Fission Theory for nuclear data needs

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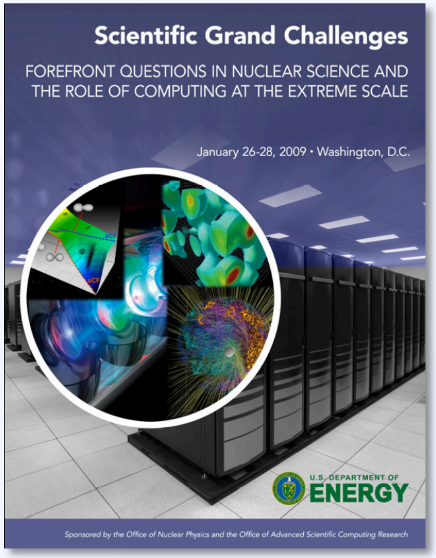
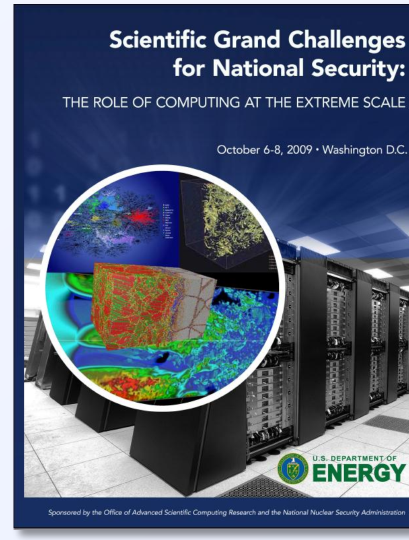
Fission theory and the future of nuclear physics



Two recent DOE-sponsored workshops on exascale computing for nuclear physics, one common conclusion:

The microscopic description of nuclear fission is one of four Priority Research Directions.



Basic science

"The ultimate outcome of the nuclear fission project is a treatment of many-body dynamics that will have wide impacts in nuclear physics and beyond. The computational framework developed in the context of fission will be applied to the variety of phenomena associated with the large amplitude collective motion in nuclei and nuclear matter, molecules, nanostructures and solids"

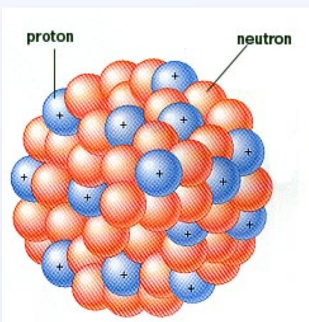
Applied science

"Understanding nuclear fission at a more comprehensive level is a critical problem in national security with important implications in nuclear materials detection and nuclear energy, as well as enhancing the quantitative understanding of nuclear weapons"

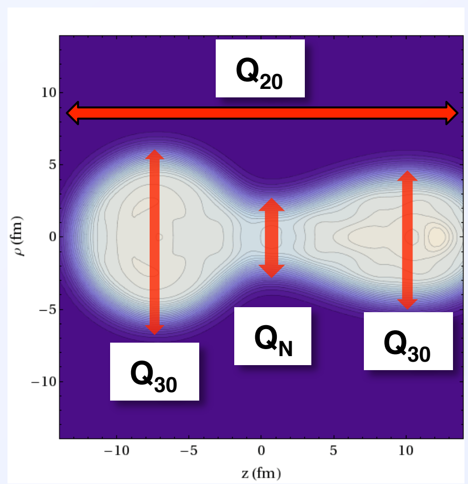
Goal and method

- <u>Goal</u>: starting from an effective interaction between nucleons, solve equations of quantum mechanics to derive a <u>comprehensive and predictive theory of fission</u>
  1) Fragment properties: energies, mass distributions,…
  2) Fission probabilities and cross sections
- <u>Method</u>: microscopic theory

Individual nucleons

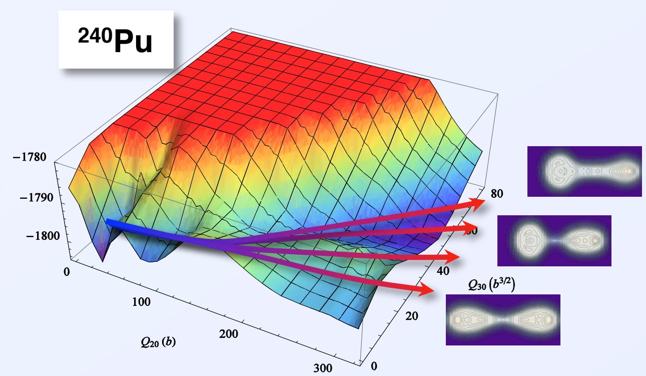


Effective interaction



Global constraints to explore nuclear configurations (Statics)
Collective (+ single-particle)

Least-action principle for evolution in time (dynamics)



