Aspects of nuclear theory for AFC

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Nuclear Data and Standards

The systematic collection and availability of nuclear data and associated standards is a pre-requisite for reactor applications.

→Worldwide network of nuclear data centers:

- **→ Collect nuclear data (experiment and theory)**
- **→ Evaluate the quality**
- **→ Make the data available in the appropriate form for the user**

Present Status:

Evaluated Nuclear Data Files represent a consistent set of cross sections and associated quantities for all relevant reaction processes.

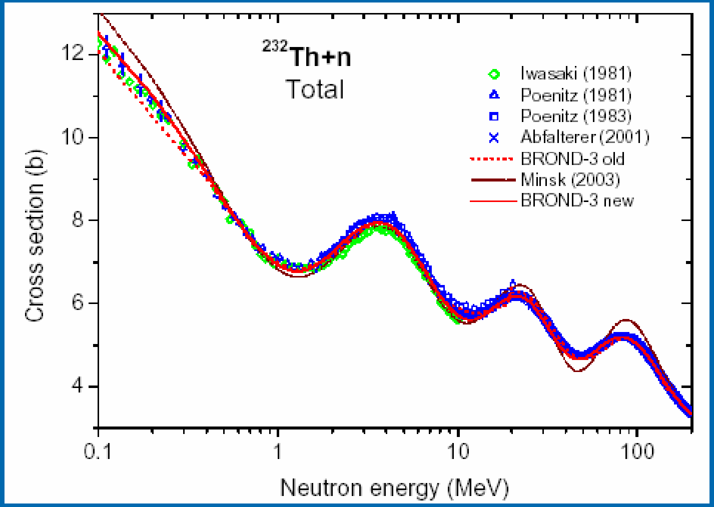
EXFOR, ENSDF
ENDF, Mass Data Library

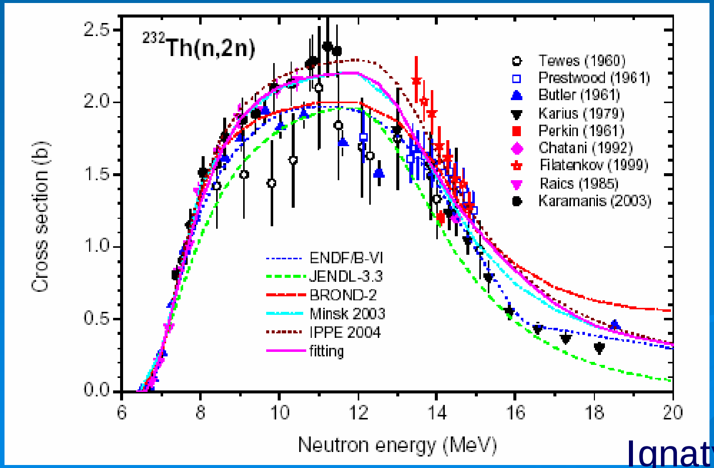
Maintained by Centers: IAEA, NNDC,…

Future facilities (and user) requirement:
Data files should contain the values of the cross sections and appropriate information about the uncertainty and reliability of the nuclear data.
Directly impacts safty and economic issues.

Nuclear Data: Quality

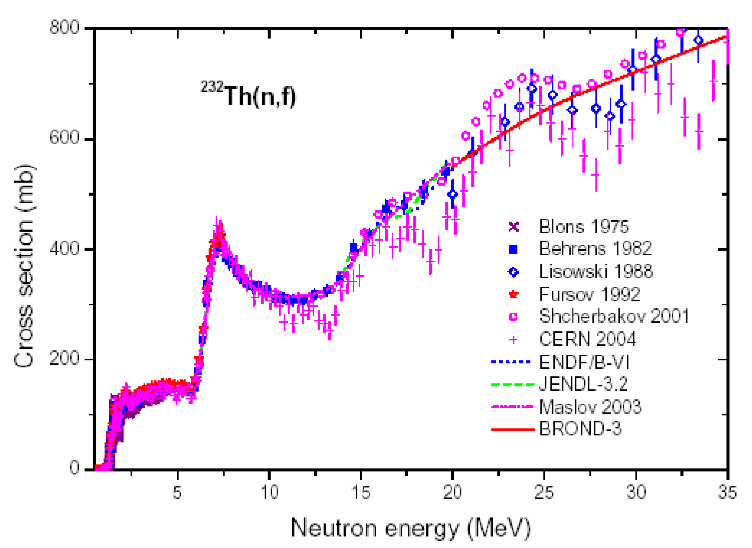
Nuclear data required for standard applications are of satisfactory quality – i.e. for thermal reactors and dosimetry

