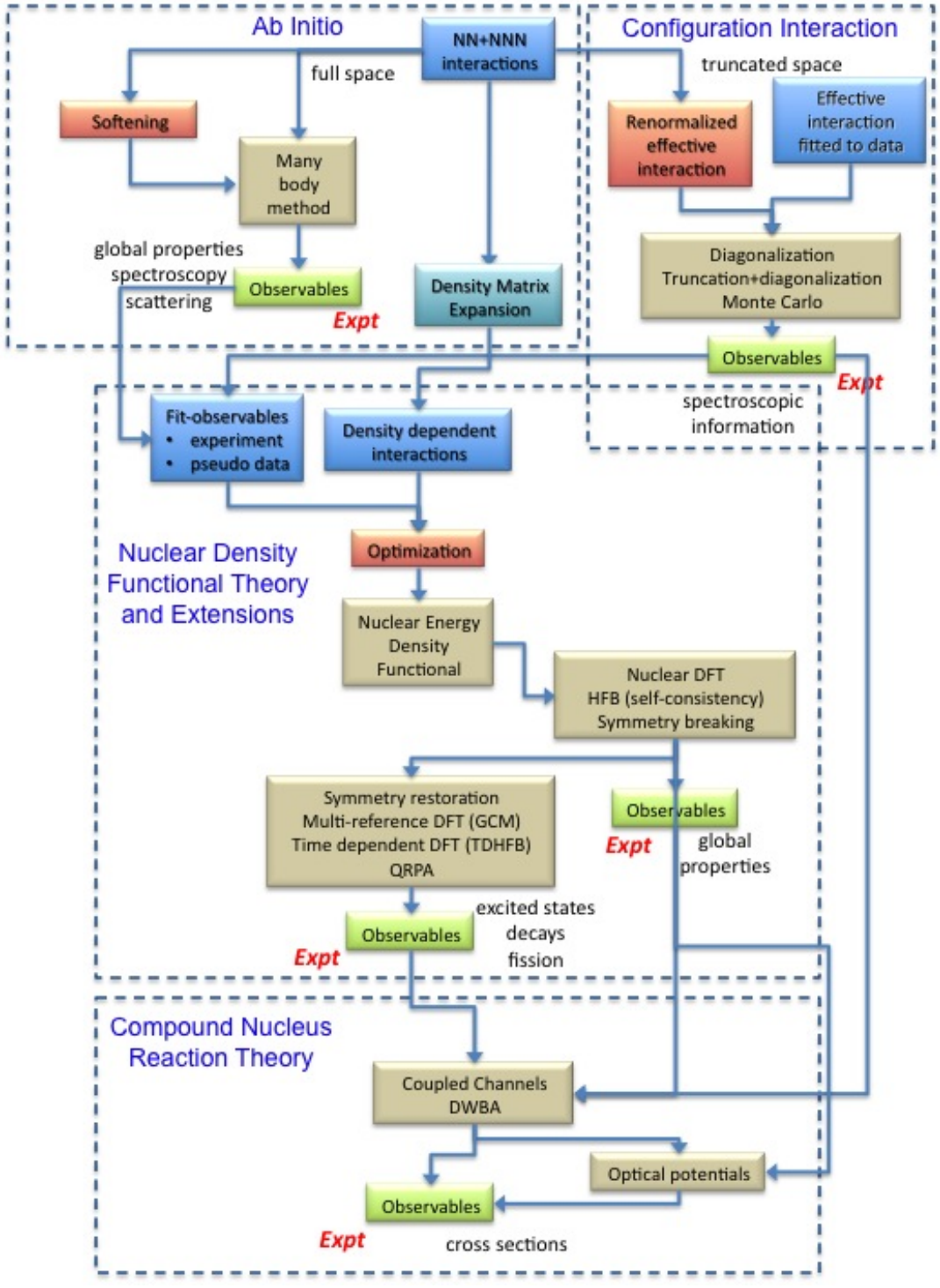
Deliverables, Highlights, and Reports

- status and plans
- news and one-pagers
- annual and exit reports
- points of emphasis



Year-5 Deliverables (from Year-4 annual report summary)

- Ab-initio Deliverables (Monday)
  - Further calculate homogeneous neutron matter and neutron drops in external fields using GFMC and AFDMC to create pseudo-data for constraining energy density functionals.
  - Calculate the Hoyle state with GFMC.
  - Continue improvements to ADLB resulting in community usable code.
  - The LCCI project will deliver final UNEDF versions of LCCI codes, scripts, and test cases and the prototype DBMS will be completed and released.
  - Study role of NNN forces in medium mass nuclei with CC.
  - Analyze LQCD calculations of multi-baryon systems at sufficiently low pion mass to permit extrapolation to the physical point.
  - Complete CUDA hybrid Monte Carlo (HMC) codes and apply them to the first large-scale HMC calculations of the unitary Fermi gas.

