Quantifying Uncertainties in Nuclear Density Functional Theory

P(ND)2-2 – Second International Workshop on Perspectives on Nuclear Data for the Next Decade

October 14 – 17, 2014

Nicolas Schunck
The NUCLEI SciDAC 3 Collaboration

NUCLEI Mission Statement

The NUCLEI (Nuclear Computational Low-Energy Initiative) SciDAC project builds upon recent successes in large-scale computations of atomic nuclei to provide results critical to nuclear science and nuclear astrophysics, and to nuclear applications in energy and national security.

SciDAC Mission Statement

The U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program was created to bring together many of the nation's top researchers to develop new computational methods for tackling some of the most challenging scientific problems.
The INCITE Program

The U.S. Department of Energy (DOE) Office of Science provides a portfolio of national high-performance computing facilities housing some of the world’s most advanced supercomputers. These leadership computing facilities enable world-class research for significant advances in science.

- 4th largest allocation for 2014-2017
- Supports 6 programs solving the nuclear many-body problem
- Hybrid MPI/OpenMP model, some with GPU, scale up to full machine

INCITE Mission Statement

The INCITE Program provides a portfolio of national high-performance computing facilities housing some of the world’s most advanced supercomputers. These leadership computing facilities enable world-class research for significant advances in science.

Types of jobs

- 4th largest allocation for 2014-2017
- Supports 6 programs solving the nuclear many-body problem
- Hybrid MPI/OpenMP model, some with GPU, scale up to full machine
The Nuclear Hierarchy
The Nuclear Hierarchy

- Hierarchy of degrees of freedom
  - Quarks and gluons in relativistic quantum field theory
  - Structure-less nucleons in non-relativistic quantum mechanics
  - Densities of nucleons in quantum mechanics and/or classical physics
The Nuclear Hierarchy

- Hierarchy of degrees of freedom
  - Quarks and gluons in relativistic quantum field theory
  - Structure-less nucleons in non-relativistic quantum mechanics
  - Densities of nucleons in quantum mechanics and/or classical physics

- The physics of nuclei is based on nucleons and densities of nucleons, not quarks or gluons
### The Nuclear Hierarchy

- **Hierarchy of degrees of freedom**
  - Quarks and gluons in relativistic quantum field theory
  - Structure-less nucleons in non-relativistic quantum mechanics
  - Densities of nucleons in quantum mechanics and/or classical physics

- The physics of nuclei is based on nucleons and densities of nucleons, not quarks or gluons

- **Nuclear density functional theory (DFT)**
  - Built on effective nuclear forces between protons and neutrons
  - Uses densities of nucleons as fundamental degrees of freedom
  - Relies on symmetry breaking
The Realm of Nuclear DFT

DFT is the only microscopic theory for heavy nuclei
Nuclear DFT for Dummies
Nuclear DFT for Dummies

- System of independent particles $\Rightarrow$ uncorrelated wave-function
Nuclear DFT for Dummies

- System of independent particles $\Rightarrow$ uncorrelated wave-function
- Total energy is a functional of the density of nucleons: energy density functional (EDF)
Nuclear DFT for Dummies

- System of independent particles $\Rightarrow$ uncorrelated wave-function
- Total energy is a functional of the density of nucleons: energy density functional (EDF)
- Cannot build the EDF from realistic nuclear forces: induced many-body physics cut-off by assumption of independent particles
  - Design and optimize “hand-made” effective nuclear forces
  - Symmetry breaking the key to success
Nuclear DFT for Dummies

- System of independent particles $\Rightarrow$ uncorrelated wave-function
- Total energy is a functional of the density of nucleons: energy density functional (EDF)
- Cannot build the EDF from realistic nuclear forces: induced many-body physics cut-off by assumption of independent particles
  - Design and optimize “hand-made” effective nuclear forces
  - Symmetry breaking the key to success
- Compared to direct approaches with realistic potentials, EDFs
  - Encode physics beyond independent particle level = the magic of producing correlations with independent particles!
  - Are phenomenological by construction. Ex.: density dependencies
Nuclear DFT for Dummies

- System of independent particles \(\Rightarrow\) uncorrelated wave-function
- Total energy is a functional of the density of nucleons: energy density functional (EDF)
- Cannot build the EDF from realistic nuclear forces: induced many-body physics cut-off by assumption of independent particles
  - Design and optimize “hand-made” effective nuclear forces
  - Symmetry breaking the key to success
- Compared to direct approaches with realistic potentials, EDFs
  - Encode physics beyond independent particle level = the magic of producing correlations with independent particles!
  - Are phenomenological by construction. Ex.: density dependencies
- Examples: Skyrme (zero-range) and Gogny (finite-range) forces