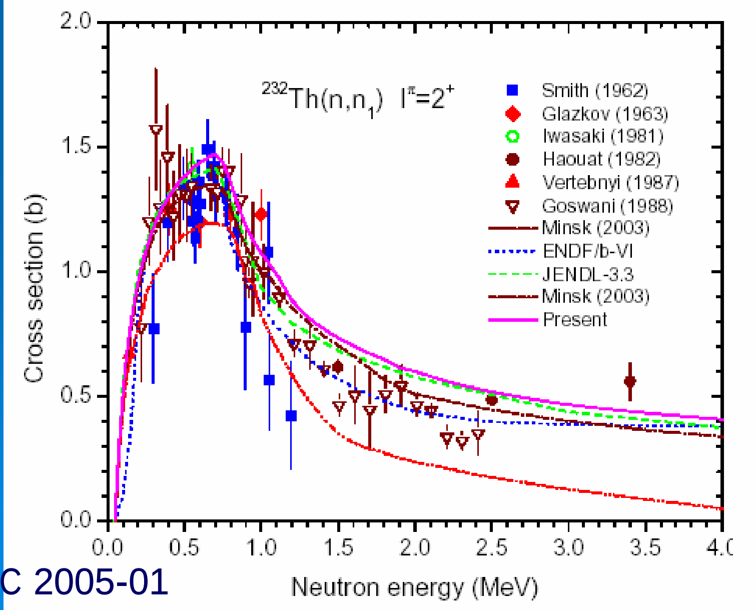




Nuclear Data Limitations

Standard evaluation techniques have a limited predictive power





Ignatyuk et al., ATI-NDC 2005-01

Emerging nuclear technologies and the data need

New nuclear technologies are emerging:
- Generation IV reactors with high burnup
- Transmutation of radioactive waste
- Use of Thorium-Uranium cycle
- Aspects of Materials research

→ Need to quantify shielding, activation, burn, and dosimetry at higher energy and intensities.

'Incomplete' experiments → nuclear theory with higher predictive power
→ reliable estimates of the quality of the nuclear theory
→ realistic margins for the observables

Reason for improved theory:

Number of open channels significantly increased –experiments cannot cover the whole variety. Because of budget limitations, feed back (Validation) experiments are limited and an optimization must be achieved already at the level of the prototype.

Theoretical inputs to the reaction problem….

from TALYS – Calculational Scheme

Loop possible over
- **incident energies**
- **Natural isotopes**

Input:
projectile p
element Fe
size 16
energy 22

Optical Model:
- **Phenomenology local/global**

Direct Reaction:
- **Spherical Optical model**
- **DWBA**
- **Rotational CC**
- **Giant Resonances**
- **Vibrational CC**

Pre-equilibrium:
- **Exciton model 1+2 component**
- **p-h LD phenom.**
- **Kalbach systematics**
  - **angular distributions**
  - **cluster emission**
  - **surface effects**
- **γ-ray emission**

Nucl. Structure
- **Abundances**
- **Discrete levels**
- **Deformations**
- **Masses**
- **Level density par.**
- **Resonance par.**
- **Fission barrier par.**
- **Microscopic LD**
- **Pre-scission shapes**