Year-5 Deliverables (from Year-4 annual report summary)

- Ab initio Functionals Deliverables (Tuesday/Wednesday)
  - Perform neutron drop benchmarks starting from realistic NN and NNN interactions and validate against ab-initio calculations.
  - Develop the Optimized Effective Potential method for 3D-HFB; compare with HF, HF-DME, and ab initio.
  - Develop improved DME functionals that go beyond Hartree-Fock.
  - Use in-medium SRG to develop valence shell model Hamiltonians and effective operators for open-shell nuclei.

Year-5 Deliverables (from Year-4 annual report summary)

- DFT Infrastructure/Applications Deliverables (Tues./Wed.)
  - Full implementation of ADIOS in HFODD; set up framework for automatic restart.
  - Optimize generalized Skyrme functionals and DME functionals by considering additional constraints on states at large deformation, shell structure, giant resonances, and neutron droplets pseudo-data from ab-initio calculations.
  - Use UNEDF functionals in large-scale surveys, spectroscopy, and description of fission.
  - Develop open-source implementation of POUNDERS.
  - Continue development of model-based optimization algorithms for noisy and constrained calculations. Global explorations of the parameter space by means of a space-filling design in order to delineate regions of stability of EDF.
  - Further optimize the ASLDA DFT solver.
  - Implement the constrained 3D Skyrme-HFB-MADNESS framework and apply to fission and cold fermions.

Year-5 Deliverables (from Year-4 annual report summary)

- DFT Extensions Deliverables (Wednesday)
  - Use the new QRPAdef code to complete the beta decay calculation
  - Develop DFT-consistent code beyond QRPA
  - Use the TDSLDA code to describe collective motion in nuclei
  - Develop and test the J-Moments nuclear level density code that removes the center- of-mass spurious states
  - Use the new J-Moments code to calculate reaction rates in the rp-process path
  - Understand the scalability barriers in NuShellX to enable the most effective use of Graphic Processing Units (GPUs) and leadership-class machines.
  - Improve the scalability of BIGSTICK CI code up to 50,000 cores
  - Use BIGSTICK code to investigate isospin breaking in pf shell

Year-5 Deliverables (from Year-4 annual report summary)

- Reaction Deliverables (Thursday)
  - Investigate reactions in light nuclei using NCSM with RGM: Benchmark n-8He, and n-9Li scattering. Investigate p-7Be and 3H+4He scattering and capture reactions. Use two-, three-, and four-body transition densities for $A = 3, 4$ nuclei. Development of three-body transition density calculation for $A > 4$.
  - Analyze Ab initio nuclear scattering in HO traps to three and four-body systems such as n-d and n-t.
  - Consistent nucleon-nucleus optical potentials within elastic and all inelastic and transfer channels.
  - Fold QRPA transition densities with density-dependent and spin-orbit forces. Include effective masses, and direct charge-exchange.
  - Calculate and investigate effects of exchange nonlocalities.

Year-5 Deliverables (from Year-4 annual report summary)

- (more) Reaction Deliverables (Thursday)
  - Systematic generation of optical potentials for a wide range of near-spherical nuclei.
  - First nucleon-nucleus calculations with deformed QRPA transition densities.
  - Examine role of optical-potential L-dependences & non-localities in direct reaction calculations.
  - Examine energy-dependence of eigensolutions in the expansion for the KKM theory.

Preparation for UNEDF annual and final reports

- Needed from each section leader
  - Progress reports on Year-5 deliverables
  - Plans for carry-over funds (if any)
- To me by email ASAP (`furnstahl.1@osu.edu`)
  - Papers acknowledging UNEDF (both published and preprints)
  - ***UNEDF-related invited talks*** (non-collaboration meeting)
  - Check unedf.org for what is missing since Year-4 CPR!
  - UNEDF-related “Good News” and “UNEDF in the News”
  - Highlights — a new one (or more) from every sub-project!
- Guidelines for continuation progress report and final report
  - CPR like last year (but less time pressure)
  - Final exit report due June, 2012

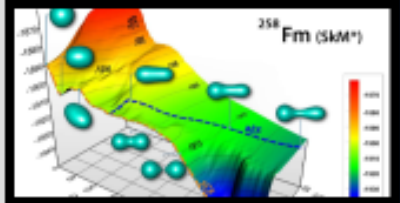
UNEDF Highlights and News

- One-page highlights are needed for our sponsors
  - to tell our successes to DOE NP, ASCR, NNSA
  - to give them success stories to tell
  - for DNP and NSAC and ...
  - also for broader science community and general public
- Website unedf.org is repository for highlights and news
  - Status of website going forward?
- Nuclear Physics News articles on UNEDF physics in June
  - project overview (copies available), NCSM, FUSTIPEN
  - linked on unedf.org

