Open Questions

TALENT Summer School
July, 31st 2014

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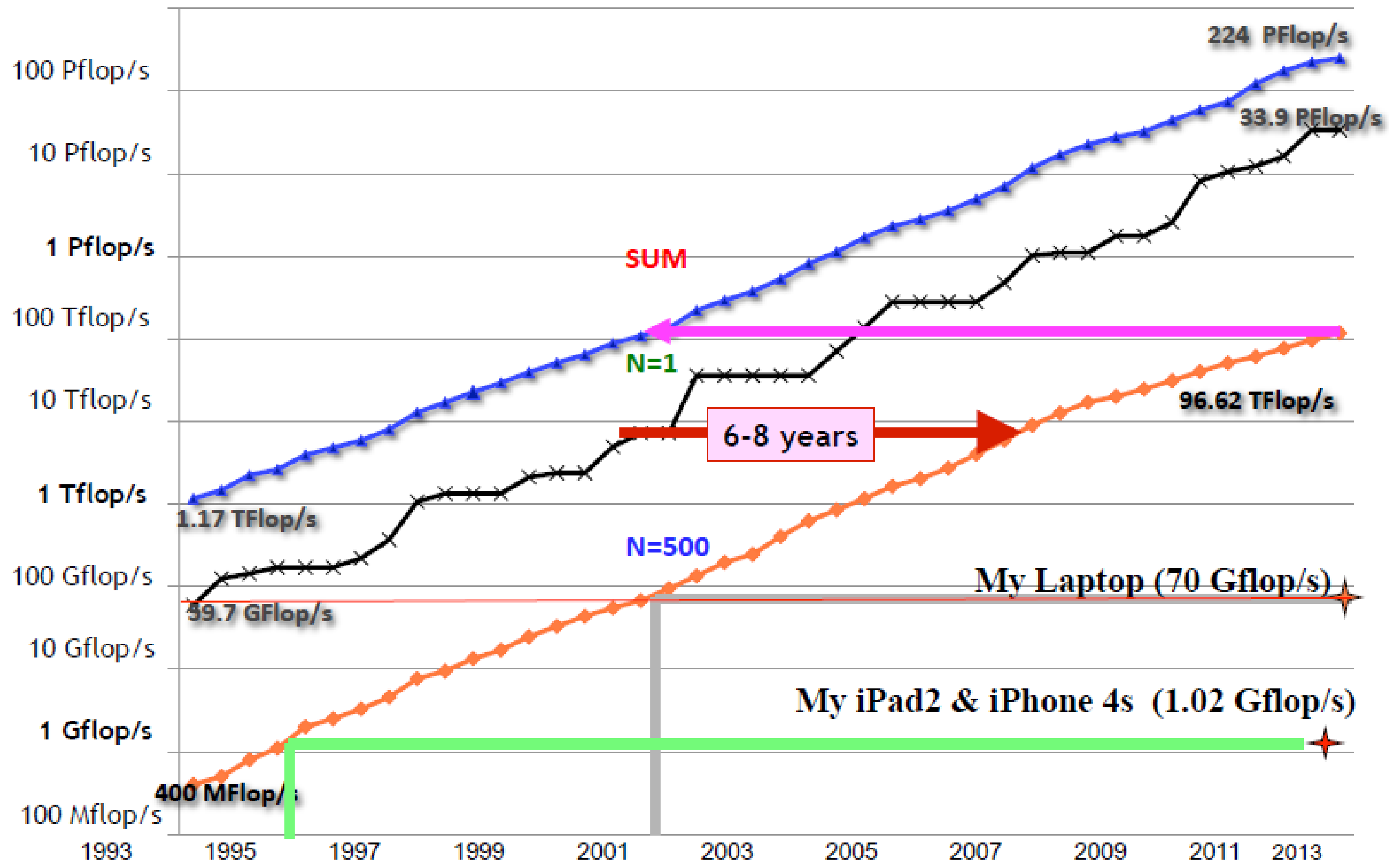
1. Computational Nuclear Physics