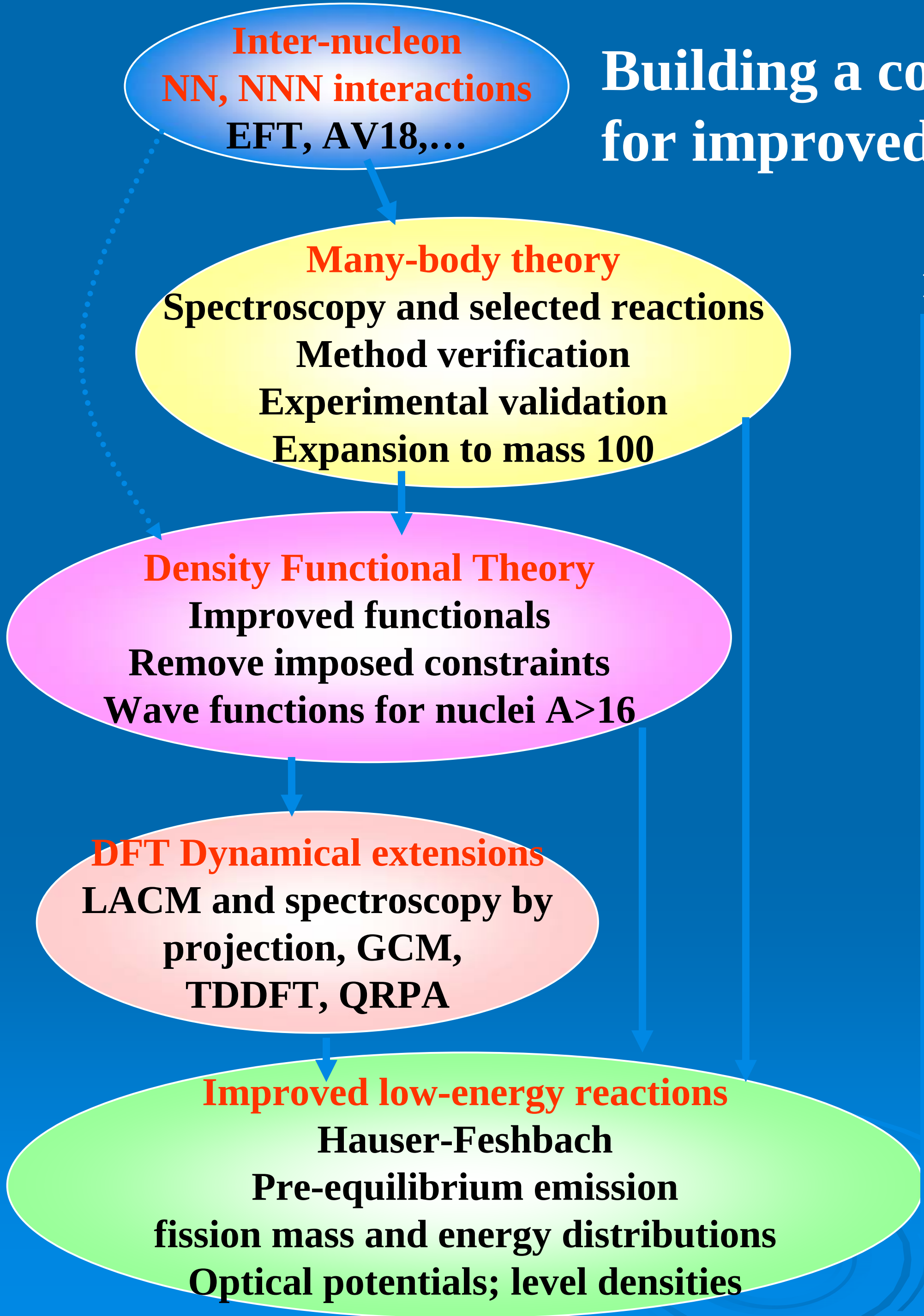
Compound:
- **Width fluctuations**
  - **Moldauer**
  - **GOE**
  - **HRTW**
- **Hauser-Feshbach**
- **Fission competition**
- **γ-ray emission**
- **GC+ Ignatyuk**

Multiple emission:
- **Exciton (any order)**
- **Hauser-Feshbach**
- **Fission competition**
- **All flux depleted γ-ray cascade**
- **Exclusive channels**
- **Recoils**

Output:
- **File containing useful output.**

ENDF:
- **transport libs.**
- **activation libs.**

Building a coherent theoretical path forward for improved nuclear reactions models.