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

MTEX



SRG+MFD

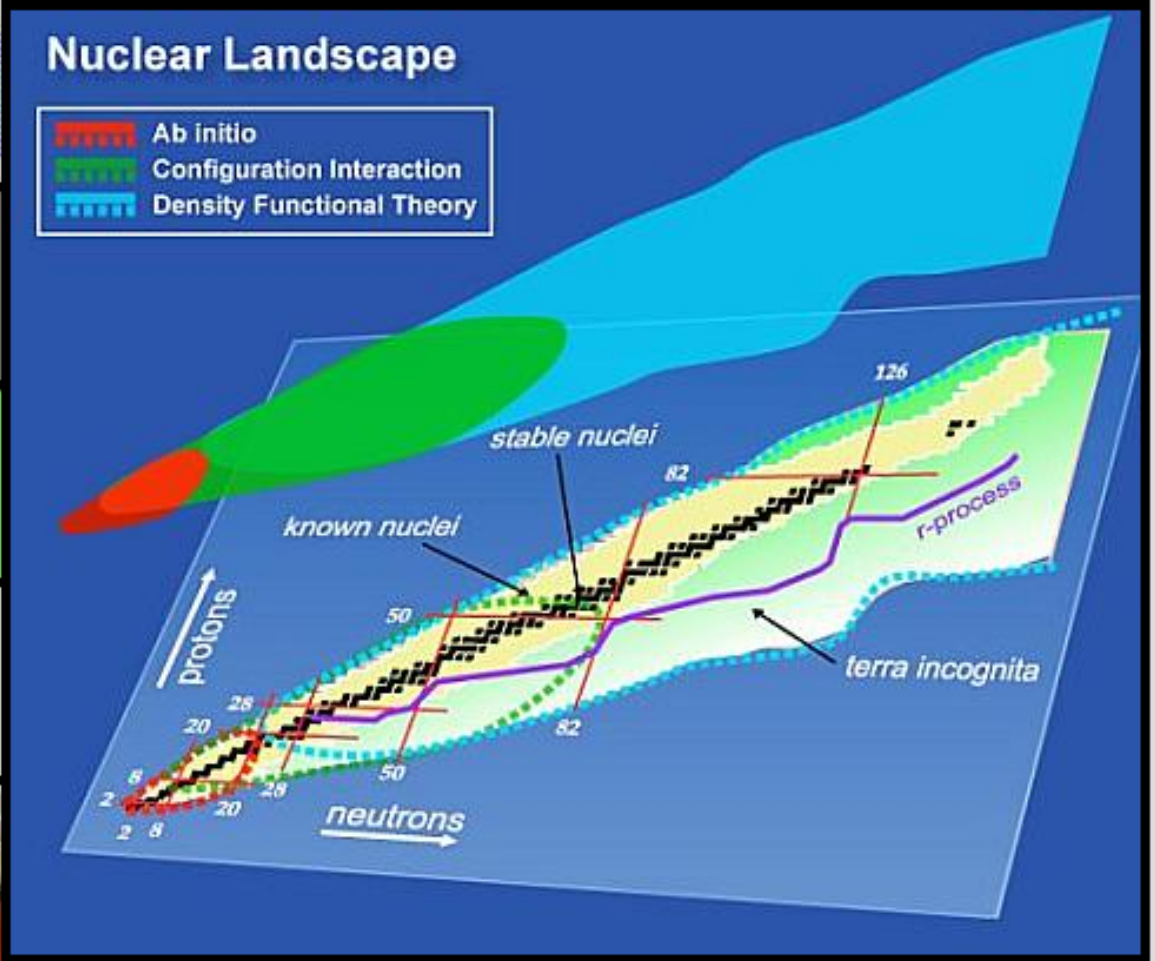
λ =4.0 fm^{-1} λ =2.0 fm^{-1}

^{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 (see also UNEDF in the News and the Good News Archive)

Pioneering calculations of quantized vortices appear in Science magazine

A team led by UNEDF researcher Aurel Bulgac of the University of Washington has developed a computational framework that describes the superfluid dynamics of fermions. The June 10 issue of Science features a paper describing real-time evolution and interaction of quantized vortices based on the solution of up to hundreds of thousands of coupled nonlinear partial differential equations. A press release with further details on the work and all the researchers can be found here.

