

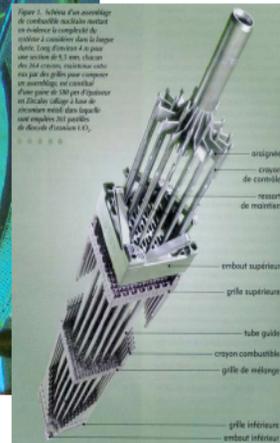
Group D Breakout DOE AFC Workshop

What's the big idea?

- Simulate the core of a reactor at higher accuracy. Explore new designs.
- 2-3% improvements (sometimes 10-20%) in key reactor parameters (Keff,...) result in tremendous improvements in economics and safety.
- One major avenue is the nuclear cross sections!!

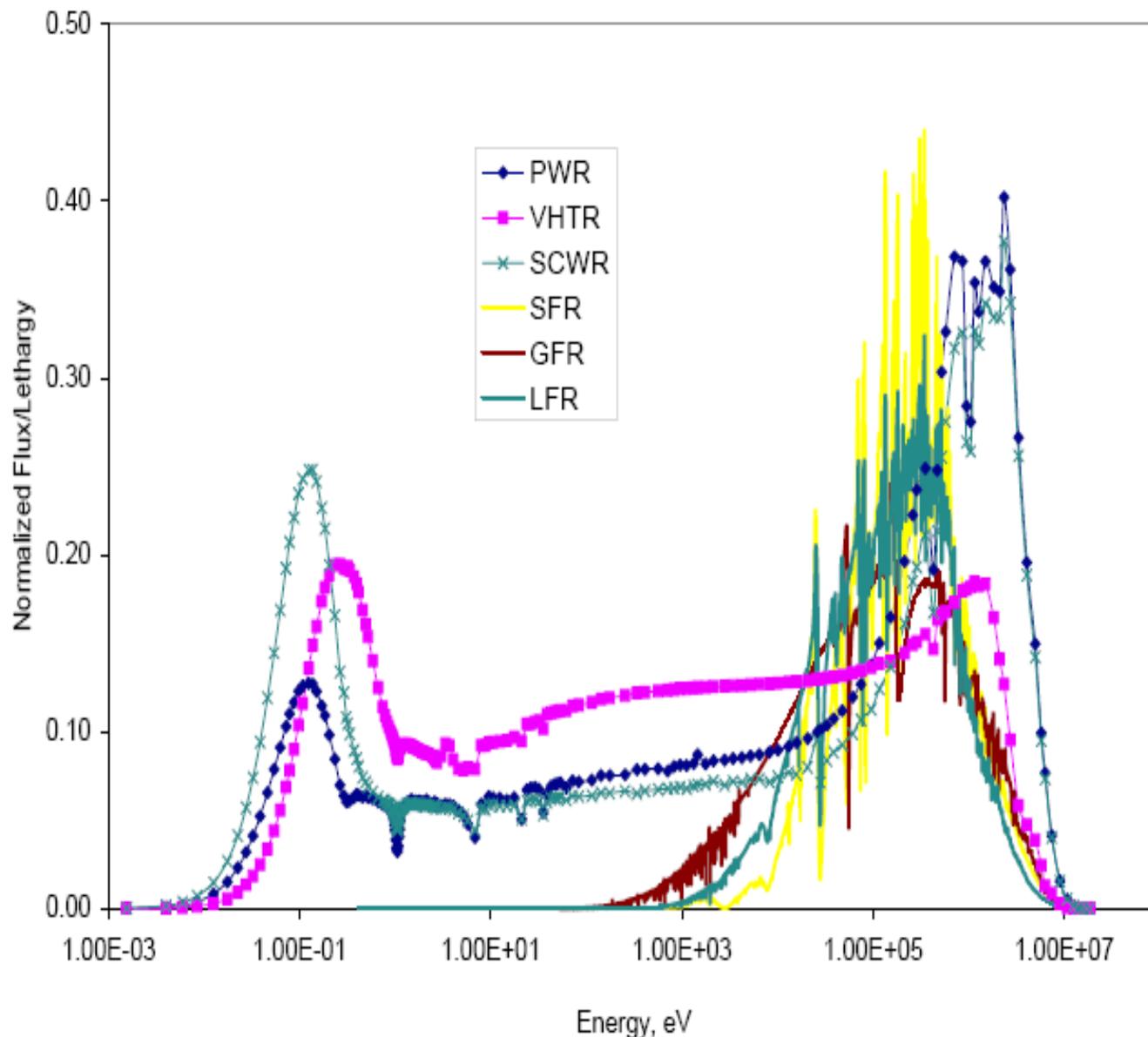


The big picture: example of a PWR core