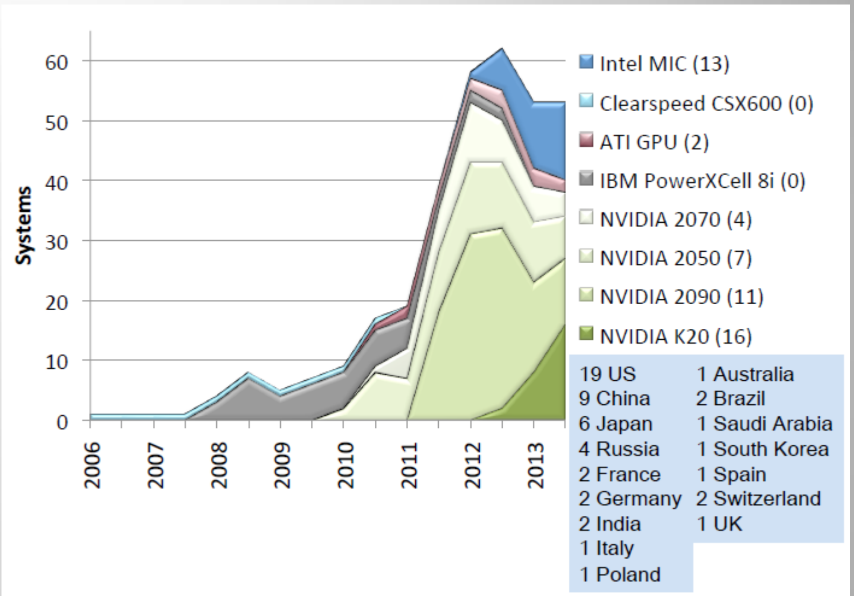
Leadership Computing Facilities

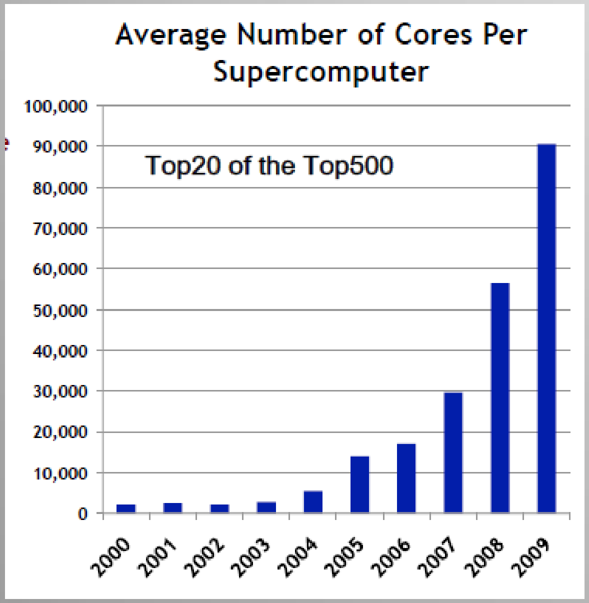
Performance Development of HPC Over the Last 20 Years



Technological Constraints

- More cores, less memory
- More exotic architectures (heterogeneity)
- More redtape to get runtime…
- … and less runtime when you get it





Job Priority by Processor Count

Jobs are *aged* according to the job's requested processor count (older age equals higher queue priority). Each job's requested processor count places it into a specific *bin*. Each bin has a different aging parameter, which all jobs in the bin receive.

Bin	Min Nodes	Max Nodes	Max Walltime (Hours)	Aging Boost (Days)
1	11,250	--	24.0	15
2	3,750	11,249	24.0	5
3	313	3,749	12.0	0
4	125	312	6.0	0
5	1	124	2.0	0

Challenges

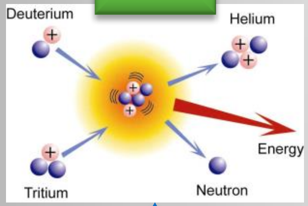
- Hardware changes much faster than software
  - Constant changes of programming paradigms: from vector (Cray) to scalar (current) to vector (GPU)
  - Biggest DFT codes are (at least) 20 years old and monolithic
- New challenges at HPC scale
  - Input/Output: How to store/access/exploit GB/TB of data
  - Fault-tolerance: the machine may crash before your run is completed
- Workforce
  - Computer scientists do computer science, nuclear theorists do nuclear theory: who does computational nuclear theory?
  - No workforce development model

The SciDAC 3 NUCLEI Collaboration

SciDAC Scientific Discovery through Advanced Computing

NUclear Computational Low-Energy Initiative

Fusion



TJNAF

NIF

LENP facilities

FRIB

Validated Nuclear Interactions

Chiral EFT
Ab-initio

Optimization
Model validation
Uncertainty Quantification

Structure and Reactions: Light and Medium Nuclei

Neutron drops
EOS
Correlations

Structure and Reactions: Heavy Nuclei

Ab-initio
RGM
CI

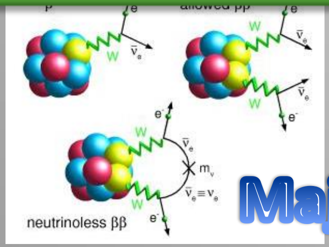
Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification