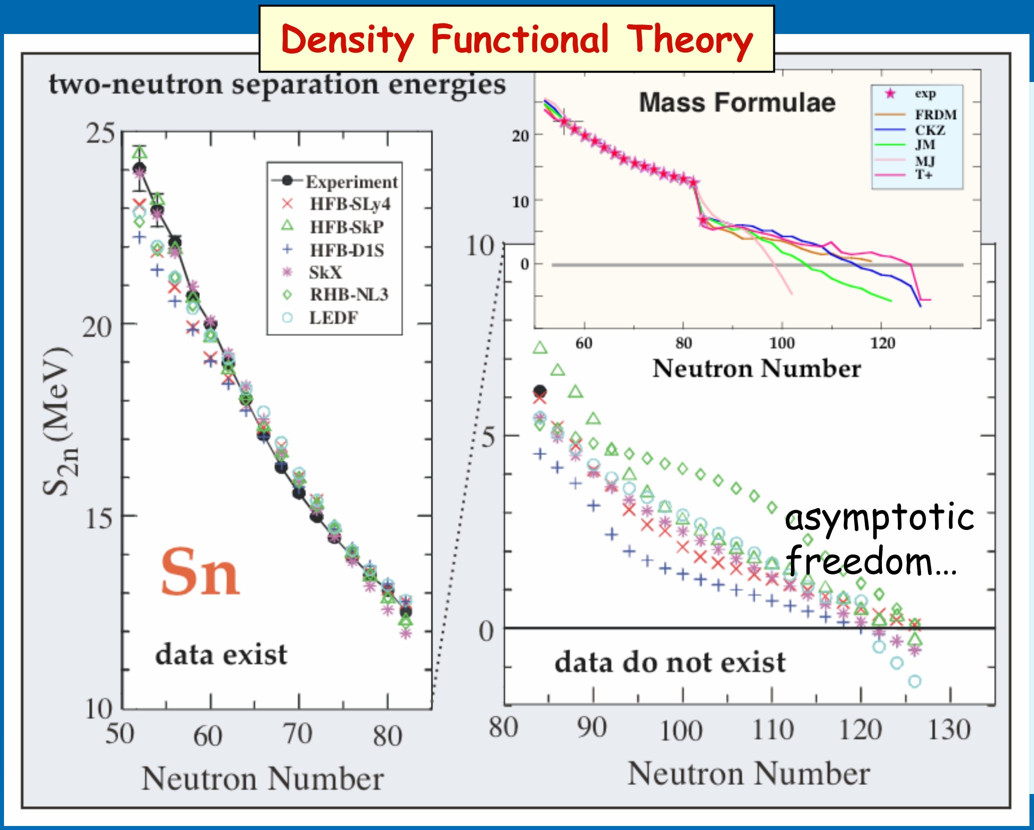


RIA Theory Blue Book (2005)

Theoretical challenges:

- Development of ab initio approaches to medium-mass nuclei
- Development of self-consistent nuclear density-functional theory methods for static and dynamic problems.
- Development of reaction theory that incorporates relevant degrees of freedom for weakly bound nuclei.
- Exploration of isospin degrees of freedom of the density-dependence of the effective interaction in nuclei.
- Development and synthesis of nuclear theory, and its consequent predictions, into various astrophysical models to determine the nucleosynthesis in stars.
- Development of robust theory and error analysis for nuclear reactions relevant to NNSA and GNEP

The mean field picture of the nucleus



This is Nuclear DFT (not HF from the initial NN interaction) – "HFB".

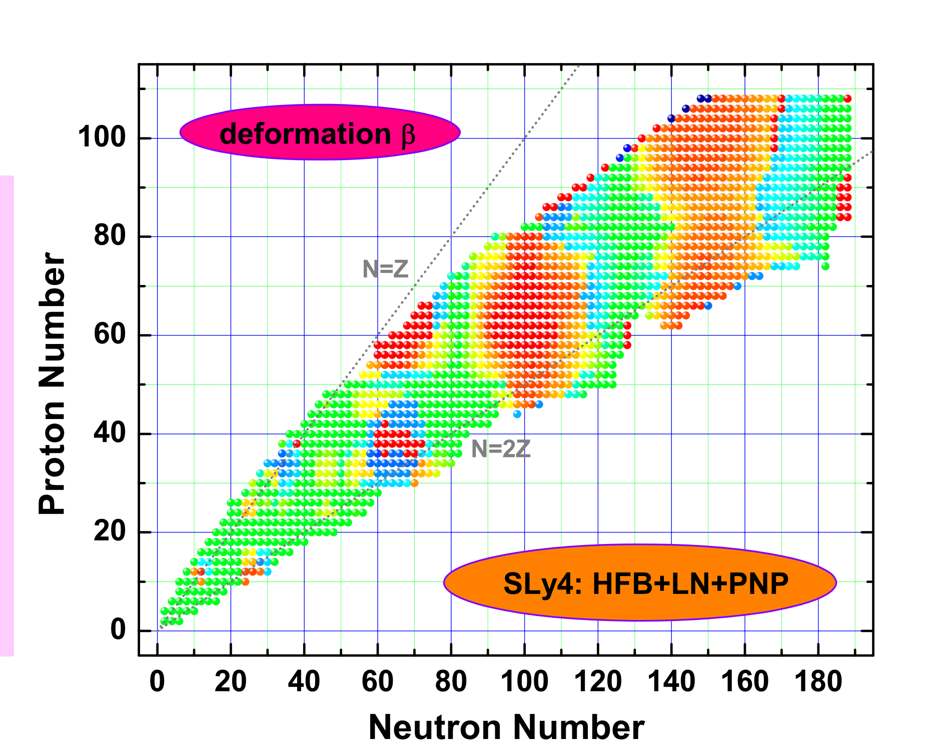
Nuclear DFT functionals (Skyrme) predict different behaviors near the drip lines. Which one is correct?

Can we include further density operators in energy density functional?

Can we use the unitary limit to constrain the form of the potential?