Nature is challenging : Typical spectrum per reactor type



Data was discussed in another group.

Our question: can high-performance simulation and physics inputs yield improved input data?

YES: Simulations of the reactor core and integral experiments

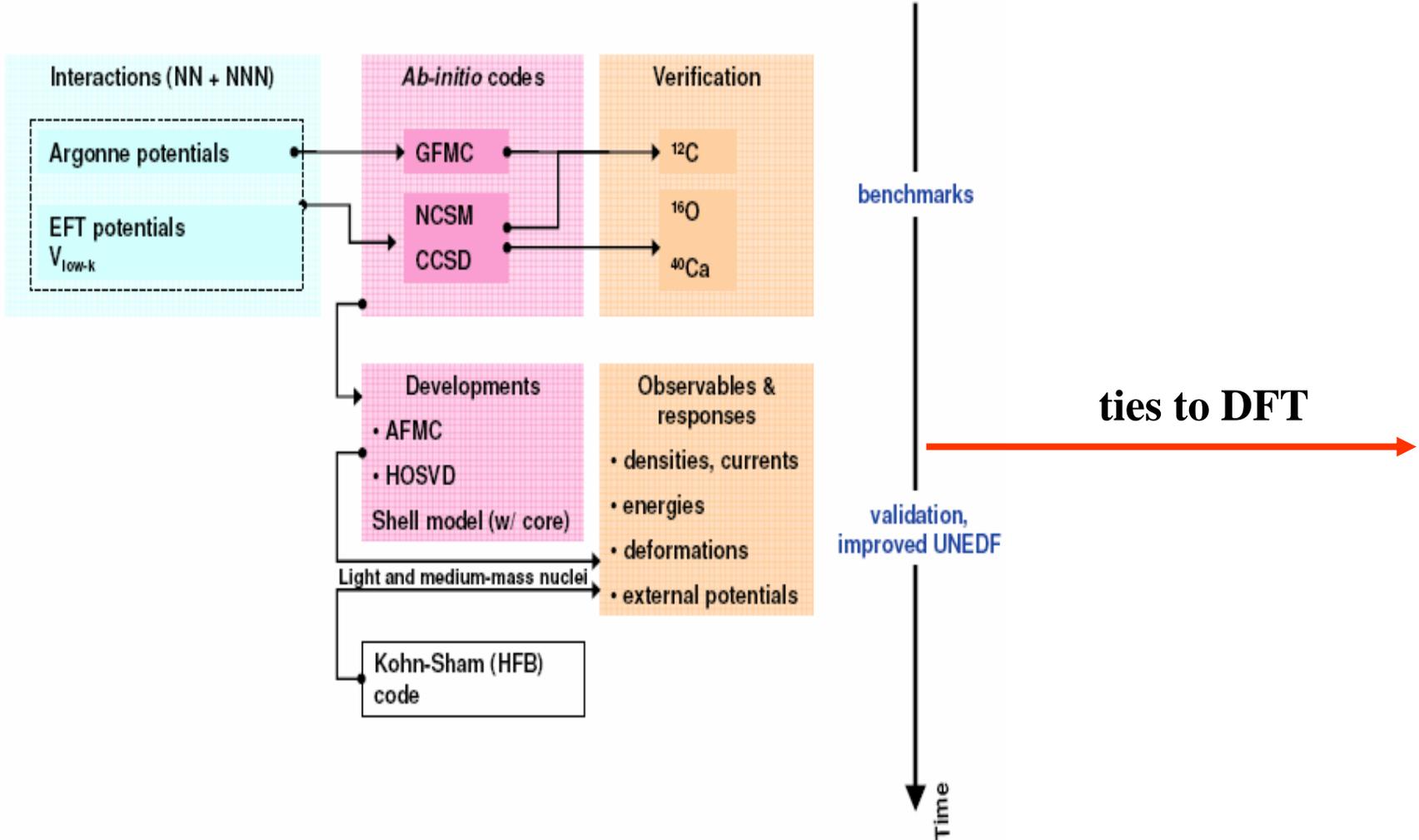
YES: Nuclear data analysis with theory and experiments

YES: Nuclear theory improvements to reaction processes

Time scales vary.