DFT
TDDFT

Load balancing
Optimization
Model validation
Uncertainty Quantification
Eigensolvers
Nonlinear solvers
Multiresolution analysis

Stellar burning

Neutrinos and Fundamental Symmetries

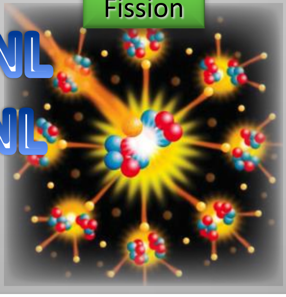


SNS

Majorana

Neutron Stars

Fission



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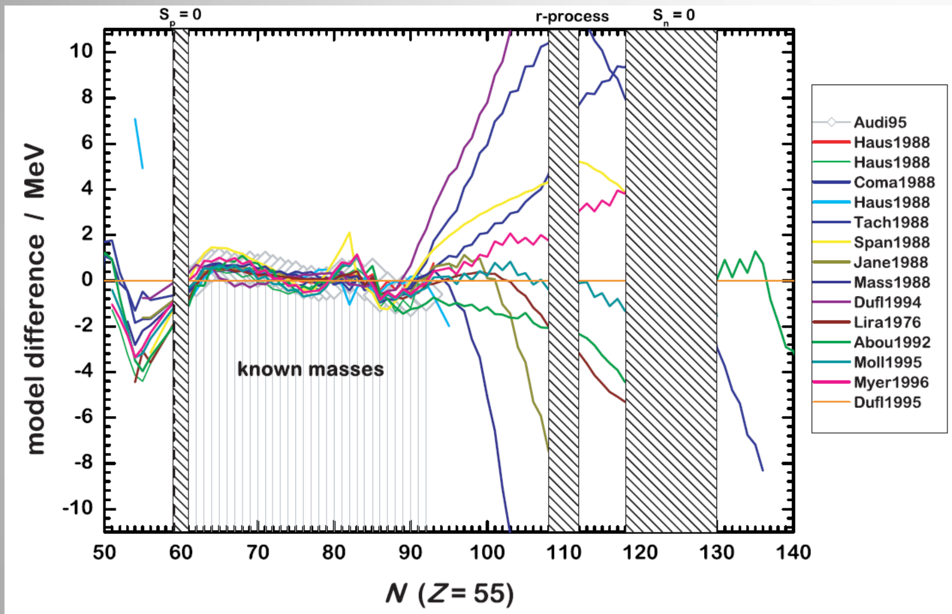
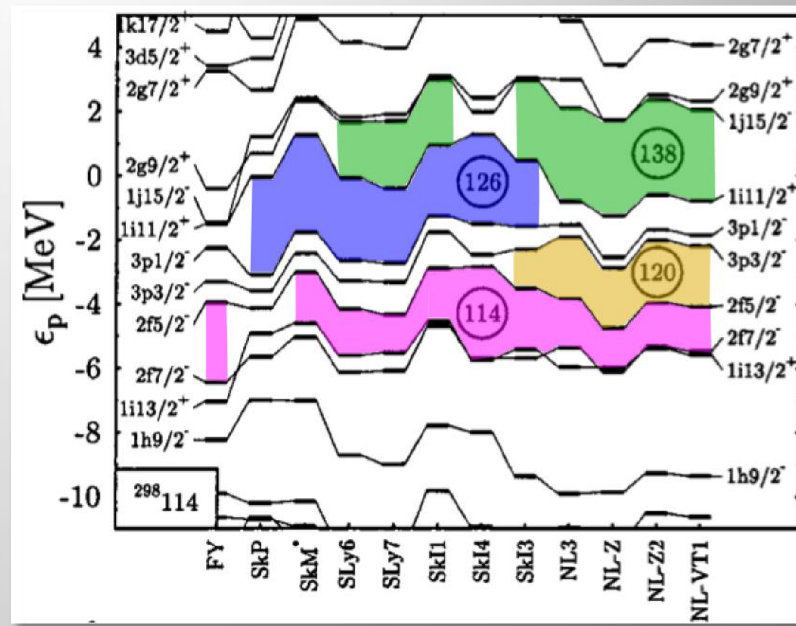
2. Uncertainty Quantification

