Theories of Fission

Topical Program: FRIB and the GW170817 Kilonova

July, 19th 2018

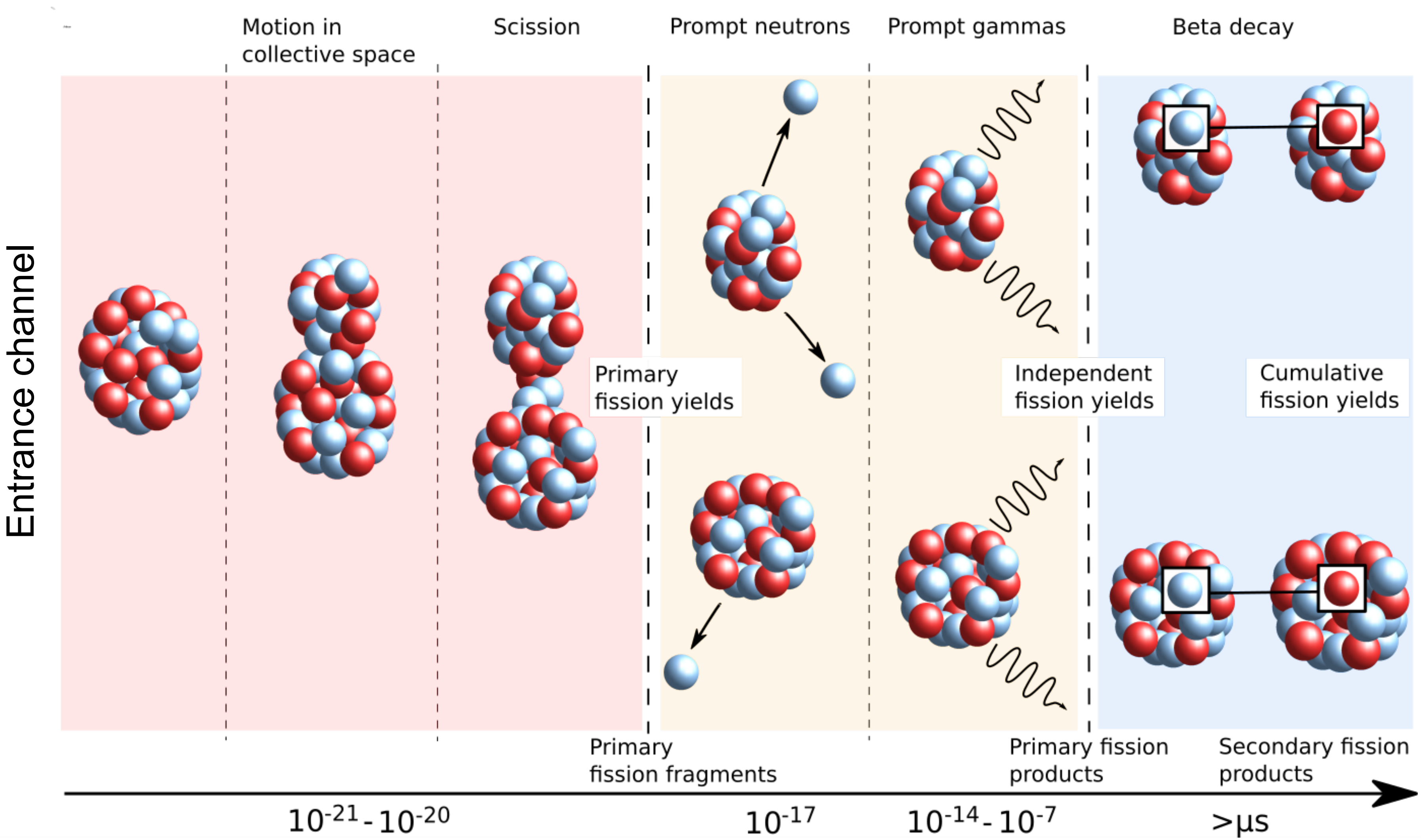
Nicolas Schunck

LLNL-PRES-737743
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

Characteristics of Fission

Multi-scale Quantum Dynamical Process

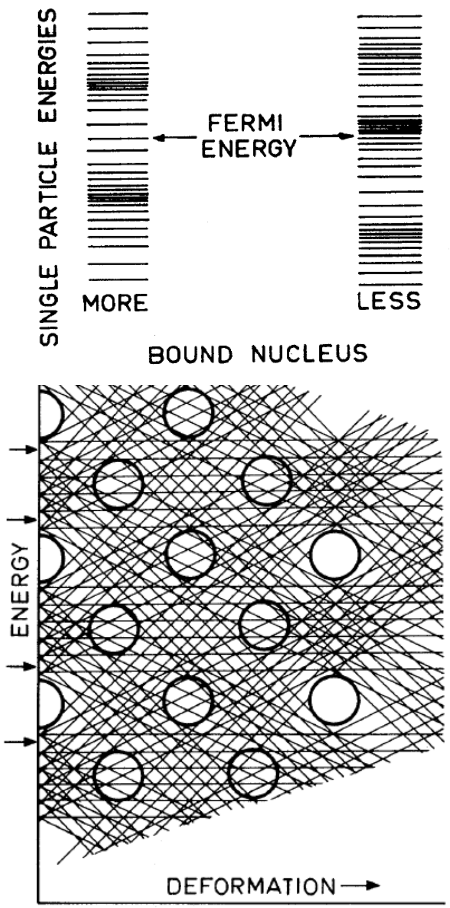


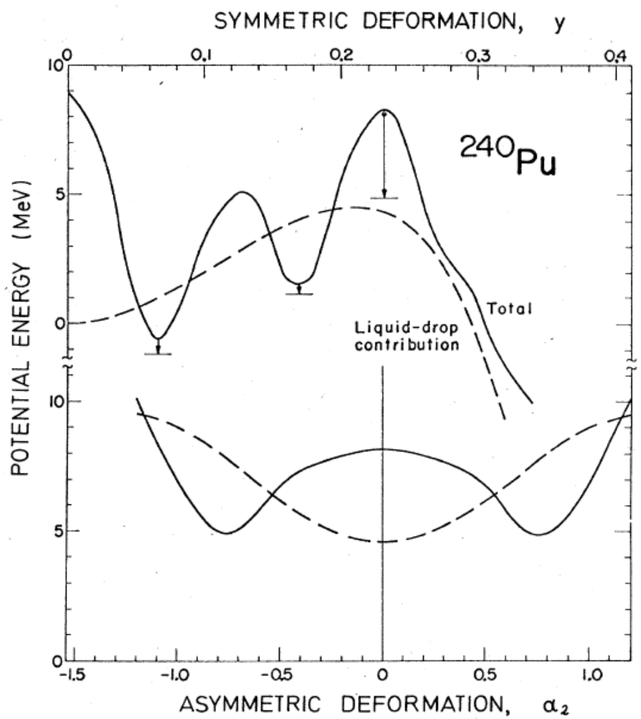
Outline

- Introduction
- Static Nuclear Properties
  - Macroscopic-Microscopic Approach
  - Nuclear Density Functional Theory
- Fission Dynamics
  - Classical Dynamics (Stochastic Langevin Equations)
  - Quantum Dynamics (“Collective”)
  - Quantum Dynamics (“Non-collective”)
- Fission Spectrum
- Concluding Remarks

Macroscopic-microscopic Models (1/4)

A phenomenological approach to nuclear structure





M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, PRC **5**, 1050 (1972); M. Brack, J. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinsky, and C. Y. Wong, RMP **44**, 320 (1972); J. Dudek, B. Herskind, W. Nazarewicz, Z. Zymanski, T.R. Werner, PRC **38** 940 (1988)

- Start with deformed liquid drop(let)
- Take into account nucleon degrees of freedom
  - Shell correction coming from the distribution of single-particle levels