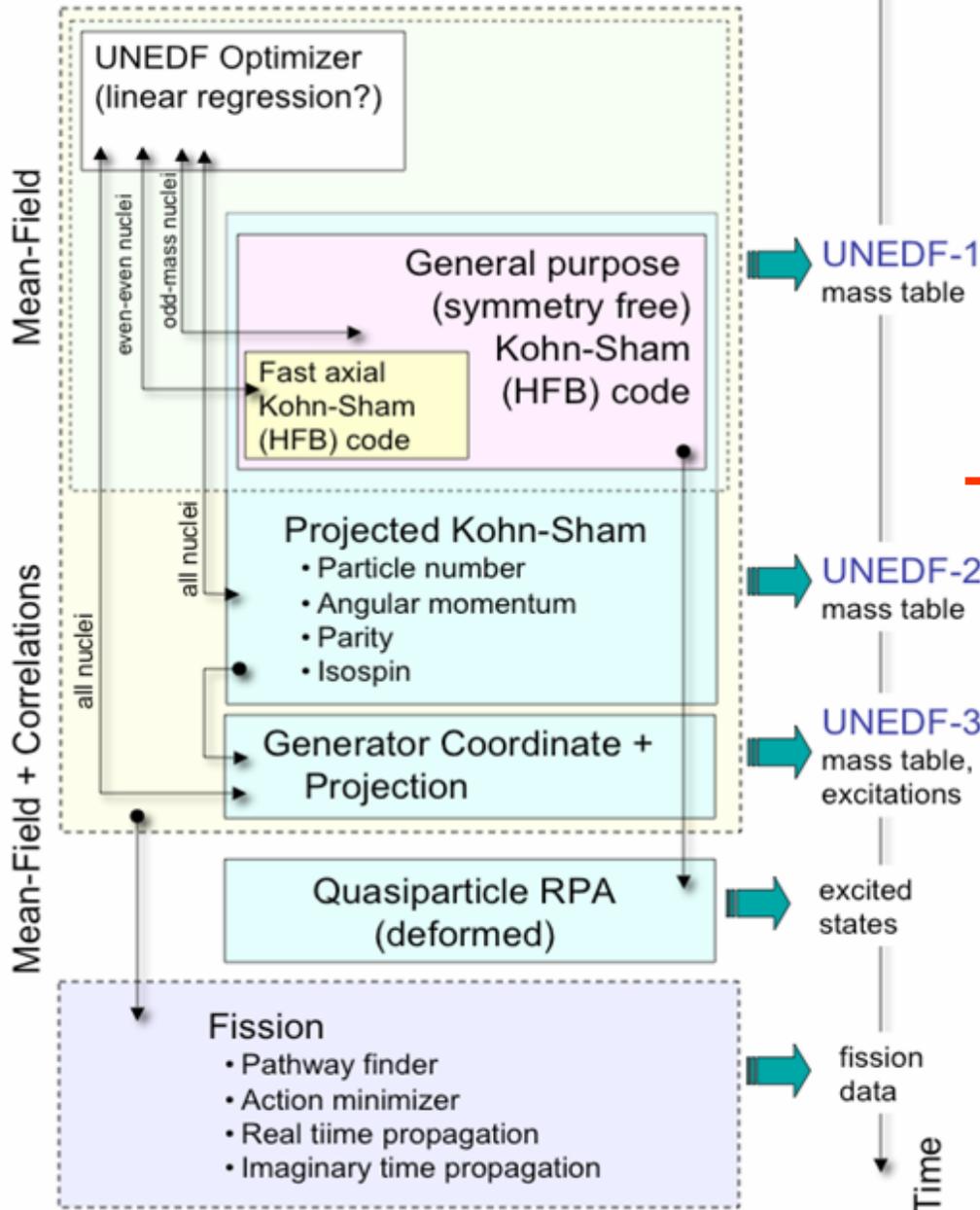
Activity coordination is important.

