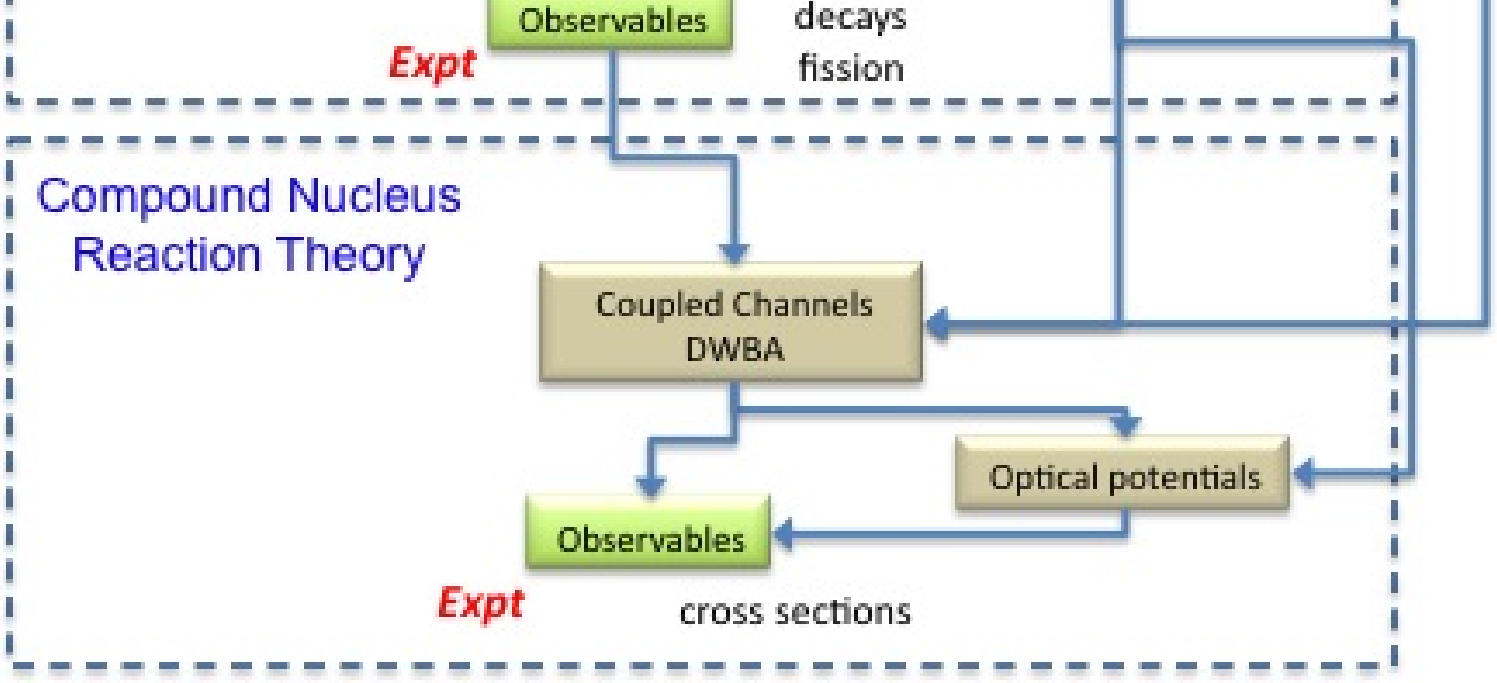
  OR

  Are there general capabilities of your computer science work that might be of interest to other physicists than the ones you are currently working with?
- What is the detailed roadmap of your project for the remaining part of Year-4 and Year-5?
- Are there any ”showcase” (i.e., of Nature/Science caliber) physics and computational questions that you are hoping to answer in Years 4 and 5?


Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Fit-observables
• experiment
• pseudo data
Density dependent interactions


Configuration Interaction
NNN
ctions
truncated space
Renormalized
effective
interaction
Effective
interaction
fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Matrix
nsion
Observables
Expt
spectroscopic
information


spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)
Symmetry breaking
Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA
Observables
Expt
global properties
Observables
Expt
excited states
decays
fission
Compound Nucleus


Observables
Expt
decays
fission
Compound Nucleus
Reaction Theory
Coupled Channels
DWBA
Optical potentials
Observables
Expt
cross sections