  - Pairing correction to mock up effects of residual interactions
- Extensions to finite angular momentum or temperature

Macroscopic-microscopic Models (2/4)

The total binding energy is a sum of several components

- Total energy is written

$$E(\boldsymbol{q}) = E_{\mathrm{mac}}(\boldsymbol{q}) + \delta R_{\mathrm{shell}}(\boldsymbol{q}) + \delta R_{\mathrm{pair}}(\boldsymbol{q})$$

- Macroscopic liquid drop energy

$$E_{\mathrm{mac}}(\boldsymbol{q}) = E_{\mathrm{vol}} + E_{\mathrm{surf}}(\boldsymbol{q}) + E_{\mathrm{asym}}(\boldsymbol{q}) + E_{\mathrm{Coul.}}(\boldsymbol{q})$$

- Shell correction

$$\delta R_{\mathrm{shell}}(\boldsymbol{q}) = \sum_n e_n - \left\langle \sum_n e_n \right\rangle$$

- Pairing correction

$$\delta R_{\mathrm{pair}}(\boldsymbol{q}) = E_{\mathrm{pair}} - \tilde{E}_{\mathrm{pair}}$$

- Shell and pairing corrections require a set of single-particle energies e_n: need to solve the Schrödinger equation

J. Dudek, T. Werner, ADNDT 50, 179 (1992)J. Dudek, T. Werner, ADNDT 59, 1 (1995); N. Schunck, J. Dudek, B. Herskind, PRC **75** 054304 (2007); P. Möller, A. Sierk, T. Ichigawa, H. sagawa, ADNDT **109**, 1 (2012)