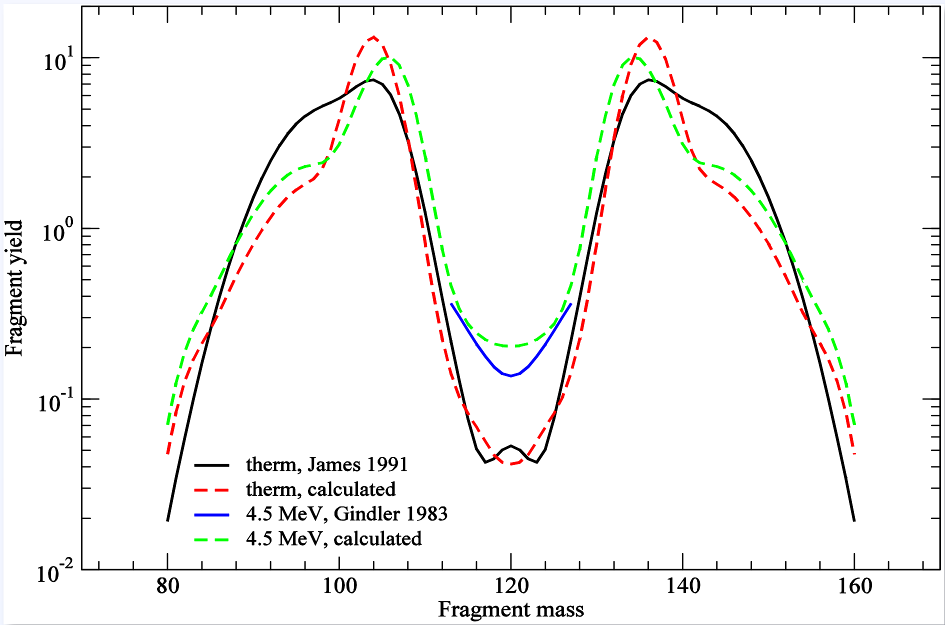
Statics gives fragment properties, dynamics gives their population distribution

Milestones and deliverables for the ARRA project

FY	Milestones	Deliverables
10	• calc PES • time-dependent formalism • microscopic theory of scission • N. Schunck hired	• 1st time-dependent calcs of $^{239}Pu(n_{th},f)$ presented at DNP meeting
11	• coll-s.p. formalism with BIII • dynamics with > 2 d.o.f. with BIII	• PRC submitted on collective-s.p. coupling • PRL submitted on microscopic theory of scission
12	• continue development of collective-s.p. coupling • implement and calculate effect of coupling on fragment properties	• report on $^{239}Pu(n,f)$ fragment properties for thermal and low energies

Results so far: Mass yields

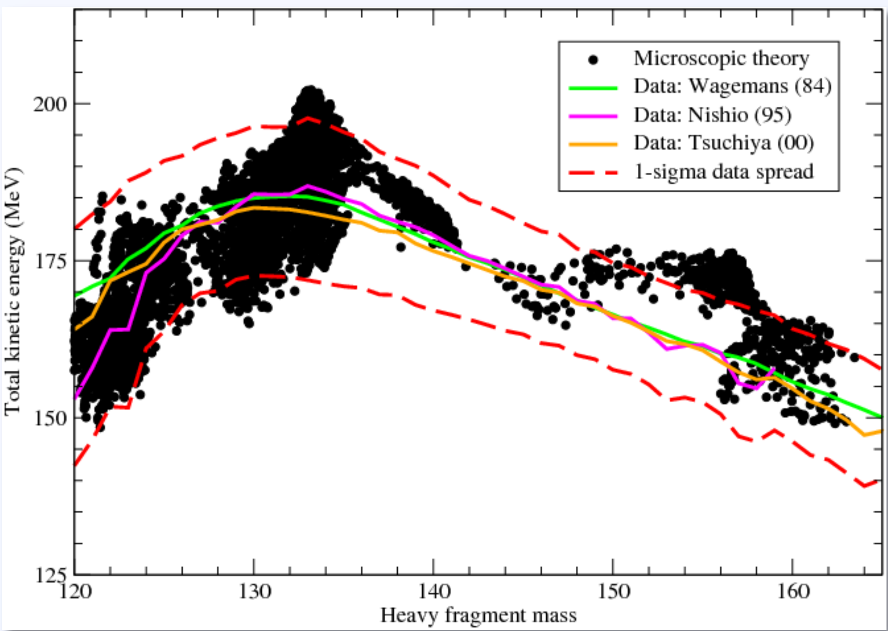
Fragment mass yields for ^{239}Pu fission: data vs theory