Challenge: Find the appropriate energy density functional that describes nuclei (Find connection to the ab initio potentials)

Self-consistent mean field theory: Nuclear DFT



Recent developments:
- General nuclear energy density functional that allows proton-neutron couplings
- First fully self-consistent QRPA+HFB
- Development of formalism for exact particle number projection before variation (but problematic)
- Mass tables calculated

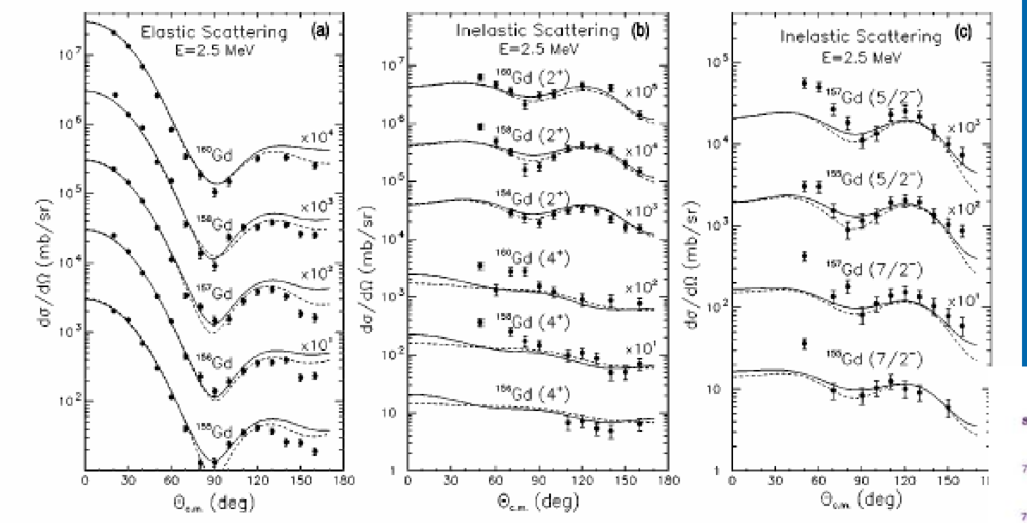
Nuclear DFT Challenges:
- Implement exact particle number projection (and others) before variation
- Improvement of the density dependence of the effective interaction
- Proper treatment of time-odd fields
- Inclusion of dynamical zero-point fluctuations
- Provide proper continuum basis for QRPA calculations

Stoitsov, Dobaczewski, Nazarewicz, Engel, Van Gai, Gorioly, Heenen, Duguet, Furnstahl, Bertsch ….
Basic focus of the UNEDF SciDAC effort

Example: Evaluation of EU - Semi-microscopic neutron-nucleus optical potentials

$$U(\vec{r},E)=\left(t/\sqrt{\pi}\right)^{-3}\int \rho(\vec{r}\,')\,U\left(\rho(\vec{r}\,'),a(\vec{r}\,'),E\right)\exp\left(-\left|\vec{r}-\vec{r}\,'\right|^{2}/t^{2}\right)d\vec{r}\,'$$

Deformed Lane-consistent optical potential with eff. NN-potential in NM-approach



E. Bauge et al., Phys. Rev. C 61, 034306 (2000)

Satisfactory description of elastic and inelastic scatt.