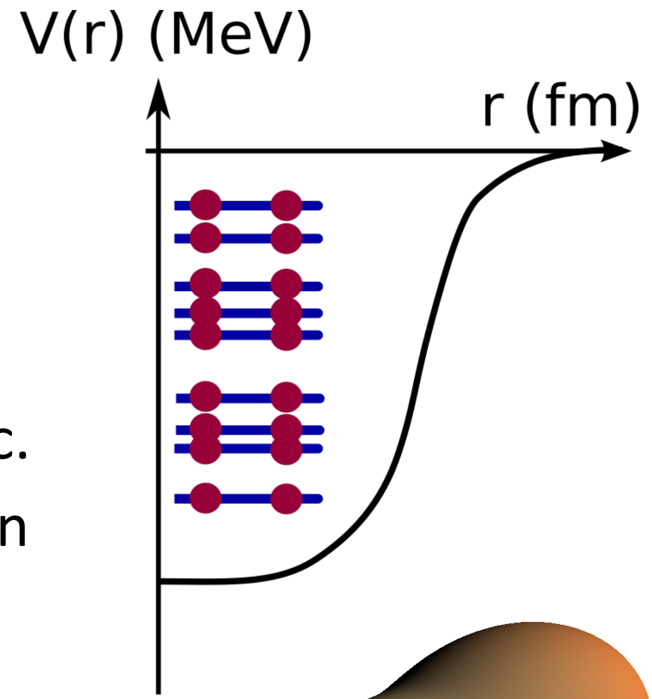
Macroscopic-microscopic Models (3/4)

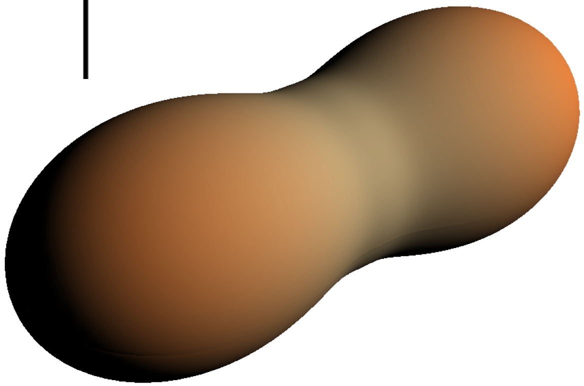
Deformations are collective d.o.f, single particles intrinsic d.o.f

- (One-body) Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\boldsymbol{q}}(\boldsymbol{r})\right]\varphi_n(\boldsymbol{r}) = e_n\varphi_n(\boldsymbol{r})$$

- Nuclear mean-field potential can be Nilsson, Woods-Saxon, Folded-Yukawa, etc.
- Solve BCS equation to compute occupation of s.p. states and extract pairing energy
- How does that apply to fission?
  - Deformation of the nuclear shape drive the fission process (=collective variables)
  - Compute energy for different deformations → potential energy surfaces

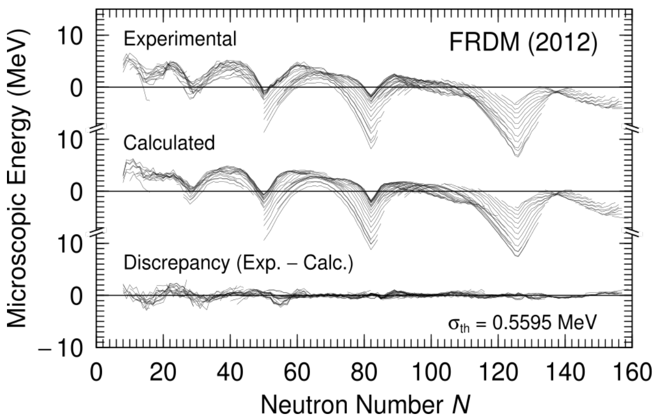


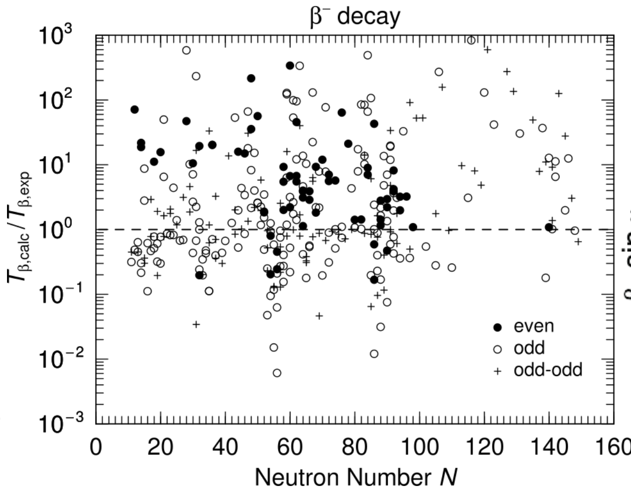


Macroscopic-microscopic Models (4/4)