UNEDF collaboration member receives early career grant from DOE

Sofia Quaglioni of Lawrence Livermore National Laboratory was recently awarded a grant from the Department of Energy Office of Science Early Career Research Program (ECRP). Sofia is one of 65 ECRP recipients and she will use the grant to continue her research to achieve an accurate prediction of fusion reactions. Sofia has been partially supported by the UNEDF project over the past few years, working alongside Petr Navratil to derive and apply an ab initio framework to describe nucleon scattering on light nuclei. The list of Early Career award recipients may be found here and the Livermore press release may be found here.

UNEDF project featured in DOE Office of Science "Science Highlights Series"

An article entitled "Universities and DOE National Laboratories Join Forces to Understand the Nucleus of an Atom" about the UNEDF collaboration is the February, 2011 highlight.

UNEDF collaboration member wins CMU President's Award for Outstanding Research

Prof. Mihai Horoi of Central Michigan University was one of two recipients recognized for "scholarship and research of national and international merit" (see video and press release).

UNEDF researcher to join University of Tsukuba high performance computing effort

Dr. Jun Terasaki, UNEDF collaboration member at the University of North Carolina, will take his expertise to a five-year UNEDF-like project using massively parallel computers.

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

Annual UNEDF Collaboration Meeting, MSU (local website)

June 19-24, 2011

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

UNEDF in the News

Calculations by UNEDF researchers at Iowa State and LBNL featured in ScienceNewsline

An article entitled "Proton dripping tests a fundamental force in nature" about calculations of the exotic, short-lived fluorine-14 nucleus was posted on May 11, 2011. ScienceNewsline.com is a news portal about science and technology that is targeted at industry, science and educational experts.

UNEDF project featured in DOE Office of Science "Science Highlights Series"

An article entitled "Universities and DOE National Laboratories Join Forces to Understand the Nucleus of an Atom" about the UNEDF collaboration is the February, 2011 highlight.

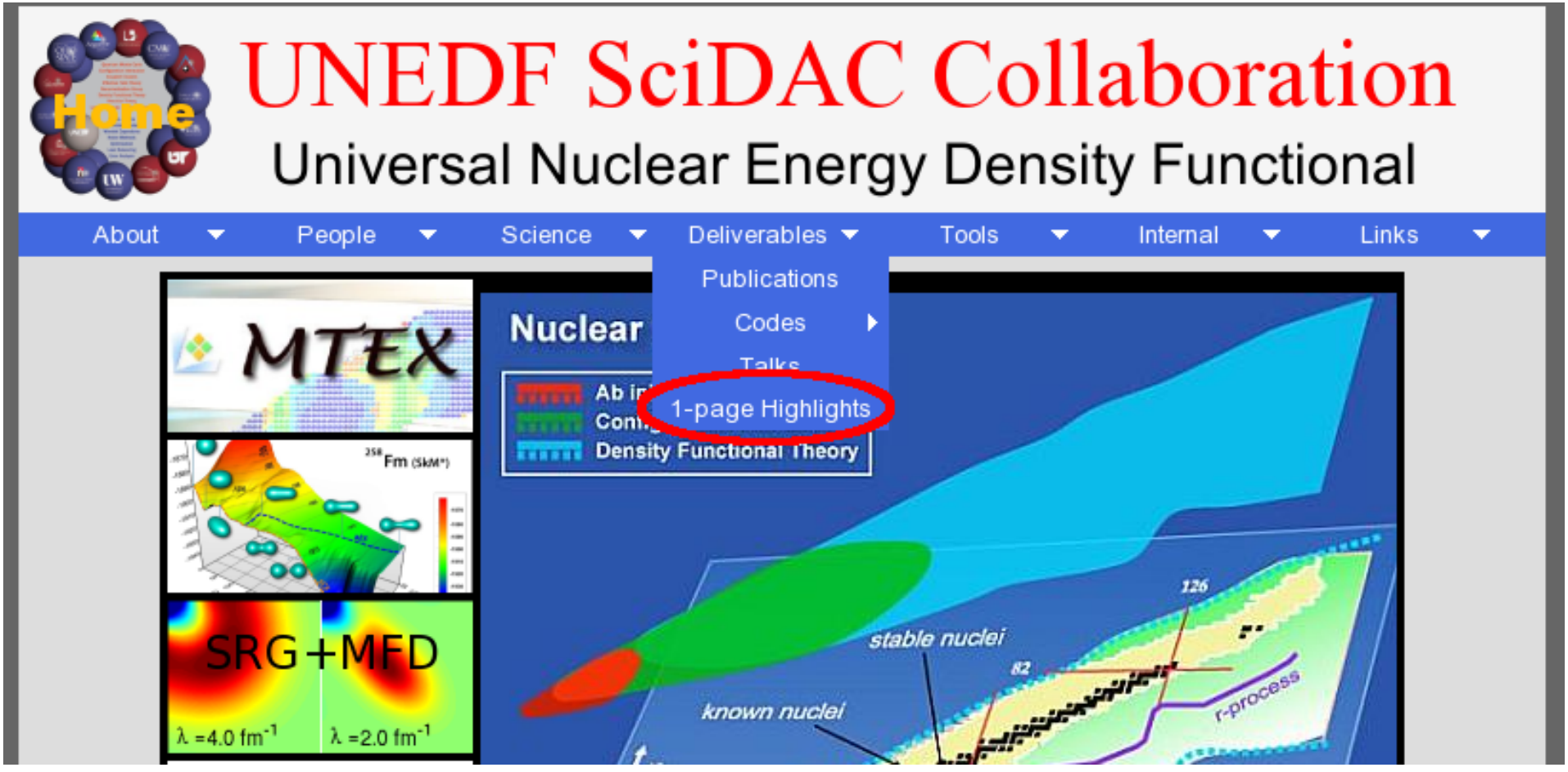
Improving density functionals for the UNEDF project is featured in DEIXIS