Most theoretical predictions are unreliable

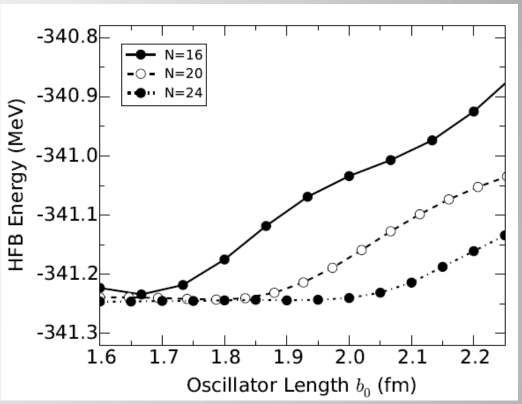


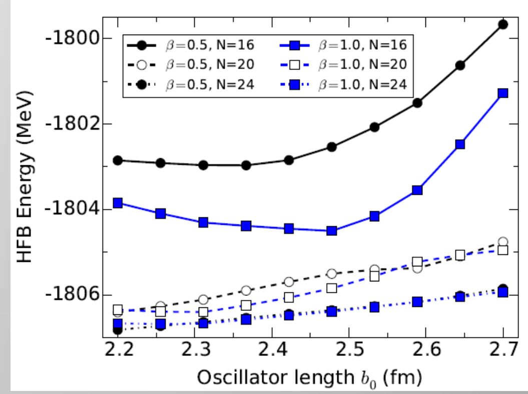


- Extrapolations of current models (DFT and others) beyond stability leads to large discrepancies: where is the truth?
- Until recently, no effort was made to try to quantify the uncertainties of each approach

How to quantify the unknown?

- **Model errors**: Non-relativistic vs. relativistic, zero-range vs. finite-range, EDF vs. mean-field + correlations, etc.
- **Fitting errors**: Choice of experimental data, of the optimization method,
- **Numerical errors**: Numerical implementation, truncation effects, numerical simplifications



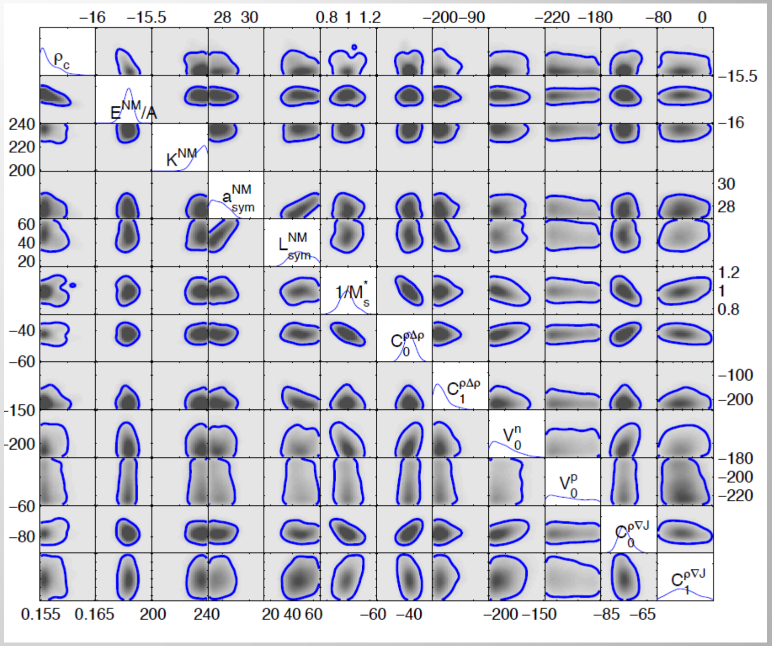


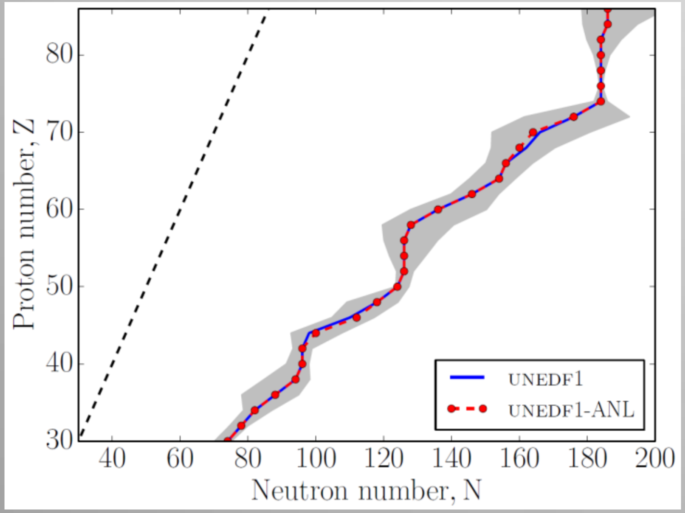
R.m.s.	UNEDF1	UNEDF1-HFB
Deformed masses	0.721	0.776
Spherical masses	1.461	1.836
Proton radii	0.016	0.022
OES neutrons	0.023	0.051
OES protons	0.080	0.075
Fission isomer	0.208	0.558