Interface DFT – *ab-initio* calculations



TIMESCALE → 1-3 years

NDFT COMPUTATIONAL STRATEGY

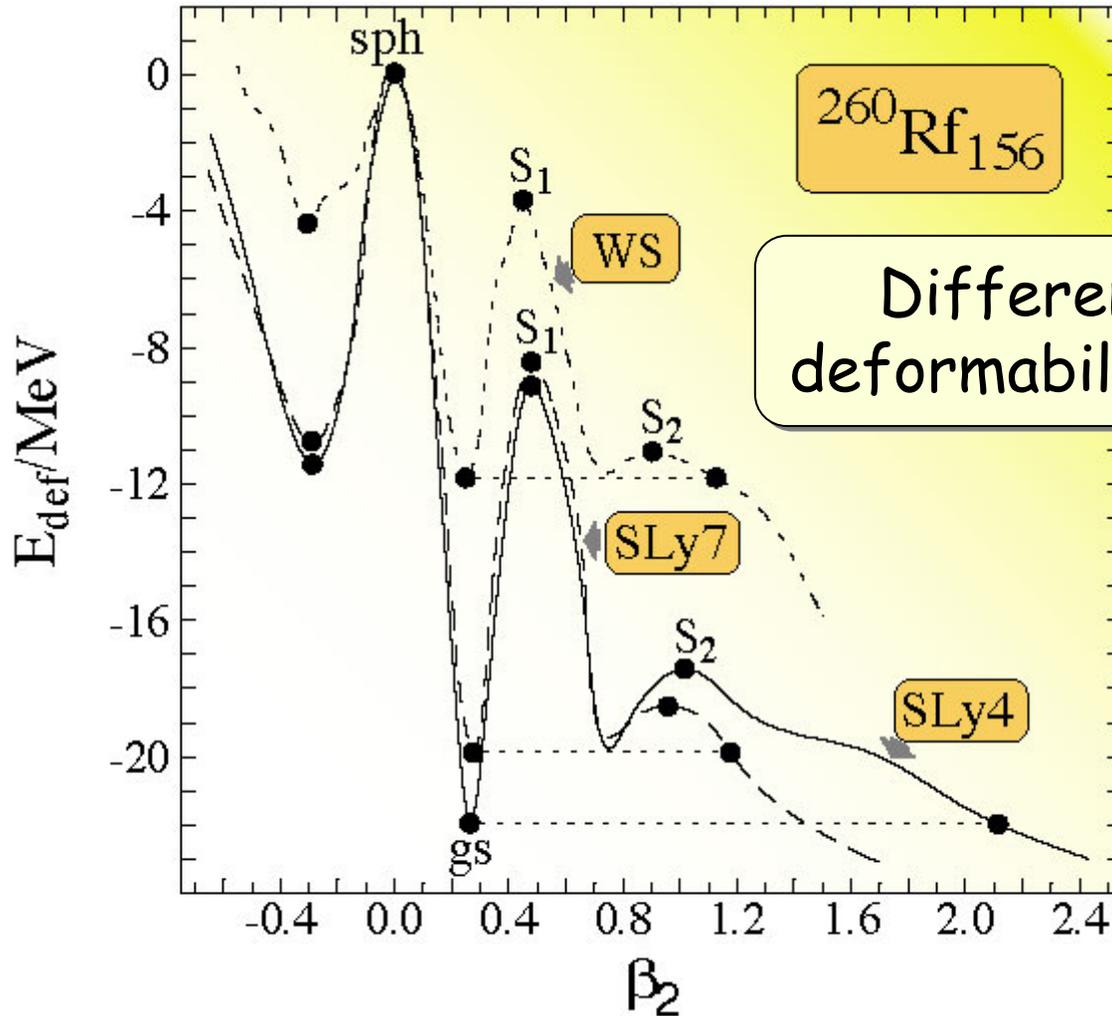


On to reactions

Timescale → 3-5 years

Timescale → 5-10 years

Collective potential $V(q)$



Universal nuclear energy density functional is yet to be developed

Different deformabilities!