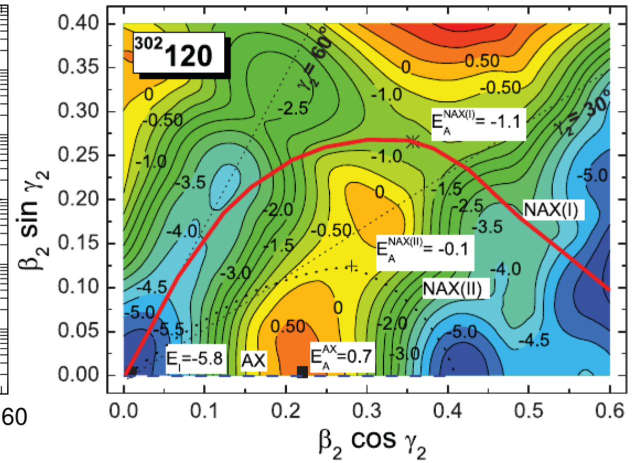
Examples

P. Möller, et al, ADNDT **109**, 1 (2012)





M. Kowal, et al, PRC **82**, 014303 (2010)



- Global theory: many properties of all nuclei in the nuclear chart
- Fast: many calculations need only a laptop
- Inconsistent framework
  - Each theoretical piece (macro, micro, pairing, RPA, etc.) is treated independently of the others
  - Predictive power has not really changed since the 1970ies

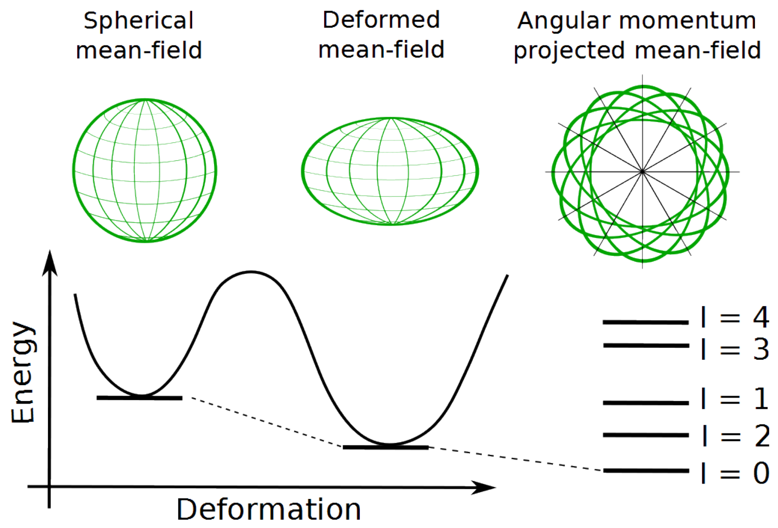
Nuclear Density Functional Theory (1/3)

DFT is a remapping of the quantum many-body problem

- Quantum mechanics rules: Start with best estimate of a realistic nuclear Hamiltonian
- Replace the exact wave function by a simpler form, the reference state: a product state
- Replace exact Hamiltonian with effective one such that

$$\langle \Psi | \hat{H} | \Psi \rangle \approx \langle \Phi | \hat{H}_{\mathrm{eff.}} | \Phi \rangle = E[\rho, \kappa]$$

- Energy is a functional of density of particles and pairing tensor
- Spontaneous symmetry breaking



P. Hohenberg and W. Kohn, PR **136**, B864 (1964); W. Kohn and L. J. Sham, PR **140**, A1133 (1965); J. Engel, PRC **75**, 014306 (2007); M Bender, P.H. Heenen, P.-G. Reinhard, RMP **75**, 121 (2003); J. Messud, M. Bender, and E. Suraud, PRC **80**, 054314 (2009).

Nuclear Density Functional Theory (2/3)

The densities contain all degrees of freedom of the system

- Form of the energy functional chosen by physicists, often guided by characteristics of nuclear forces (central force, spin-orbit, tensor, etc.): Skyrme, Gogny, etc.
- Variational principle: determine the actual densities of the nucleus by requiring the energy is minimal with respect to their variations
  - Resulting equation is called HFB equation (Hartree-Fock-Bogoliubov)
  - Solving the equation gives densities and characteristics of the reference state
- Any observable can be computed when we know the density