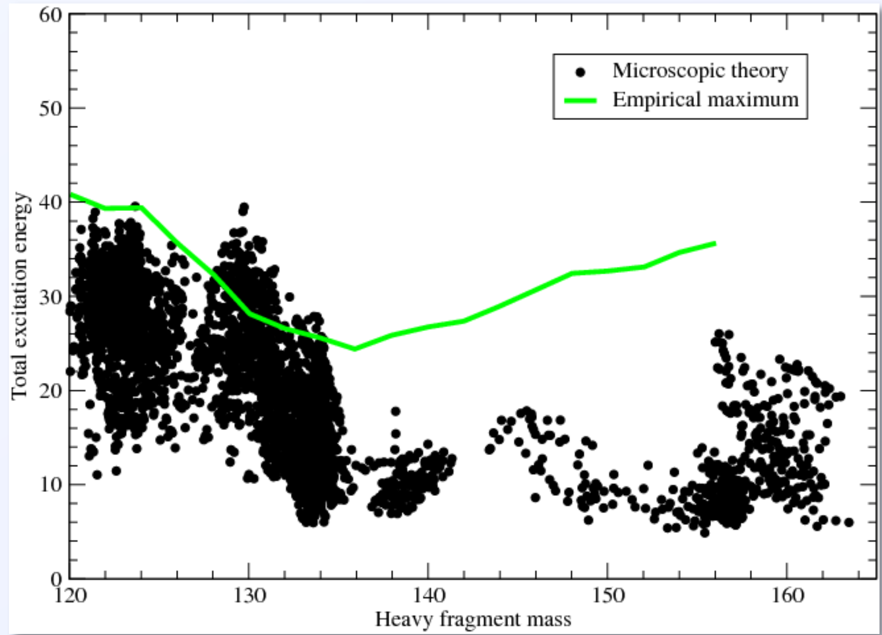


- Results are from time-dependent calculations
- Shape and trends of yields fairly well reproduced but
  - Discrepancies in mass range 135-150
  - Missing physics in energy dependence (e.g., collective-s.p. coupling)

1) Missing points/configurations?
2) Behavior at higher energies?

Results so far: fragment kinetic and excitation energies





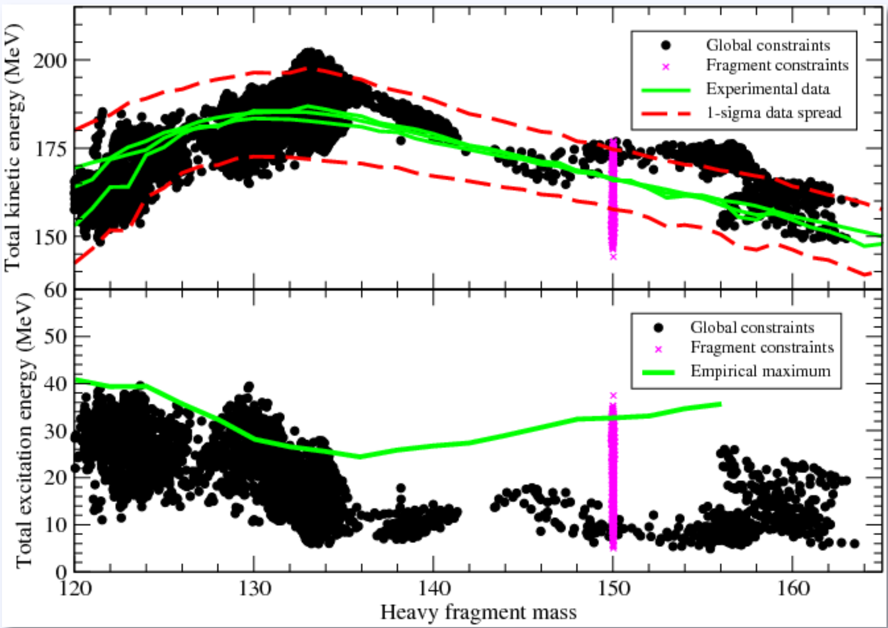
TKE calcs mostly within 1-sigma window, different Z, fission modes explains spread

TXE calcs span low-E to empirical maximum, different Z, fission modes explains spread

Remarkable agreement, but there are still questions:

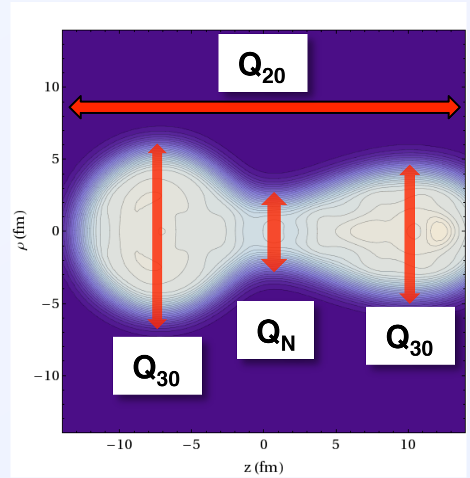
1) **Missing points for A > 134?**
2) **Microscopic calculation of contribution from dynamics?** **(currently using simplistic estimate)**
3) **Behavior at higher energies?**