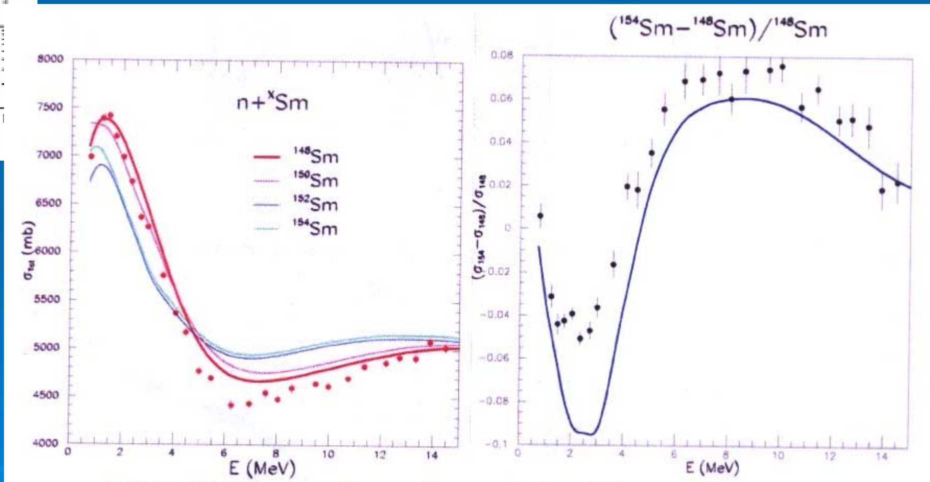
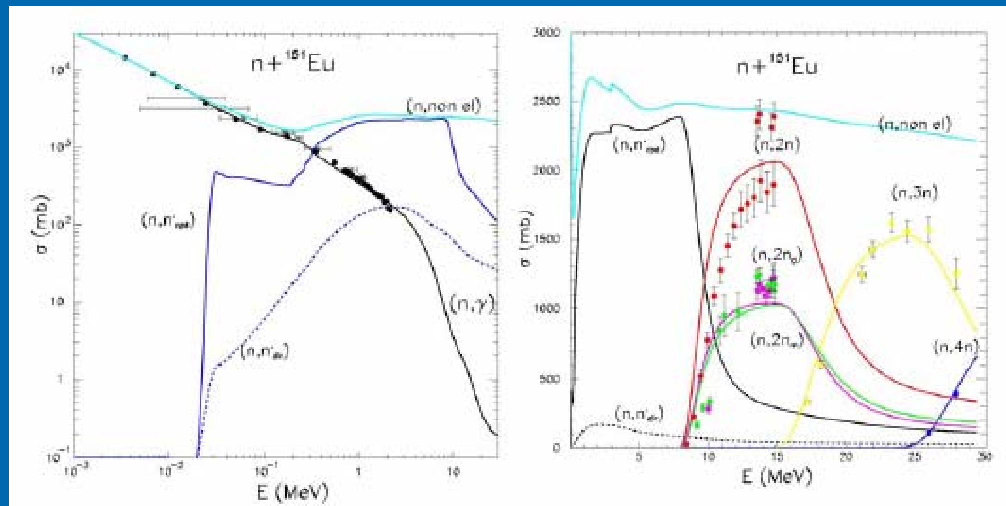
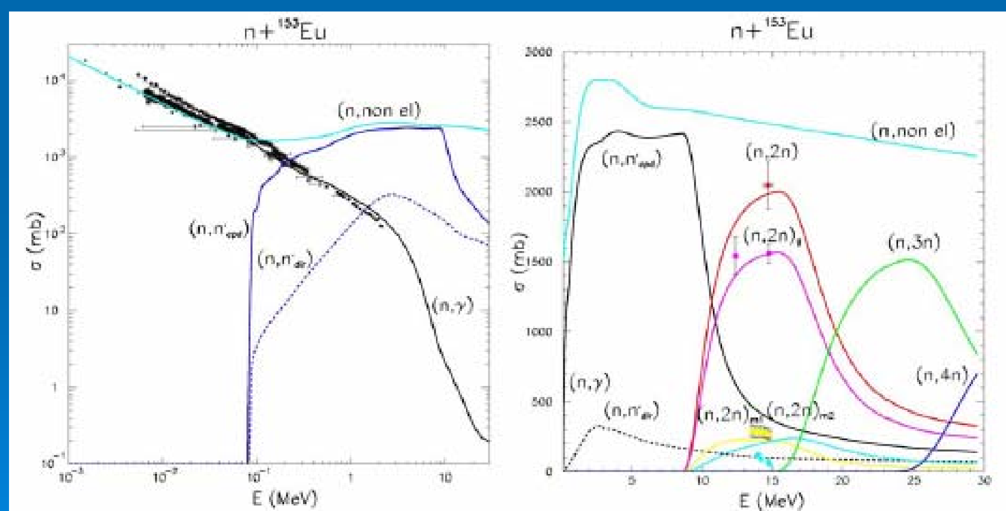


Fig. 4 : Total cross sections and cross sections differences for Sm isotopes.

The situation with odd mass nuclei is more difficult to predict.

Evalution of Eu – statistical model





Goal: Unified description of the various reaction processes
Need: good description of transmission coefficients.

Some words about codes and algorithms

Level densities → Quantum Monte Carlo → scales to 1000's of processors

DFT functional → non-linear 2nd order DIFFeq → scales to 1000's of processors

ab initio connections

→ QMC (GFMC) → scales to 1000's of processors

→ Diagonalization → scales to 1000's of processors

→ Coupled-cluster → scales to 1000+ processors

Lifetimes (DFT/QRPA)→ spherical only need to develop deformed.

Fission problem (Nazarewicz talk at breakout)

Unrestricted DFT→ need to build code (wavelet technology)