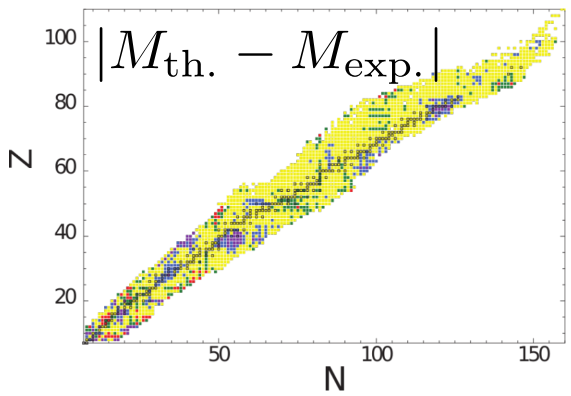
$$\langle \Phi | \hat{Q}_{20} | \Phi \rangle = \int d^3\boldsymbol{r}\ \rho(\boldsymbol{r}) Q_{20}(\boldsymbol{r})$$

- One can compute potential energy surfaces by solving the HFB equation with constraints on the value of the collective variables

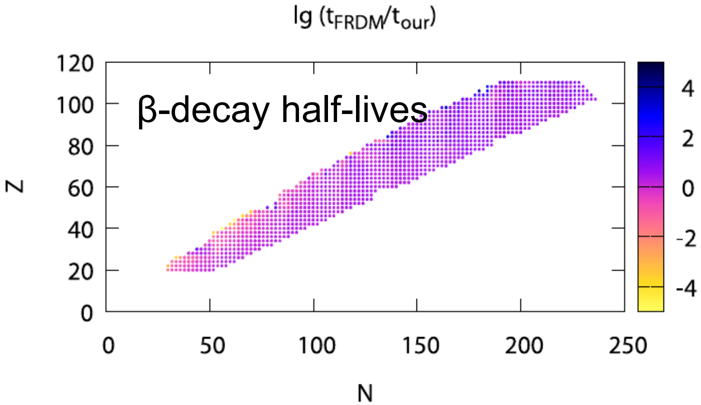
Nuclear Density Functional Theory (3/3)

Examples

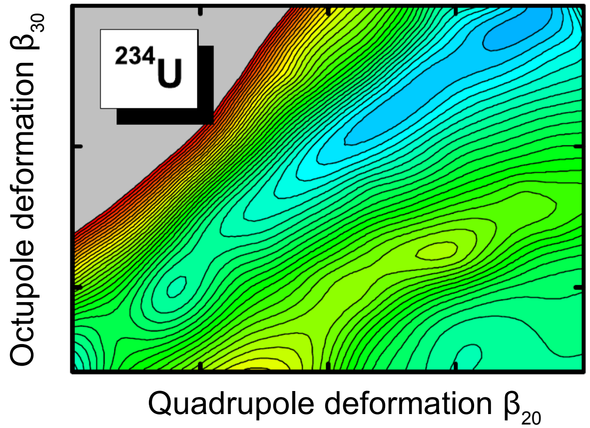
S. Goriely, R. Capote, PRC **89**, 054318 (2014)



M. Mustonen, J. Engel, PRC **93**, 014304 (2016)



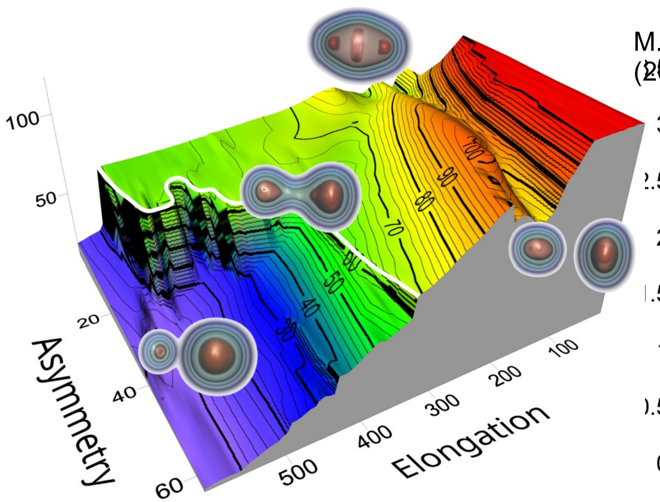
J. Zhao, et al, PRC **91**, 024321 (2015)



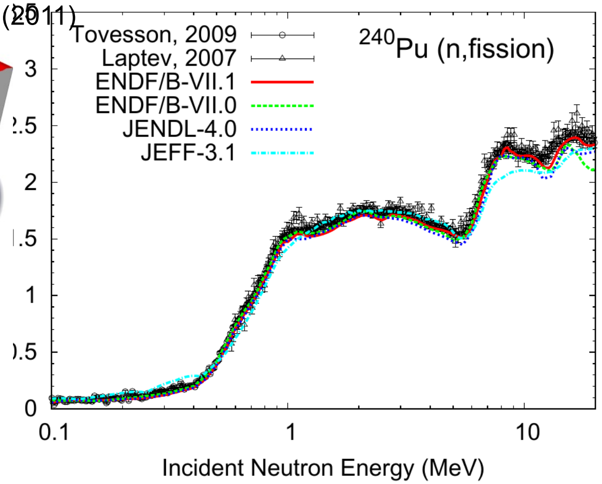
- Global theory: many properties of all nuclei in the nuclear chart
- Consistent framework: a single energy functional and quantum many-body methods
- Computationally expensive
  - Mass-table-scale calculations require supercomputers
  - Computing potential energy surfaces is an art