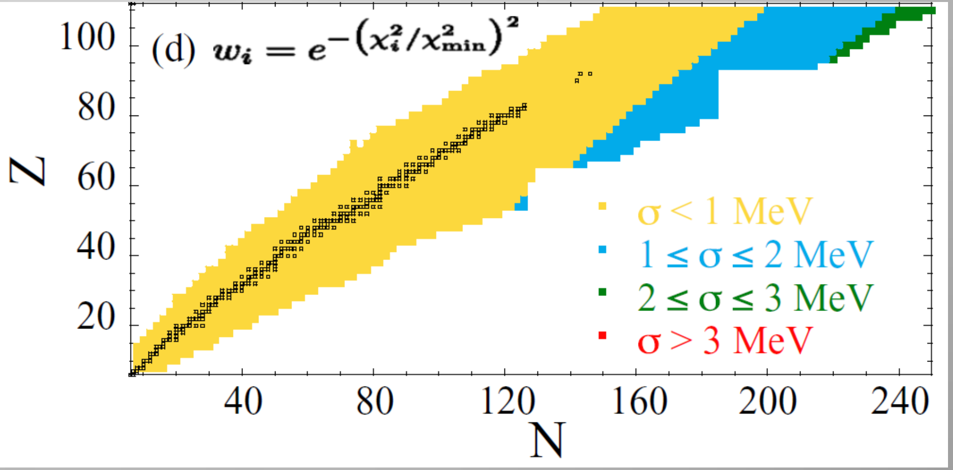
	$\sigma_{FI} = 0.25$	UNEDF1-HFB	$\sigma_{FI} = 0.75$	$\sigma_{FI} = 1.00$
Deformed masses	1.057	0.776	0.748	0.730
Spherical masses	1.808	1.836	1.879	1.893
Proton radii	0.023	0.022	0.021	0.021
OES neutrons	0.057	0.051	0.044	0.042
OES protons	0.079	0.074	0.073	0.072
Fission isomer	0.279	0.558	0.794	0.903

Advanced statistical methods are becoming available

- Bayesian inference methods treat model parameters as genuine random variables
- Posterior distribution allows to quantify uncertainties







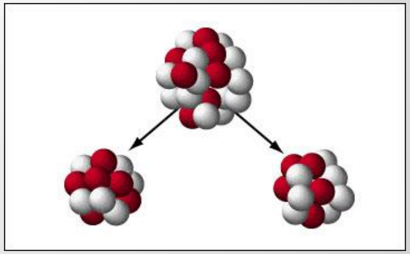
Future work

- “Know thyself”: use statistical techniques such as covariance and sensitivity analysis to better understand models
- Further explorations of Bayesian inference to quantify fitting errors
  - Thousands of Markov-Chain Monte-Carlo runs are necessary to produce a distribution: response functions are needed
  - Can we apply such techniques to quantify uncertainties on complex observables such as fission half-lives or beta-decay probabilities?
- Quantify systematic errors by rigorous model-to-model comparisons

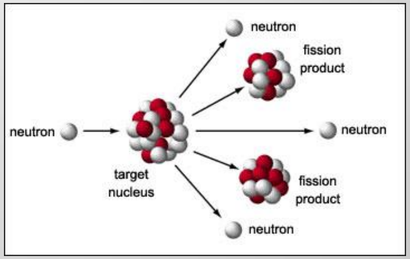
3. Microscopic Description of Nuclear Fission

Nuclear Fission: The Final Frontier...