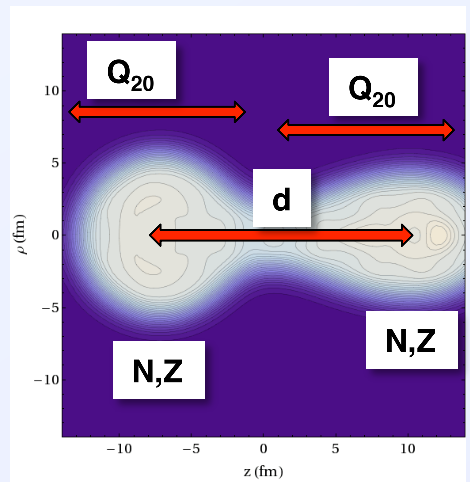
Improving the calculations: where are the missing points?



From global

To local constraints on fragments

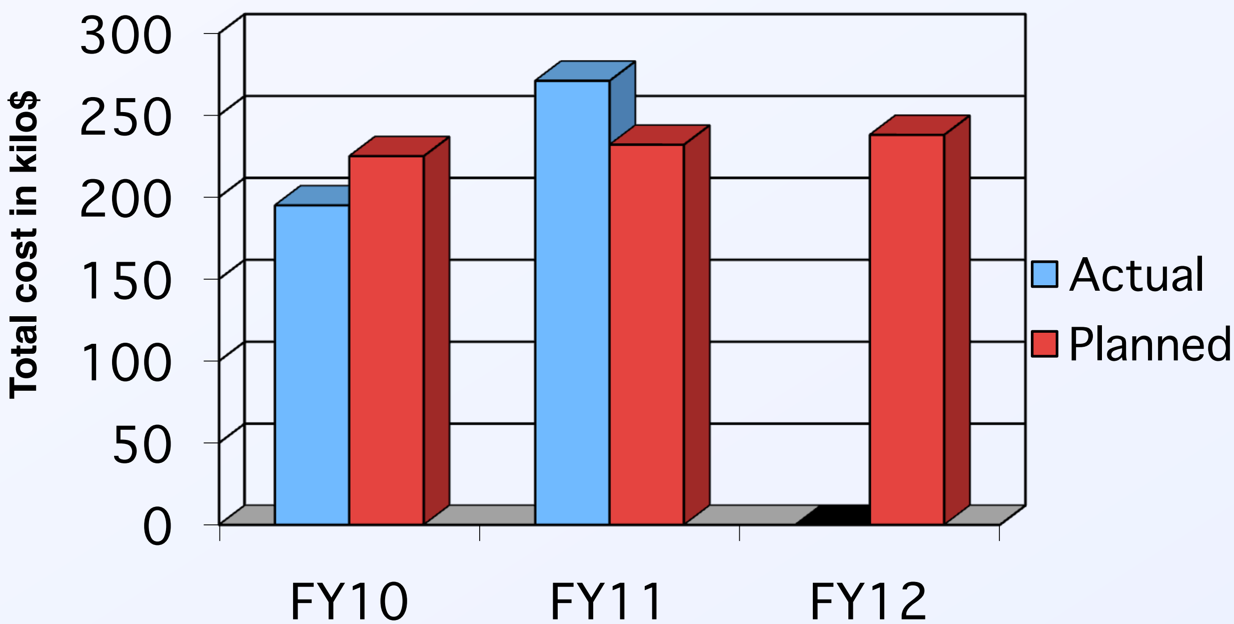




Studied $^{240}Pu \rightarrow {}^{150}Ce + {}^{90}Kr$ in particular
- **fragment constraints recover missing points**
- **more computationally intensive!**

Budget & personnel

Total budget: $695k, remaining = $229k



Personnel:

S. Quaglioni
Oct 09 – Mar 10

N. Schunck
Sep 10 -

W. Younes
Oct 09 -

Plan to finish work

- Focus on the two major issues
  - Missing configurations
    - Now performing preliminary calcs with constraints on fragments
    - Requested computer time for full-scale calcs
  - Coupling between single-particle and collective d.o.f.
    - Development of collective-s.p. formalism continues with BIII
- In addition
  - Improvements to computational algorithms (N. Schunck)
    - Faster calculations/analysis

Future developments (beyond this ARRA)

- Study of non-adiabatic fission, “dissipation” at microscopic level due to
  - Collective d.o.f.
  - Single-particle d.o.f.
  - Coupling
- Induced fission at higher energies (e.g., E_n >> 2 MeV)
- Spectroscopy of fission fragments
- Microscopic calculations of fission probabilities, cross sections
- …