Reviews: RMP 75, 121 (2003), Prog. Part. Nucl. Phys. 64, 120 (2010)
Skyrme: PRC 5, 626 (1972); Gogny: PRC 21, 1568 (1980)
DFT as a Model
DFT as a Model

- A mathematician view of DFT: given a set of parameters, we produce a set of outputs by solving the DFT equations (to determine the actual density $\rho(r)$ in the system)
DFT as a Model

- A mathematician view of DFT: given a set of parameters, we produce a set of outputs by solving the DFT equations (to determine the actual density $\rho(r)$ in the system)

- Sources of uncertainties
  - Numerical errors due to implementation of DFT equations on a CPU

Numerical errors

arXiv:1406.4383
DFT as a Model

- A mathematician view of DFT: given a set of parameters, we produce a set of outputs by solving the DFT equations (to determine the actual density $\rho(r)$ in the system)

- Sources of uncertainties
  - Numerical errors due to implementation of DFT equations on a CPU
  - Statistical errors induced by the fit of model parameters on data

Numerical errors

Statistical errors

**arXiv:1406.4383**

**PRC 89, 054314 (2014)**
DFT as a Model

- A mathematician view of DFT: given a set of parameters, we produce a set of outputs by solving the DFT equations (to determine the actual density $\rho(r)$ in the system)

- Sources of uncertainties
  - Numerical errors due to implementation of DFT equations on a CPU
  - Statistical errors induced by the fit of model parameters on data
  - Systematic errors caused by the choice of the functional

**Numerical errors**  
*arXiv:1406.4383*

**Statistical errors**  
*PRC 89, 054314 (2014)*

**Systematic errors**  
*From PRC 61, 034313 (2000)*
Skyrme Energy Density
Skyrme Energy Density

- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

\[ E = \int d^3r \left[ \mathcal{E}_{\text{kin}}(r) + \mathcal{E}_{\text{Cou}}(r) + \mathcal{E}_{\text{pair}}(r) + \sum_{t=0,1} \chi_t(r) \right] \]
Skyrme Energy Density

- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

\[
E = \int d^3r \left[ \mathcal{E}_{\text{kin}}(r) + \mathcal{E}_{\text{Cou}}(r) + \mathcal{E}_{\text{pair}}(r) + \sum_{t=0,1} \chi_t(r) \right]
\]

- Nuclear potential term
Skyrme Energy Density

- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

\[ E = \int d^3 r \left[ \mathcal{E}_{\text{kin}}(r) + \mathcal{E}_{\text{Cou}}(r) + \mathcal{E}_{\text{pair}}(r) + \sum_{t=0,1} \chi_t(r) \right] \]

- Nuclear potential term

\[ \chi_t(r) = C_{\rho}^{\rho \rho} \rho_t^2 + C_{\rho}^{\rho \tau} \rho_t \tau_t + C_{t}^{J J} \sum_{\mu \nu} J_{\mu \nu, t} J_{\mu \nu, t} \]

\[ + C_{t}^{\rho \Delta \rho} \rho_t \Delta \rho_t + C_{t}^{\rho \nabla J} \rho_t \nabla \cdot J_t \]
Skyrme Energy Density

- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

\[
E = \int d^3r \left[ \mathcal{E}_{\text{kin}}(r) + \mathcal{E}_{\text{Cou}}(r) + \mathcal{E}_{\text{pair}}(r) + \sum_{t=0,1} \chi_t(r) \right]
\]

- Nuclear potential term

\[
\chi_t(r) = C^\rho_\rho_\rho_\rho t^2 + C^\rho_\tau_\rho_\tau t + C^J_JJ \sum_{\mu \nu} J_{\mu \nu, t} J_{\mu \nu, t}
\]

\[
+ C^\rho_\Delta_\rho_\rho_\Delta_\rho t + C^\rho_\nabla_\rho_\nabla J_\rho_\nabla \cdot J_\rho
\]
Skyrme Energy Density

- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

\[ E = \int d^3r \left[ \mathcal{E}_{\text{kin}}(r) + \mathcal{E}_{\text{Cou}}(r) + \mathcal{E}_{\text{pair}}(r) + \sum_{t=0,1} \chi_t(r) \right] \]

- Nuclear potential term

\[ \chi_t(r) = C_t^{\rho \rho} \rho_t^2 + C_t^{\rho \tau} \rho_t \tau_t + C_t^{J J} \sum_{\mu \nu} J_{\mu \nu, t} J_{\mu \nu, t} + C_t^{\rho \Delta \rho} \rho_t \Delta \rho_t + C_t^{\rho \nabla J} \rho_t \nabla \cdot J_t \]
Skyrme Energy Density

- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

\[
E = \int d^3r \left[ \mathcal{E}_{\text{kin}}(r) + \mathcal{E}_{\text{Cou}}(r) + \mathcal{E}_{\text{pair}}(r) + \sum_{t=0,1} \chi_t(r) \right]
\]

- Nuclear potential term

\[
\chi_t(r) = C_t^{\rho_\rho} \rho_t^2 + C_t^{\rho \tau} \rho_t \tau_t + C_t^{JJ} \sum_{\mu \nu} J_{\mu \nu, t} J_{\mu \nu, t}
\]
Optimization Strategies
Optimization Strategies

- Given the form of the functional, how do we fit model parameters?
Optimization Strategies

- Given the form of the functional, how do we fit model parameters?
- Experimental data
  - Find data such that each term in the functional is constrained
  - Choose data as model-independent as possible. Ex.: atomic masses
  - Avoid evaluated data, stay away from large error bars
Optimization Strategies

- Given the form of the functional, how do we fit model parameters?
- Experimental data
  - Find data such that each term in the functional is constrained
  - Choose data as model-independent as possible. Ex.: atomic masses
  - Avoid evaluated data, stay away from large error bars
- A philosophical choice: A little or a lot of data?
Optimization Strategies

- Given the form of the functional, how do we fit model parameters?

- Experimental data
  - Find data such that each term in the functional is constrained
  - Choose data as model-independent as possible. Ex.: atomic masses
  - Avoid evaluated data, stay away from large error bars

- A philosophical choice: A little or a lot of data?
  - Mass models (Bruxelles-Montréal)
    - Take all available data on masses and fit the parameters
    - r.m.s. values: 0.50 MeV (Skyrme), 0.80 MeV (Gogny), 0.57 MeV (FRLDM)
    - May introduce uncontrolled bias because too much data hides model limitations
Optimization Strategies

- Given the form of the functional, how do we fit model parameters?
- Experimental data
  - Find data such that each term in the functional is constrained
  - Choose data as model-independent as possible. Ex.: atomic masses
  - Avoid evaluated data, stay away from large error bars
- A philosophical choice: A little or a lot of data?
  - Mass models (Bruxelles-Montréal)
    - Take all available data on masses and fit the parameters
    - r.m.s. values: 0.50 MeV (Skyrme), 0.80 MeV (Gogny), 0.57 MeV (FRLDM)
    - May introduce uncontrolled bias because too much data hides model limitations
  - Not mass models (UNEDF project)
    - Choose limited amount of (usually heterogeneous) data
    - Predictive power constrained by model limitations
    - Choice of data also introduces bias
Optimization Strategies

- Given the form of the functional, how do we fit model parameters?

- Experimental data
  - Find data such that each term in the functional is constrained
  - Choose data as model-independent as possible. Ex.: atomic masses
  - Avoid evaluated data, stay away from large error bars

- A philosophical choice: A little or a lot of data?
  - Mass models (Bruxelles-Montréal)
    - Take all available data on masses and fit the parameters
    - r.m.s. values: 0.50 MeV (Skyrme), 0.80 MeV (Gogny), 0.57 MeV (FRLDM)
    - May introduce uncontrolled bias because too much data hides model limitations
  - Not mass models (UNEDF project)
    - Choose limited amount of (usually heterogeneous) data
    - Predictive power constrained by model limitations
    - Choice of data also introduces bias

The UNEDF Protocol

- Fit at deformed HFB level
- Composite $\chi^2$
  
  $$\chi^2 = \frac{1}{n_d - n_x} \sum_{t=1}^{T} \sum_{i=1}^{n_T} \left( \frac{y_{it}(x) - d_{it}}{\sigma_t} \right)^2$$

- Supplement “best-fit” with full covariance and sensitivity analysis
  - Provide sensitivity on data points
  - Covariance matrix allows uncertainty propagation

<table>
<thead>
<tr>
<th></th>
<th>UNEDF0</th>
<th>UNEDF1</th>
<th>UNEDF2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of parameters $n_x$</td>
<td>12</td>
<td>12</td>
<td>14</td>
</tr>
<tr>
<td>Type of data $t$</td>
<td>Masses, r.m.s. radii, OES ($T=3$)</td>
<td>Masses, r.m.s. radii, OES, E* fission isomer ($T=4$)</td>
<td>Masses, r.m.s. radii, OES, E* fission isomer, s.p. splittings ($T=5$)</td>
</tr>
<tr>
<td>Number of data points $n_d$ (total)</td>
<td>108</td>
<td>115</td>
<td>130</td>
</tr>
</tbody>
</table>