+correlations → need to implement consistently

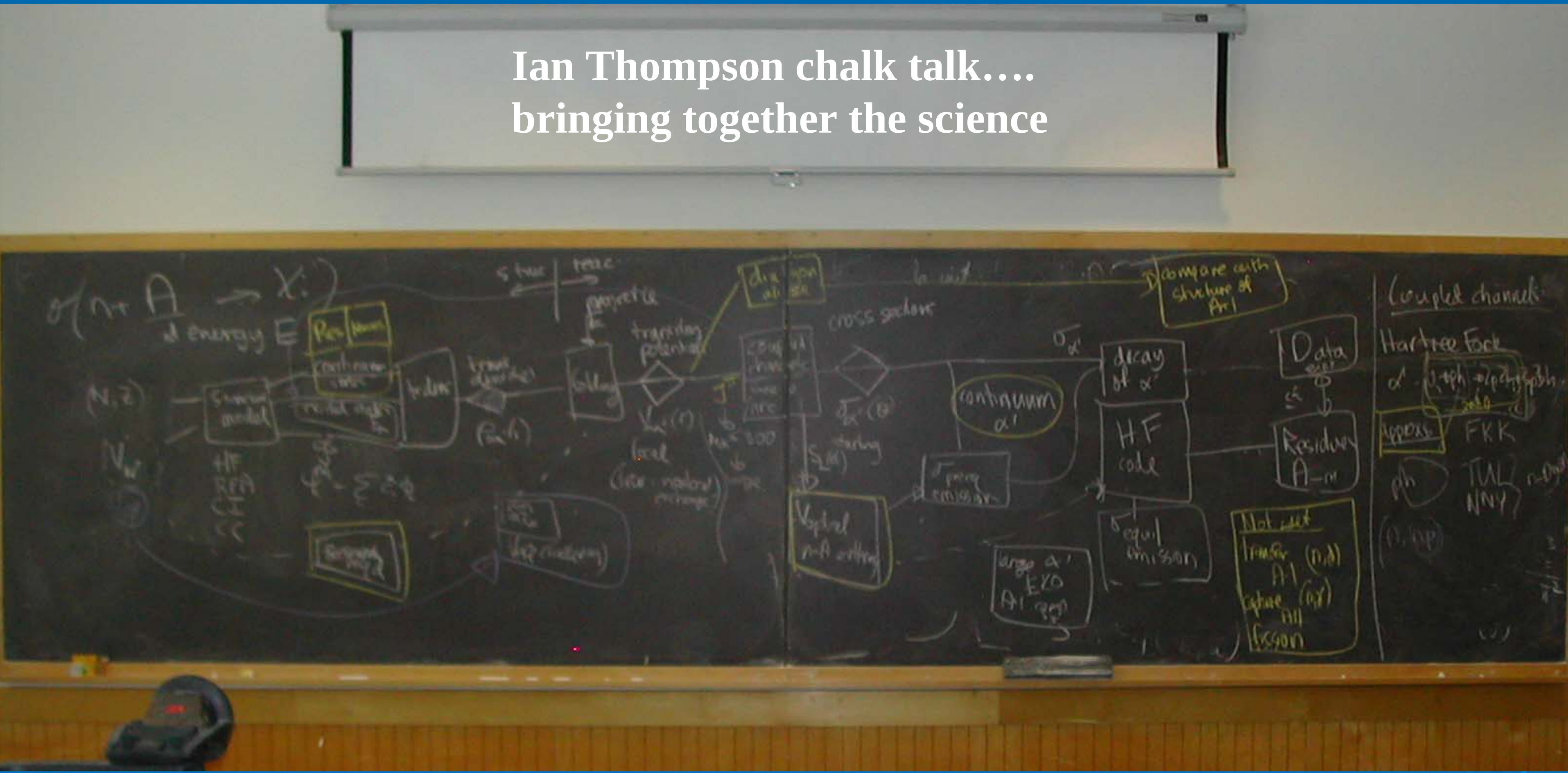
Improved optical potentials

→ Diagonalization and others (need to build up using existing technology)

Coupled-channels calculations → non-linear equations → 10-100 processors.

Some details discussed in the break out session.

COMPUNET: COMPUtational Nuclear EnvironmenT



The COMPUNET will bring together under one common component architecture the various codes and algorithms that can be used by others to calculate cross sections of interest. ---- SHOULD BE A KEY OUTCOME OF THE UNEDF SCIDAC EFFORT.

Some key areas of improvement

- Microscopic nucleon-nucleus optical potentials for the energy range up to 20-40 MeV (and higher)
- Microscopic formulation of composite particle optical potentials
- Nuclear structure (deformation) of odd-mass nuclei
- Quantitative description of (n,xn) cross sections and charged particle emission
- Level densities at high excitations
- Improved description of fission
- Improved description of resonant scattering

Problems to be solved

- Higher order method for microscopic nucleon-nucleus optical model closing the gap between NS- and NM-approach
- Microscopic ion-nucleus optical potential coupling of fission to OM calculations
- Quantitative preequilibrium calculations also at higher energies
- Microscopic level densities
- Theory of fission
- Estimate of global quantities of the resonance region
- Estimate of uncertainties of nuclear model calculations

Accuracy and Reliability

The extension of the energy range and isotope range implies

the uncertainties associated with nuclear model calculations should be estimated

The covariance matrix of the model is composed of the contributions

$$M^{(mod)} = M^{(par)} + M^{(num)} + M^{(def)}$$

parameter uncertainties

statistically well defined, taken into account, e.g. in the KALMAN code system

numerical implementation error

non-statistical error, usually well known, but usually small....