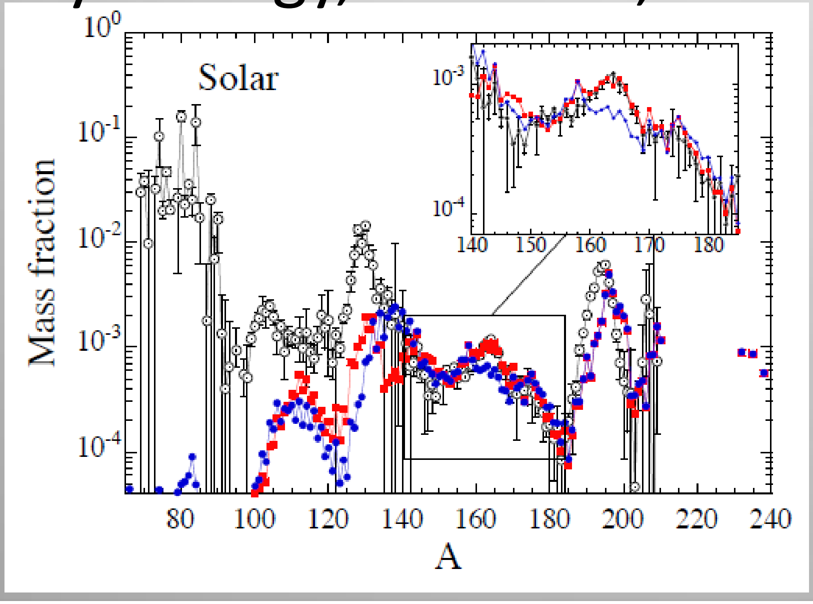
- Beautiful and challenging quantum many-body problem
- Ends nucleosynthesis and determines the limits of stability
- Important applications in society: energy, bad stuff, etc.