PRC 82, 024313 (2010), PRC 85, 024304 (2012), PRC 87, 054314 (2014)
The UNEDF Family

- UNEDF functionals are all-round functionals
- Quality degrades when more constraints added
- Skyrme form too limited
Covariance Analysis

- PRC 87, 034324 (2013)
- PRC 88, 031305 (2013)
The UNEDF Family

- **UNEDF functionals** are all-round functionals
- Quality degrades when more constraints added
- Skyrme form too limited

**Masses**

![Masses graph](image)

**Separation energies**

![Separation energies graph](image)

**Neutron droplets**

![Neutron droplets graph](image)

**Single-particle states**

![Single-particle states graph](image)

**Fission barriers**

![Fission barriers graph](image)
Quantifying the Unknown: Bayesian Inference
Quantifying the Unknown: Bayesian Inference

- DFT model parameters are treated as genuine random variables
Quantifying the Unknown: Bayesian Inference

- DFT model parameters are treated as genuine random variables.
- Reflect the fact that DFT is a model of a more complex reality.
Quantifying the Unknown: Bayesian Inference

- DFT model parameters are treated as genuine random variables
- Reflect the fact that DFT is a model of a more complex reality
- Bayesian inference techniques give access to probability distribution of parameters
Quantifying the Unknown: Bayesian Inference

- DFT model parameters are treated as genuine random variables
- Reflect the fact that DFT is a model of a more complex reality
- Bayesian inference techniques give access to probability distribution of parameters
- The posterior distribution depend the metric defined by some $\chi^2$

$$L(\text{model}) \approx e^{-\chi^2}$$
Quantifying the Unknown: Bayesian Inference

- DFT model parameters are treated as genuine random variables
- Reflect the fact that DFT is a model of a more complex reality
- Bayesian inference techniques give access to probability distribution of parameters
- The posterior distribution depend the metric defined by some $\chi^2$
  \[ L(\text{model}) \approx e^{-\chi^2} \]
- Posterior distribution generated by Markov-Chain Monte-Carlo simulations

Quantifying the Unknown: Bayesian Inference

- DFT model parameters are treated as genuine random variables
- Reflect the fact that DFT is a model of a more complex reality
- Bayesian inference techniques give access to probability distribution of parameters
- The posterior distribution depend the metric defined by some $\chi^2$

$$L(\text{model}) \approx e^{-\chi^2}$$

- Posterior distribution generated by Markov-Chain Monte-Carlo simulations
- Draw random samples of the posterior to propagate errors


UQ work: ~5 M CPU hours
Propagating Uncertainties
Propagating Uncertainties

Masses of neutron-rich nuclei
Propagating Uncertainties

- For driplines, statistical errors are comparable to systematic errors

Masses of neutron-rich nuclei

Two-neutron driplines

Closed-shell nuclei

Proton Number, Z vs Neutron Number, N
Propagating Uncertainties

- For driplines, statistical errors are comparable to systematic errors.
- Large statistical errors in fission barriers translate into orders of magnitude uncertainties for half-lives.

Masses of neutron-rich nuclei

Two-neutron driplines

Closed-shell nuclei

Fission barrier in $^{240}$Pu
Conclusions
Conclusions

- Density functional theory has entered the era of systematic, large-scale, quantitative predictions of nuclear properties thanks to the advent of leadership class computers
  - Global surveys at the scale of the mass table
  - Realistic simulations of complex phenomena such as fission
Conclusions

- Density functional theory has entered the era of systematic, large-scale, quantitative predictions of nuclear properties thanks to the advent of leadership class computers
  - Global surveys at the scale of the mass table
  - Realistic simulations of complex phenomena such as fission

- Quantifying and propagating uncertainties is crucial for applications in fundamental symmetries, nuclear astrophysics, and nuclear data needs
  - Rigorous mathematical tools to estimate statistical uncertainties exist and are being deployed on a large scale
  - Systematic errors remain significant and must be investigated in more details
Conclusions

- Density functional theory has entered the era of systematic, large-scale, quantitative predictions of nuclear properties thanks to the advent of leadership class computers
  - Global surveys at the scale of the mass table
  - Realistic simulations of complex phenomena such as fission
- Quantifying and propagating uncertainties is crucial for applications in fundamental symmetries, nuclear astrophysics, and nuclear data needs
  - Rigorous mathematical tools to estimate statistical uncertainties exist and are being deployed on a large scale
  - Systematic errors remain significant and must be investigated in more details
- Challenges
  - Improve the connection between the EDF and theory of nuclear forces
  - Propagate uncertainties in complex problems such as decays, spectroscopy