1. What is Density Functional Theory?
2. Motivation
3. Deliverables for Nuclear Physics
4. Scientific Organizational Structure
5. Challenges
6. Near-term goals
7. Milestones

UNEDF Panel Review-Bertsch introduction
Density Functional Theory--What is it?

**Conceptual**
--Ask me later

**Practical**
--Kohn&Sham, 1965

Define a set of N orbitals  \( \phi_i(r); \ i = 1, \ldots, N \)

Minimize with respect to the orbital functions

\[
\int \left( \sum_i \frac{\left| \nabla \phi_i \right|^2}{2m} + V(\{\phi\}) \right) d^3r
\]

\[
n(r) = \sum_i |\phi_i(r)|^2
\]

**Kohn-Sham equations**

\[-\frac{\hbar^2 \nabla^2}{2m} \phi_i + \frac{\delta V}{\delta n} \phi_i = \epsilon_i \phi_i\]

\[
V = V_{ext}(r)n(r) + \frac{e^2}{2} \int d^3r' \frac{n(r)n(r')}{|r - r'|} + \mathcal{E}_{xc}[n]
\]
## The DFT Success Story

### Average error for simple molecules

<table>
<thead>
<tr>
<th>Method</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hartree-Fock</td>
<td>1929</td>
</tr>
<tr>
<td>LDA</td>
<td>1965</td>
</tr>
<tr>
<td>GGA</td>
<td>1989</td>
</tr>
<tr>
<td>tau</td>
<td>1999</td>
</tr>
</tbody>
</table>

Image of vitamin C from Nobel Foundation website
What do we want to know?

Binding Energies

Nucleosynthesis

Interactions with neutrons

Inelastic cross sections: For some intermediate mass nuclei (e.g., $^{23}{\text{Na}}$ or $^{56}{\text{Fe}}$) inelastic scattering cross-section accuracies of the order of 10% are needed. Moreover, there exists a general need to improve the knowledge of inelastic scattering for actinides. Relevant experiments have proven particularly difficult. It would be worthwhile for the basic science community to investigate whether current challenges could be met with new and innovative measurement techniques.

From the report “Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles”, 2006

Radioactive decay properties

Fission properties
Challenges we face

The functional itself

The DFT solver

Extensions for dynamics

Reactions with DFT input

Utilizing leadership class machines
Building blocks: Nuclear Local Densities and Currents

\[
\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau) \\
\rho_1(\vec{r}) = \rho_1(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau) \tau
\]

isoscalar (T=0) density \( (\rho_0 = \rho_n + \rho_p) \)

isovector (T=1) density \( (\rho_1 = \rho_n - \rho_p) \)

\[
\bar{s}_0(\vec{r}) = \sum_{\sigma'\sigma} \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau) \sigma_{\sigma'\sigma} \\
\bar{s}_1(\vec{r}) = \sum_{\sigma'\sigma} \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau) \sigma_{\sigma'\sigma} \tau
\]

isoscalar spin density

isovector spin density

\[
\vec{j}_T(\vec{r}) = \frac{i}{2} \left( \vec{\nabla}' - \vec{\nabla} \right) \rho_T(\vec{r},\vec{r}') \bigg|_{\vec{r}' = \vec{r}}
\]

current density

\[
\vec{J}_T(\vec{r}) = \frac{i}{2} \left( \vec{\nabla}' - \vec{\nabla} \right) \otimes \bar{s}_T(\vec{r},\vec{r}') \bigg|_{\vec{r}' = \vec{r}}
\]

spin-current tensor density

\[
\tau_T(\vec{r}) = \vec{\nabla} \cdot \vec{\nabla}' \rho_T(\vec{r},\vec{r}') \bigg|_{\vec{r}' = \vec{r}}
\]

kinetic density

\[
\vec{T}_T(\vec{r}) = \vec{\nabla} \cdot \vec{\nabla}' \bar{s}_T(\vec{r},\vec{r}') \bigg|_{\vec{r}' = \vec{r}}
\]

kinetic spin density

+ analogous p-p densities and currents
Need to go beyond DFT for dynamics, excited states

Two strategies:

\[ \phi_i \rightarrow \phi_i(t), \phi_i(q), \ldots \]

\[ \phi_i \rightarrow a_i^\dagger \]
Near-term goals

Verification

Methodologies for ab initio wave functions

Global Benchmarking

2+ Excited states

Odd-A mass table

Pairing energies
Physics Milestones

2.2. Computational
a) Schroedinger solver with fission-quality accuracy. (June 2008)
   Note: the outcome of the comparison here may affect the choice of algorithms for the final DFT solver.
b) Medium-mass coupled-cluster calculations within a new spherical coding scheme (Dec. 2008)
c) DFT solver with fission-quality accuracy (June 2009)
d) NCSM solver and analyser program suite (June 2009)
e) Parallelized coupled-channel code including 2p2h excitations (Mar. 2009)
f) Partially fitted, energy density functional with documented global performance (Dec. 2010)

2.3. DFT
a) First comparisons of ab initio coupled-cluster and large-configuration calculations with the density matrix expansion using the same low-momentum NN + fit NNN Hamiltonian (June 2008)
b) Delivery of a complete DFT based on above Hamiltonian compatible with Skyrme DFT solvers. (Dec. 2008)
c) Completed evaluation of adequacy of the density matrix expansion (DME) for ab initio functionals. (June 2009)
d) Delivery of an energy density functional using a fine-tuned Hamiltonian (Dec. 2009)

2.4. Reactions
a) Folding treatment of full target-projectile interaction. (June 2009)
b) Dispersive optical potentials for many DFT structure models (Dec. 2009)
c) Nonlocal exchange and pickup corrections to optical potentials (Dec. 2009)

2.5. Final Deliverables (mid 2011)
a) The performance documented functional;
b) The codes to apply the functional to the nuclear energy surface including post-fission shapes;
c) The codes to apply the extension of DFT to nuclear excitations;
d) Systematic predicted optical potentials including nonlocatities;
e) DFT-based level densities for neutron reactions.

Ultimate goal:
Order-of-magnitude improvement of global systematics with respect to near-term benchmarks.
How many parameters are really needed?

Global (masses)

Bertsch, Sabbey, and Uusnakki

New optimization strategy and protocol needed
Global calculations of the lowest $2^+$ states

Deformed QRPA code including general Skyrme functional in progress (Terasaki, Engel)