Choice of collective parameters

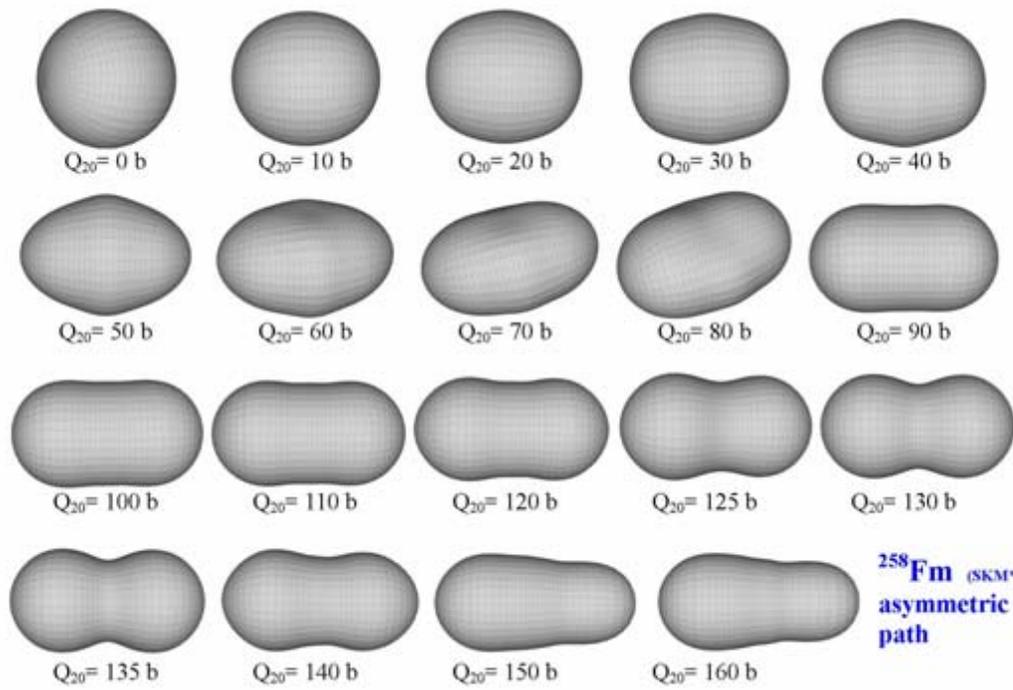
How to define a barrier?
How to connect valleys?