The universal energy density functional under development by UNEDF scientists requires the solution of density functional theory equations for nuclei and the adjustment of coupling constants to best reproduce a selected subset of nuclear properties. This optimization-minimization problem has been attacked in collaboration with applied mathematicians at Argonne National Laboratory, who have developed the POUNDERS algorithm for vastly imporved optimization.

Innovative algorithm developed for UNEDF is featured in DEIXIS

The POUNDERS algorithm, developed by Stefan Wild and collaborators at Argonne National Laboratory, addresses the critical need for rapid and detailed information to optimize energy functionals under development for the UNEDF project.

Highlights of research on unedf.org



- One-slide summaries targeted for broad audience or for specific sponsors
- Notes with details and references (usually)
- Also look under Internal⟶One-Pagers

UNEDF One-Page Highlights

On this page are links to one-slide summaries of UNEDF-related research accomplishments. All are in pdf format. See also the "UNEDF Highlights" page.

Computing and Applied Math Highlights

- NEW Anomalous Long Lifetime of Carbon-14
- NEW 2011 INCITE award to UNEDF researchers
- Proton-Dripping Fluorine-14
- Load Balancing at Extreme Scale
- Derivative-free Optimization for Density Functional
- Towards reliable cross sections for astrophysics, nuclear energy and security
- Ab initio nuclear reactions
- Time-Dependent Superfluid Local Density Approximation - TDSLDA
- MADNESS for SciDAC UNEDF

Highlights for General Audiences

These highlights also come with notes giving contacts and references along with brief explanations of the technical details.

- Nuclear excitement [notes]
- 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]