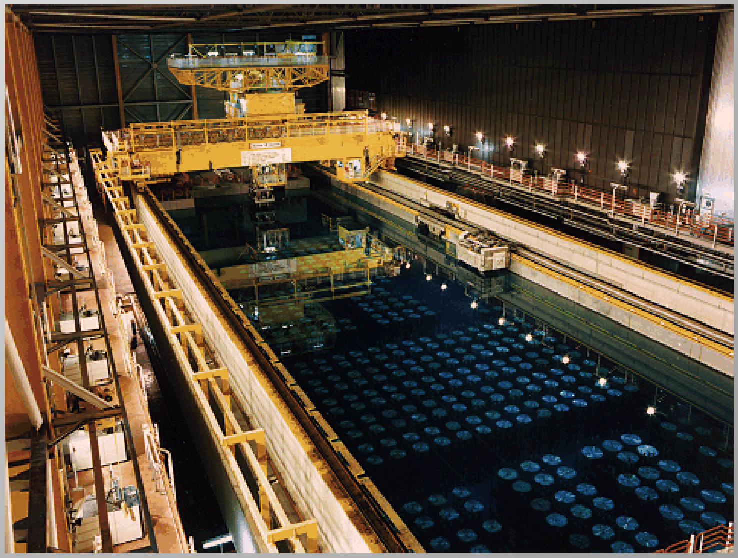


Spontaneous fission



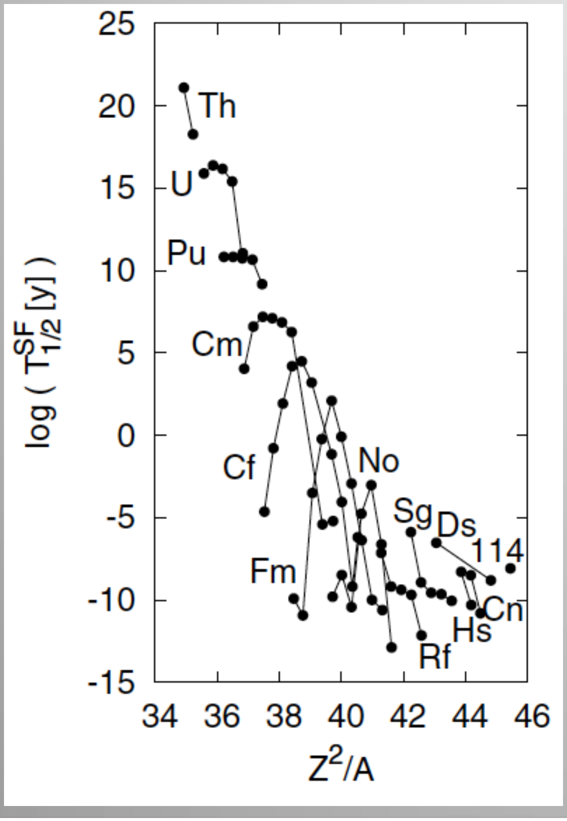
Induced fission

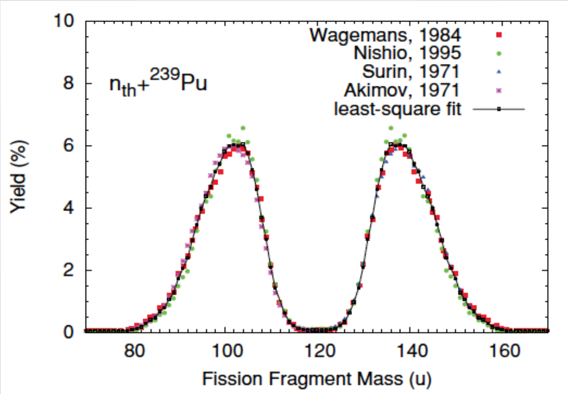


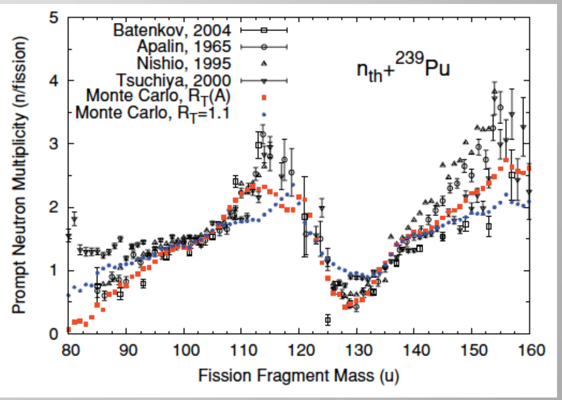


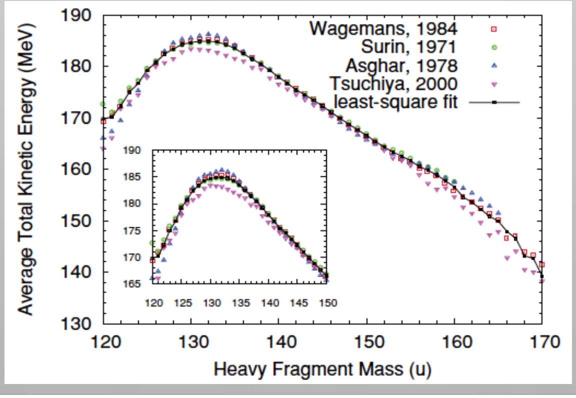
Fission Observables

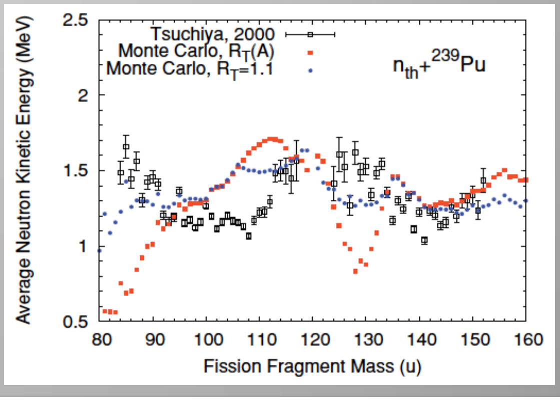
- Simple observables (energies, ratios (yields), lifetimes) are among the most difficult quantities to compute
- Example: Half-lives range from 10^{21} years (^{232}Th) to …0.25 ms (^{250}No) covering more than 30 orders of magnitude!