Dynamical corrections going beyond mean field important

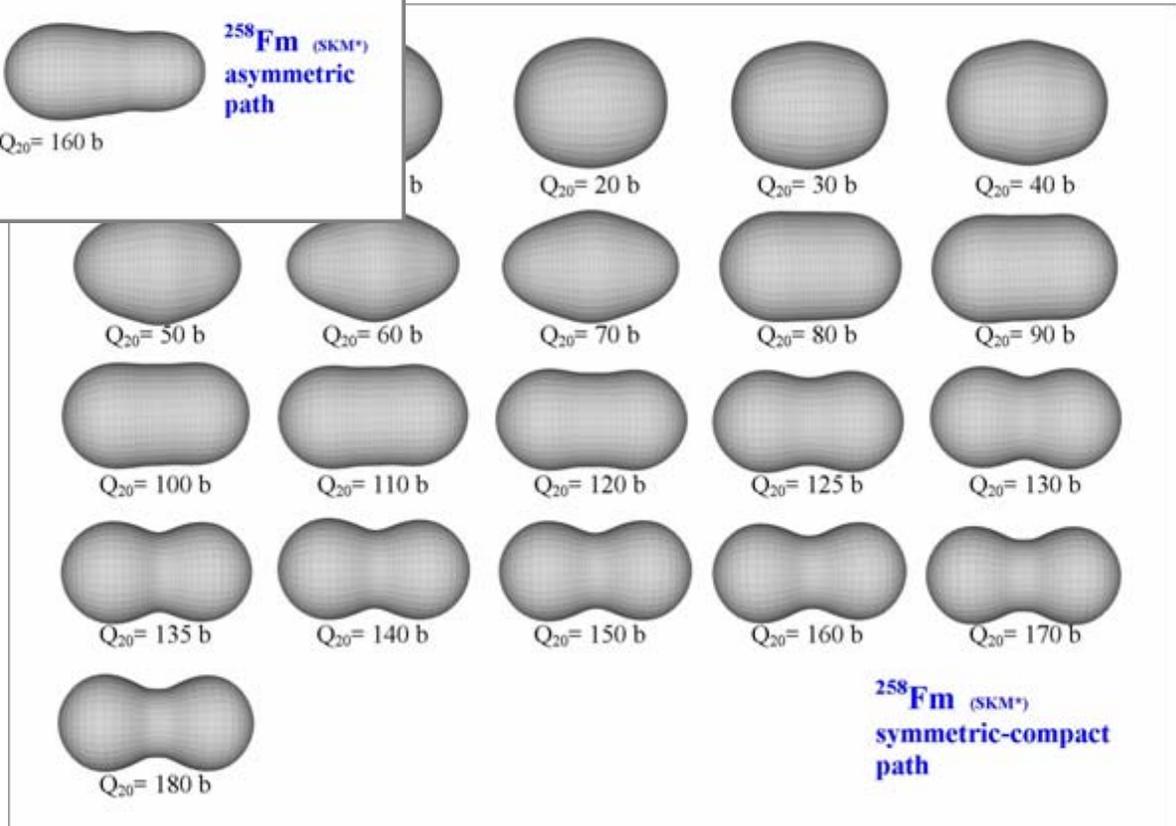
- Center of mass
- Rotational and vibrational (zero-point quantum correction)
- Particle number

$$V(q) \rightarrow V(q) - (E_{\text{ZPE},\beta} + E_{\text{ZPE},\text{rot}})$$

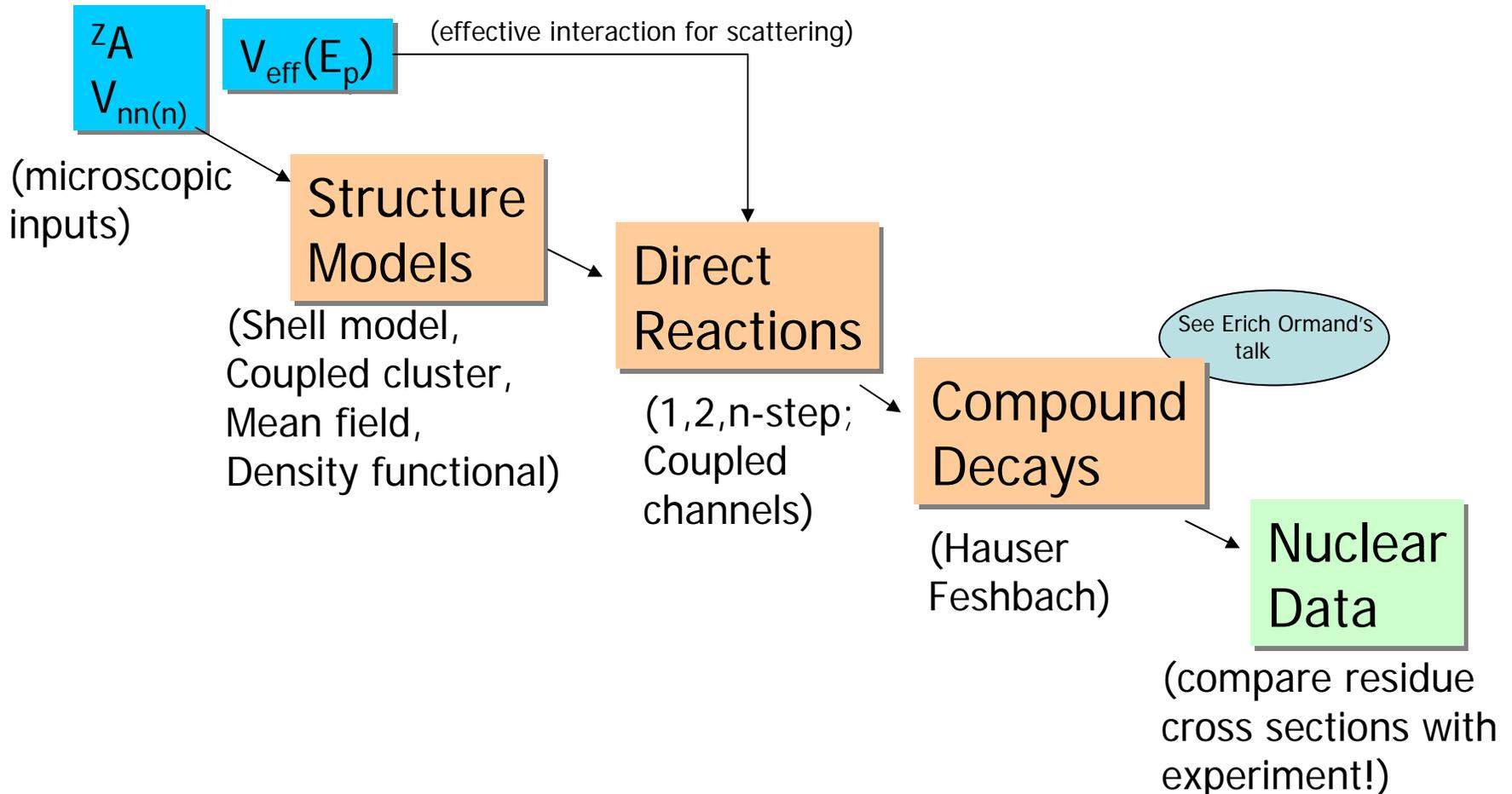
$$\log T_{\text{sf}} = -20.54 + \log [1 + \exp(2S(L_{\text{min}}))] - \log(2E_{\text{ZPE}})$$