Fission Observables

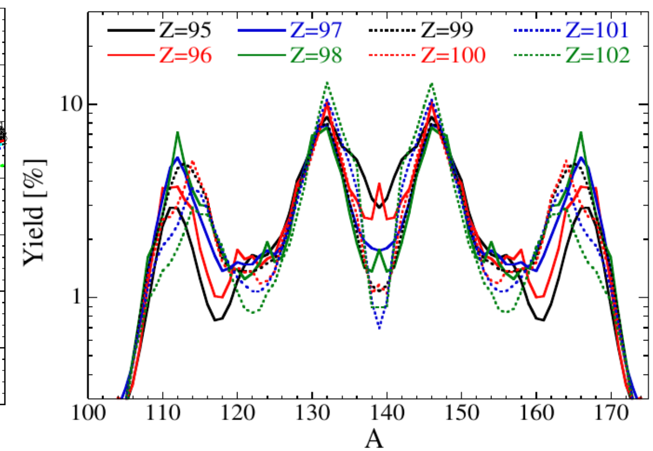
Static approaches can be used to compute some fission observables



M. Chadwick, et al, Nucl. Data Sheets **112**, 2887 (2011)



S. Goriely, et al, PRL **111**, 242502 (2013)



- Fission barriers inputs to compute fission cross-sections (=rates)
  - Reduction multi-dimensional → 1-dimensional (arbitrary)
  - Assume parabolic shape (not justified)
  - Neglect collective inertia
- Statistical theory gives (rather poor) estimates of primary fission yields

Classical Dynamics (1/3)

Fission is a stochastic diffusion process in the collective space

- How to extract fission product yields from the knowledge of the potential energy surface?
  - Analogy with classical theory of diffusion
  - Collective variable = generalized coordinate
  - Define related momentum
- Langevin equations

Fluctuation-dissipation theorem

$$\sum_k \Theta_{ik}\Theta_{kj} = \Gamma_{ij} T$$

$$\dot{q}_\alpha = \sum_\beta B_{\alpha\beta} p_\beta ,$$

Friction tensor

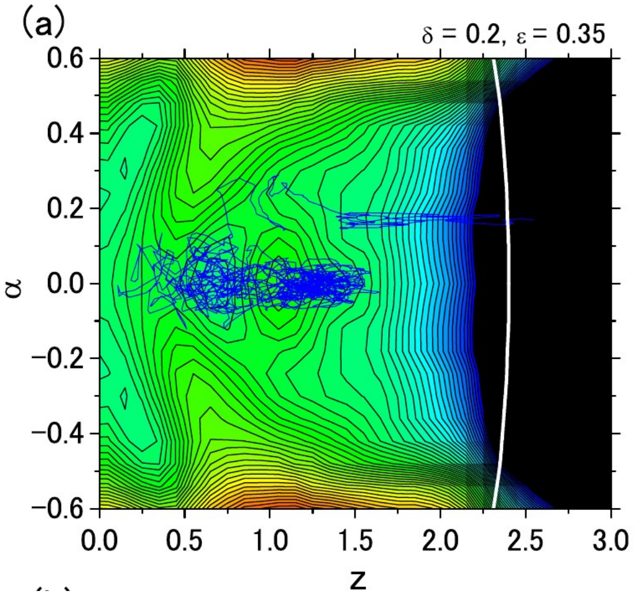
Random force

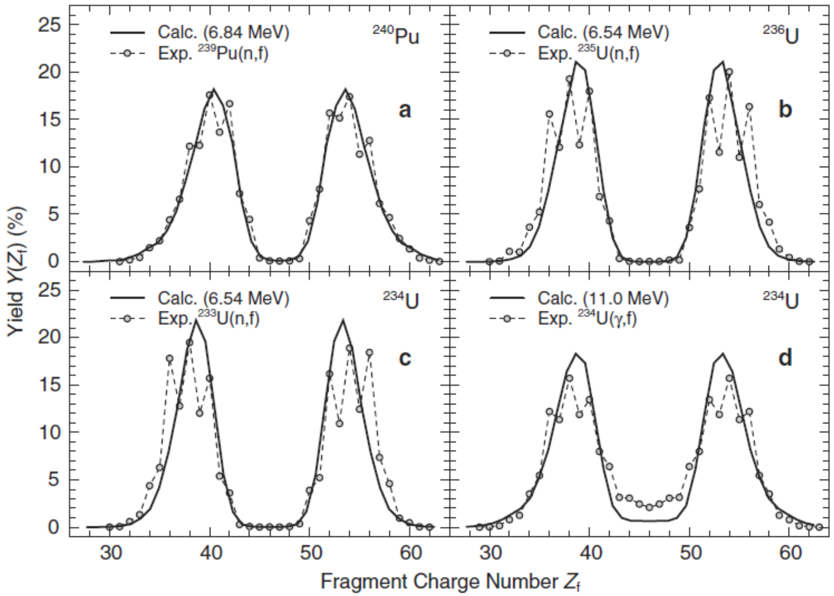
$$\dot{p}_\alpha = -\sum_{\beta\gamma} \Gamma_{\alpha\beta} B_{\beta\gamma} p_\gamma + \sum_\beta \Theta_{\alpha\beta}\xi_\beta(t)$$