For all UNEDF speakers: Points to emphasize

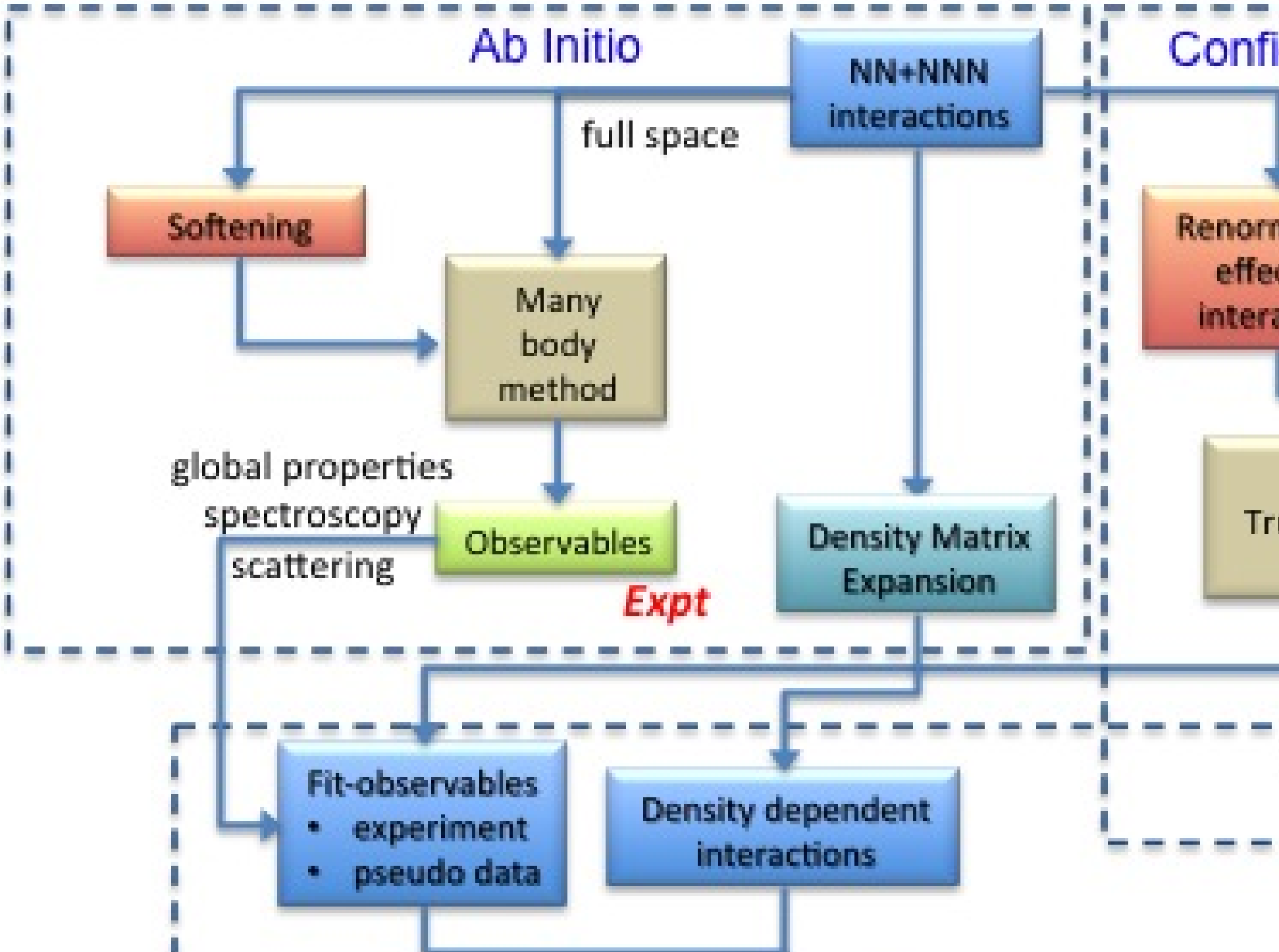
- What are the main accomplishments since the last meeting? Is your Year-5 plan well on track? If not, why?
- What are the aspects of your science that require high-performance computing?