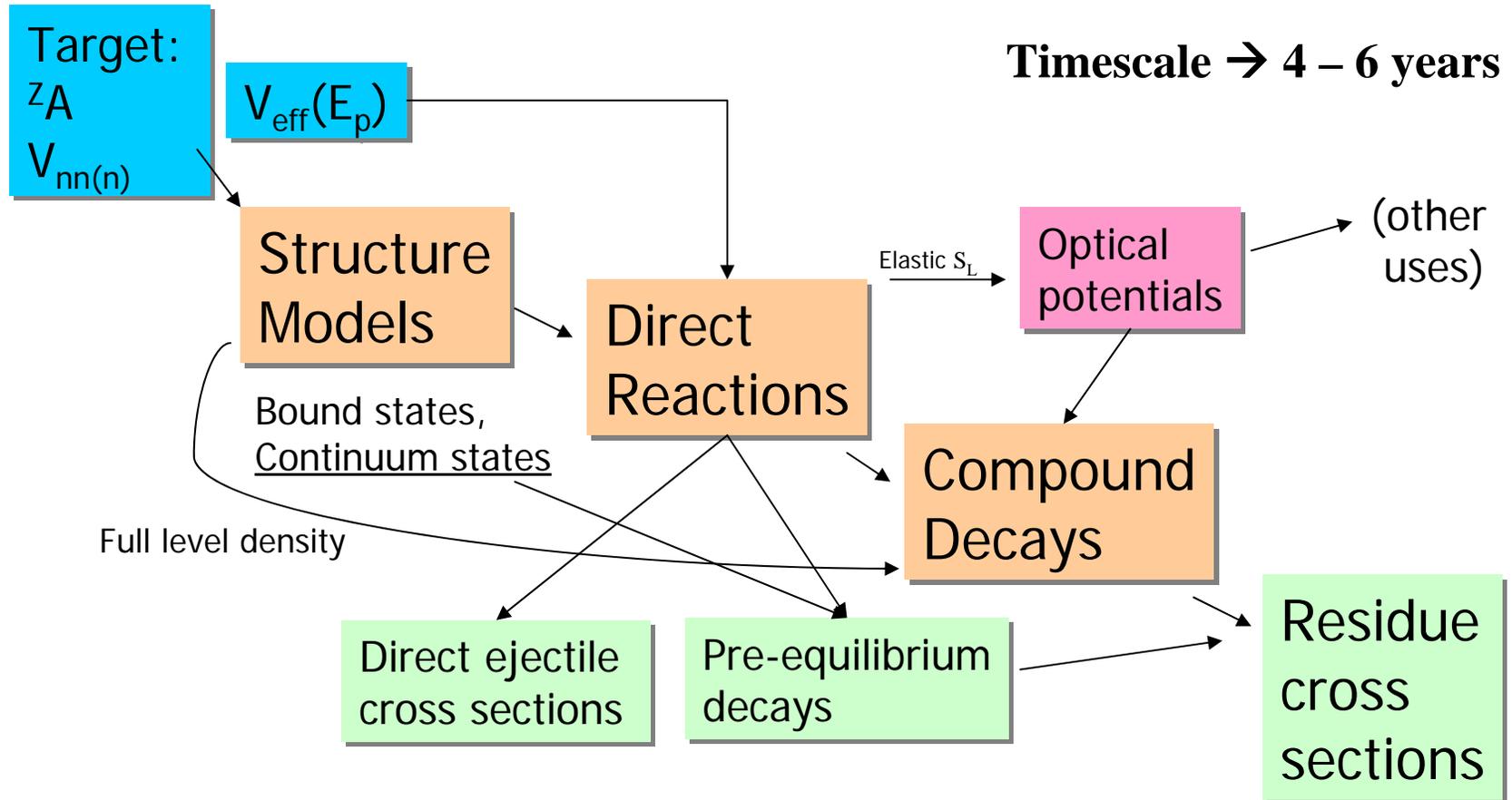
A. Staszczak, J. Dobaczewski
W. Nazarewicz, in preparation