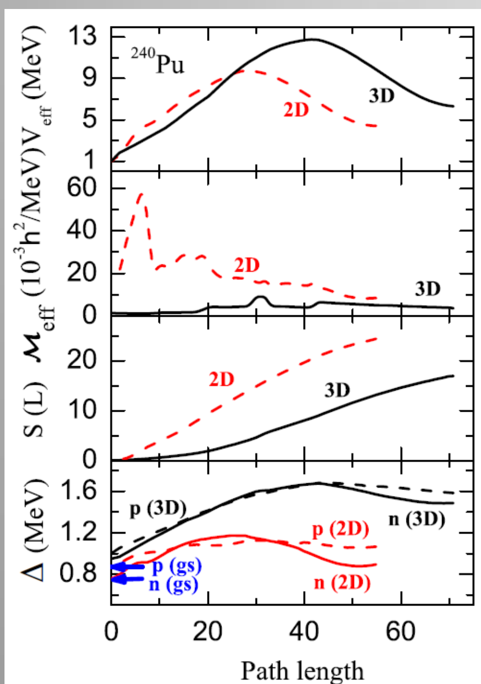


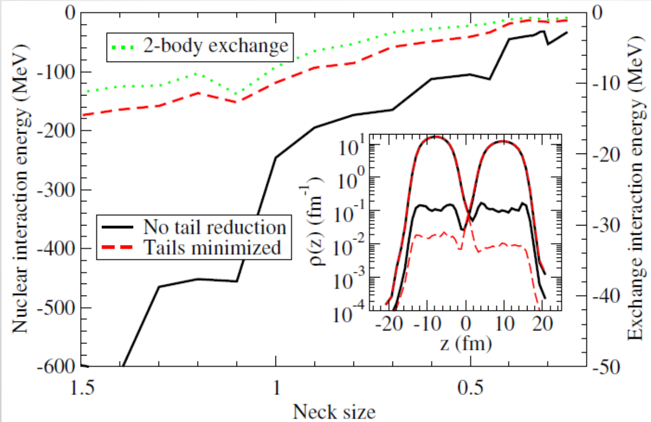


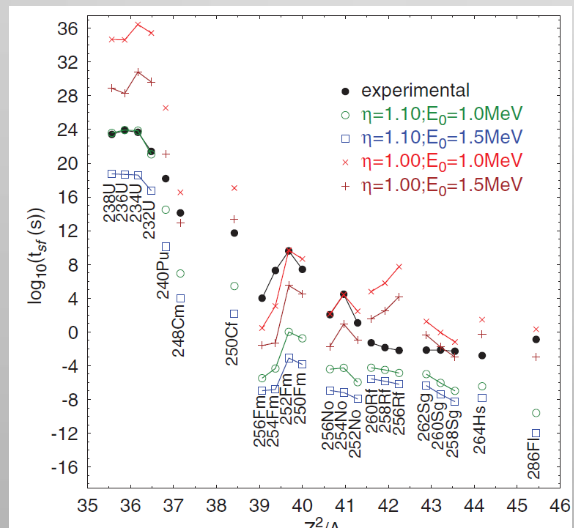


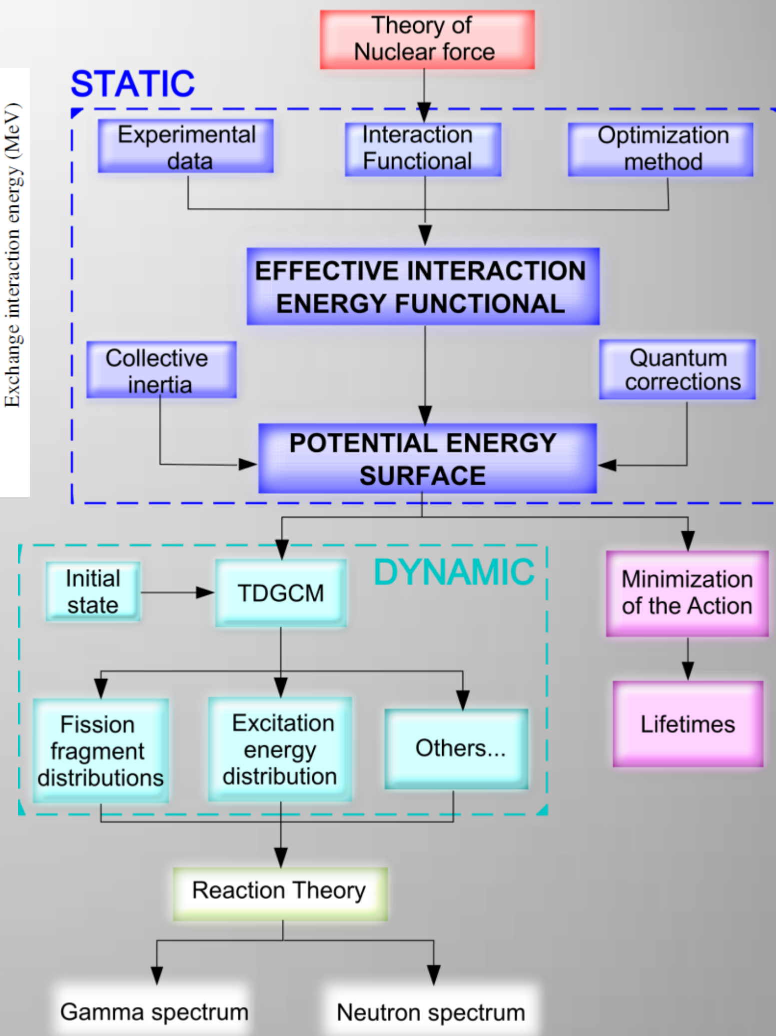
The Big Picture

Hypersensitivity to the model: the ultimate challenge









Challenges

- Tackling the computational problem
  - Near scission up to a dozen collective variables are needed
  - Numerical precision is not trivial for such geometries in such heavy nuclei
- Understanding the quantum mechanics of scission
  - When one quantum many-body problem becomes two
  - No equilibrium, highly-excited nuclei, time-dependent, etc.
- At least understanding isolating the source of major uncertainties
  - Dependence of final observables on underlying EDF and treatment of correlations
  - How much phenomenology will we have to accept?

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