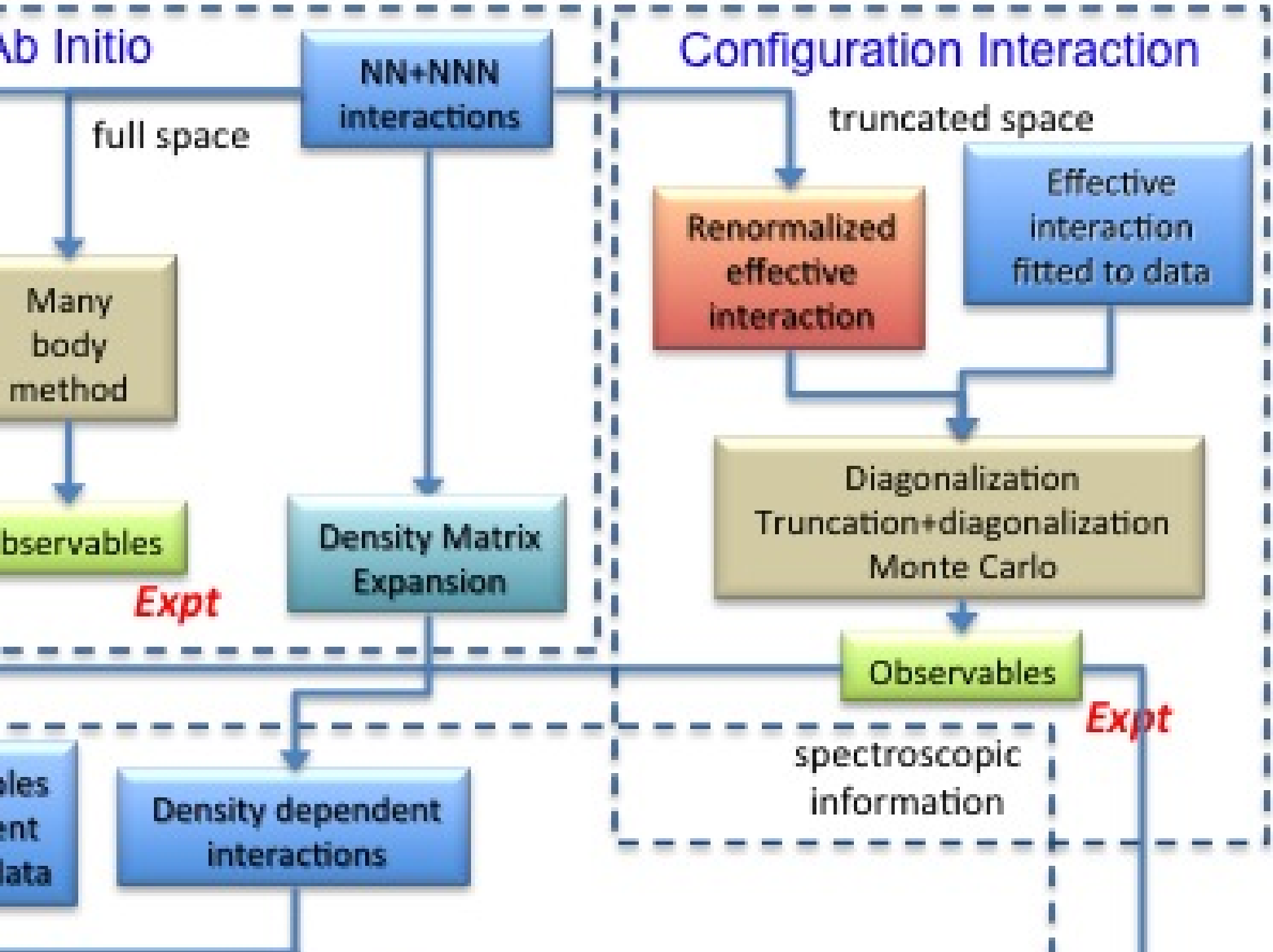
  OR

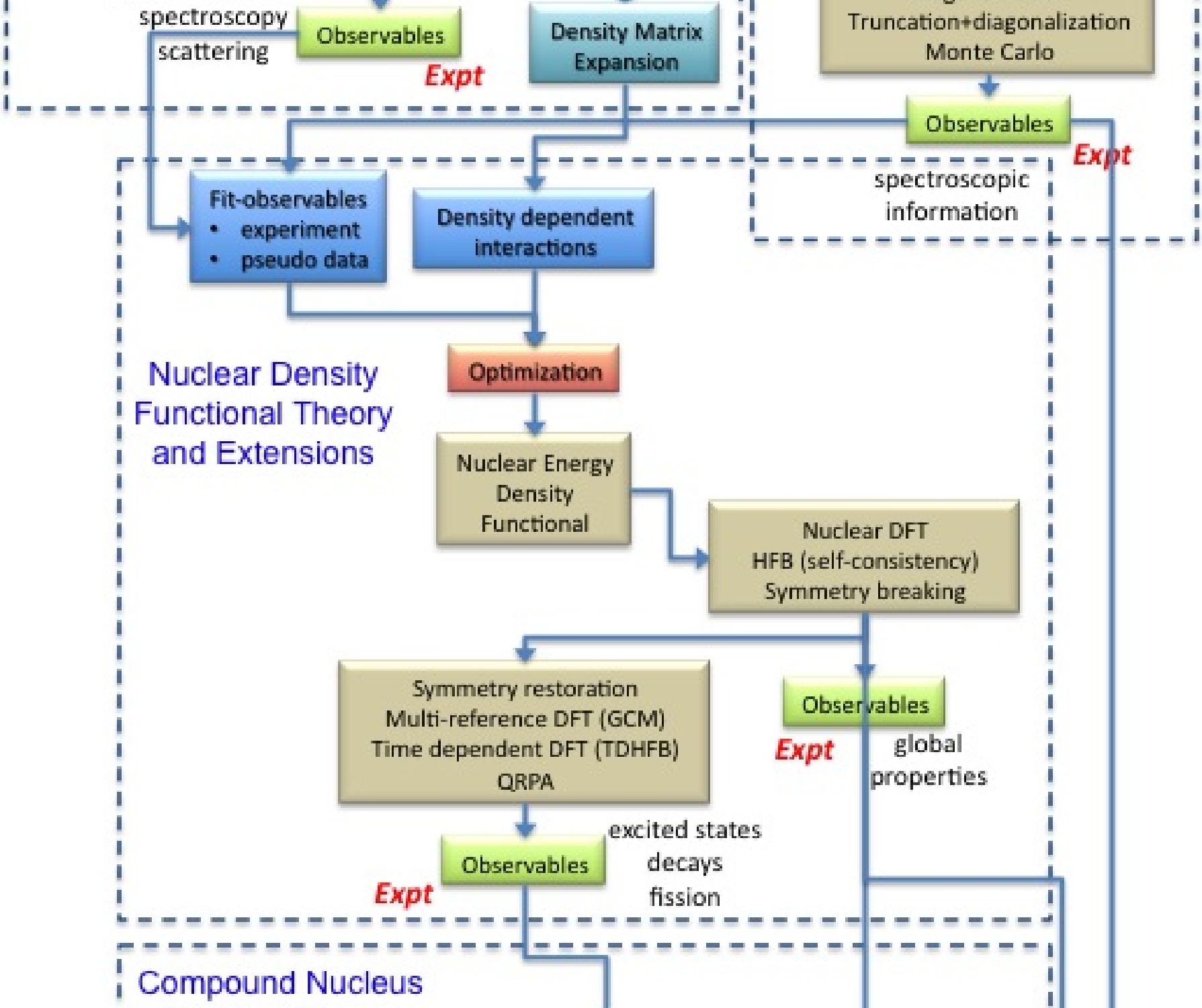
  What problems in high performance computing are you working on in general?
- What are the major computational issues? Are there any questions you would like to bring to the attention of our CS/AM collaborators?