Overall: $n+A$ scattering at E_p



More detail: n+A scattering



CPU time estimate

- Assumptions (for single 3GHz PC):
 - 400 nuclides
 - 50 parameters/nuclide
 - Single model calculation (1 nuclide up to 20 MeV)
 - 20 min
 - benchmark sensitivity to a single parameter 500 min
 - full library benchmark 400 000 min

- Single iteration (min):
 - Model calculations:
 $400 \times 50 \times 2 \times 20 = 800\,000$
 - Benchmark parameter-sensitivity:
 $400 \times 50 \times 2 \times 500 = 20\,000\,000$
 - Library benchmarking:
400 000
 - Total:
~21 000 000 min = 40 years
- 1 iteration per week - 2100 CPU's

TIMESCALE → 2-4 years

Reactor Simulations

- Boltzmann transport → well known equations
- 2 classes of formulations (deterministic and Monte Carlo)
- Quantified computing resources
 - Adequate resolution to describe reactor → petascale problem
 - Methods exist, algorithms exist, software being developed to get to the petascale (LCF)

TIMESCALE: 3-5 year development

Enabling Math and CS technologies

Enabling Math and CS technologies

- 1) parallel eigenvalue solvers for low-memory/processor machines (BG/P)
 - 1) Uncertainty propagation through large systems of ODEs
 - 2) Scalable sparse linear system solves (CG for neutronics)
- 

Time scales for various activities (to completion?)

ab initio foundations (1-3)

data evaluation loop (2-4)

**Nuclear energy density Functional (3-5)
Simulation of reactor core (3-5)**

Microscopic reactions (4-6)

Microscopic fission (5-10)

Conclusions

- **Loss of capability in reaction theory in U.S. is significant. A rebuilding program will better enable AFC (and NNSA and other) needs to be met.**
- **Rebuilding the reactions program in the light of LCF computing will be key (→ joint fellowships for nuclear theory with ASCR?)**
- **Reactors will be built. Reactor simulations to improve upon design (cut cost, improve safety) will require predictive theory in addition to new experimental data.**
- **Digital RIA is the simulation of nuclear structure and reactions given $A(N,Z)$.**
- **Certain codes are at the computing edge today...They will need an underlying help in the near term to move to peta-flop architecture.**