$$-\frac{1}{2}\sum_{\beta\gamma}\frac{\partial B_{\beta\gamma}}{\partial q_\alpha} p_\beta p_\gamma - \frac{\partial V}{\partial q_\alpha}$$

Classical Dynamics (2/3)

Practical examples





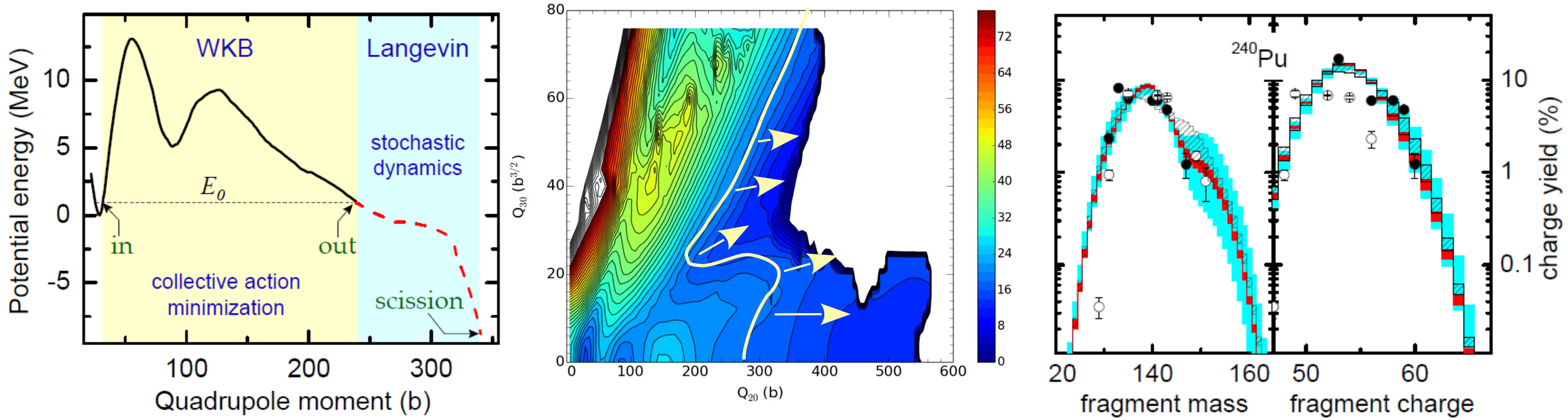
P. Nadtochy and G. Adeev, PRC **72**, 054608 (2005); P. N. Nadtochy, A. Kelić, and K.-H. Schmidt, PRC **75**, 064614 (2007); J. Randrup and P. Möller, PRL **106**, 132503 (2011); J. Randrup, P. Möller, and A. J. Sierk, PRC **84**, 034613 (2011); P. Möller, J. Randrup, and A. J. Sierk, PRC **85**, 024306 (2012); J. Randrup and P. Möller, PRC **88**, 064606 (2013); J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC **93**, 011304 (2016), J. Sadhukhan, W. Nazarewicz and N. Schunck, PRC **96**, 061361 (2017).

- Start beyond the saddle point (or close enough)
- Build trajectories through the collective space by generating at each step the needed random variable
- Enough trajectories (in the thousands) allow reconstructing FPY

Classical Dynamics (3/3)

Langevin classical dynamics is ideal tool for spontaneous fission

J. Sadhukhan, W. Nazarewicz and N. Schunck, Phys. Rev. C **93**, 011304 (2016); J. Sadhukhan, W. Nazarewicz, C. Zhang and N. Schunck, Phys. Rev. C (R) **96**, 061301 (2017)

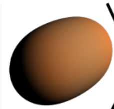
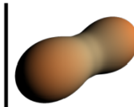
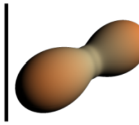