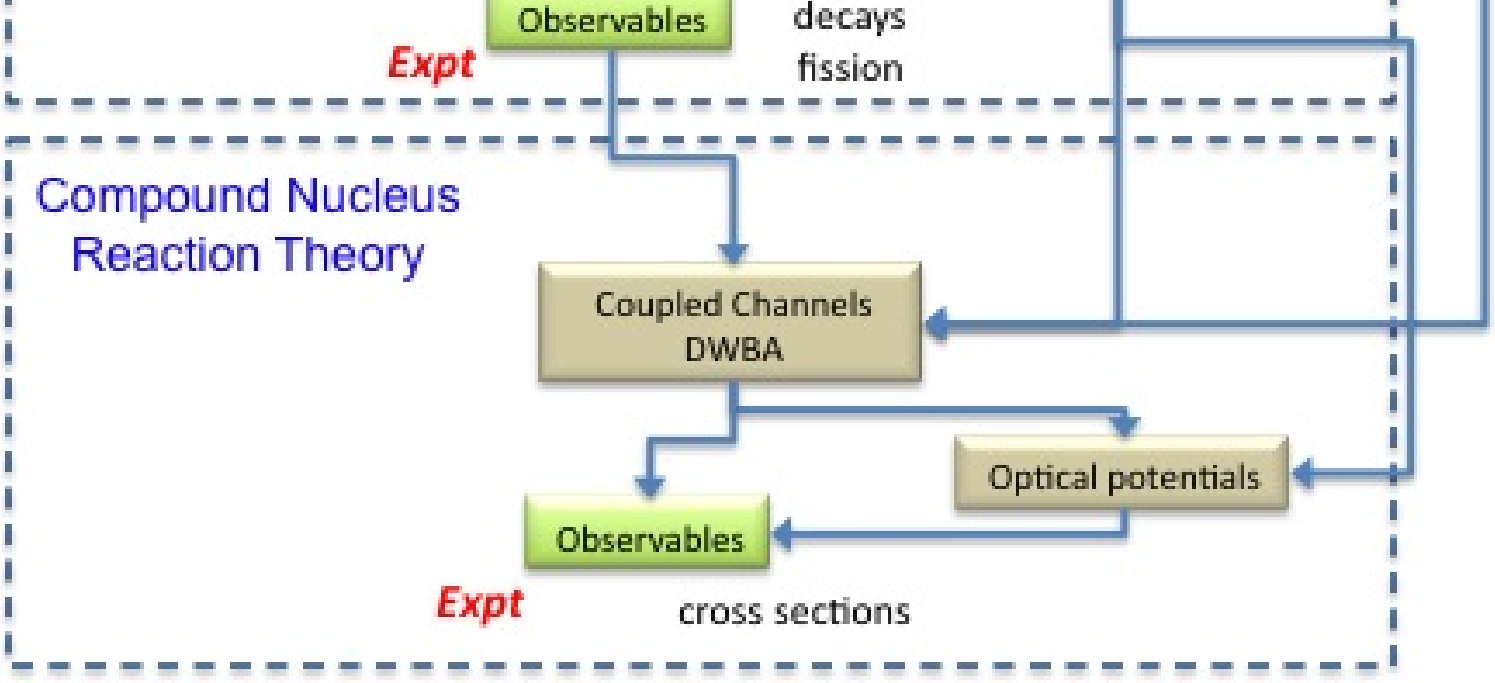
  OR

  Are there general capabilities of your CS/AM 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-5 (and beyond)?
- Are there any ”showcase” (i.e., of Nature/Science caliber) physics and computational questions that you are hoping to answer in Year 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


Ab Initio
NN+NNN interactions
full space
Many body method
bservables
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
Density dependent interactions


spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Nuclear Density Functional Theory and Extensions
Optimization
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
excited states
decays
fission
Observables
Expt
Compound Nucleus


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