Deficiency of the model

Non-statistical error, strongly related to the predictive power of the model, problem of quantitative estimate

Conclusions

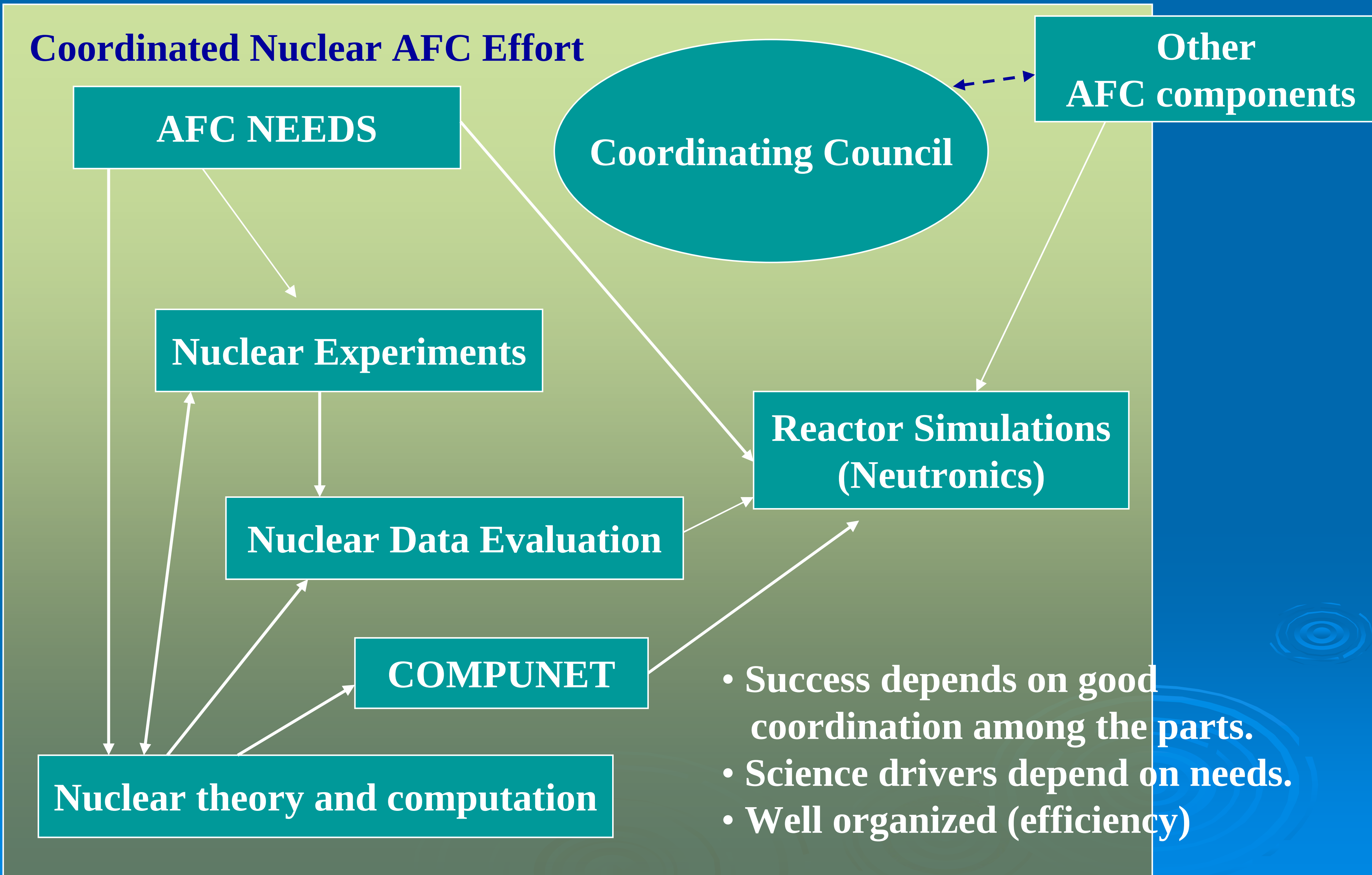
Key questions to nuclear theory in light of needs:

→ How to better describe a neutron induced cross section?
- **→ Development of theory**
- **→ Utilization of computational power**

→ How to better determine the life-times?
→ Theory of fission?
→ What are the theoretical error estimates?

Applications needs coincide with topics in nuclear structure and nuclear astrophysics (radioactive ion beam science)

Nuclear AFC coordination within the big picture



- Success depends on good coordination among the parts.
- Science drivers depend on needs.
- Well organized (efficiency)