- SF mass distributions can be obtained by combining quantum tunneling techniques (half-lives) and classical dynamics
  - Collective inertia plays critical role in determining tunneling probability (=τ_{SF})
  - Evolution from saddle to scission done with Langevin dynamics (=classical_ with microscopic inputs (energy, inertia)
  - Dissipation tensor still cause of significant uncertainty

Quantum Dynamics - TDGCM (1/3)

Computing the flow of probability in the collective space

- Ansatz for the time-dependent many-body wave function

$|\Psi(t)\rangle = f_1(t)|$  $\rangle + f_2(t)|$  $\rangle + f_3(t)|$  $\rangle \cdots$

- Minimization of the time-dependent quantum mechanical action + ansatz + Gaussian overlap approximation + some patience

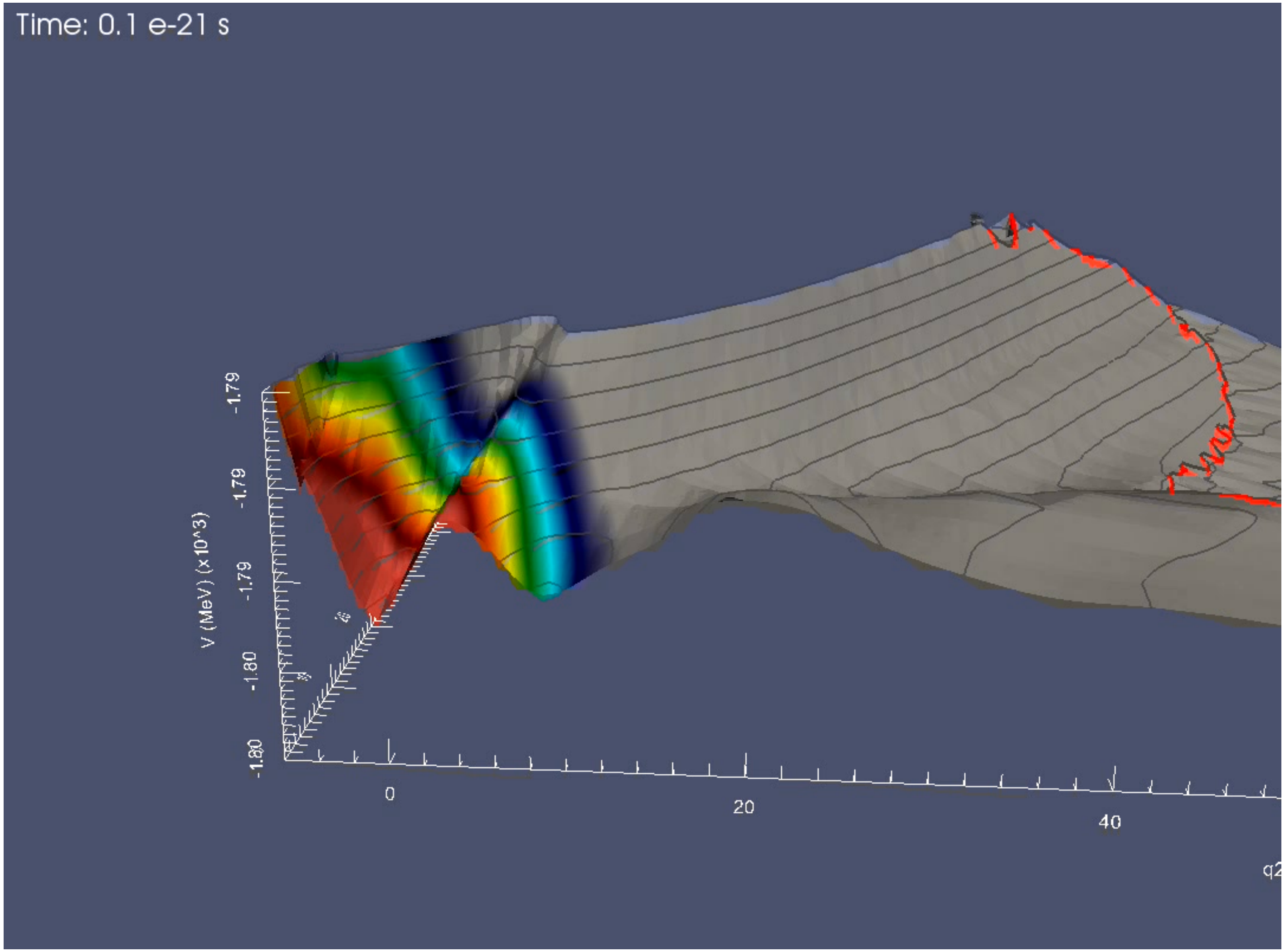
$$i\hbar\frac{\partial}{\partial t}g(\mathbf{q},t) = \left[-\frac{\hbar^2}{2}\sum_{kl}\frac{\partial}{\partial q_k}B_{kl}\frac{\partial}{\partial q_l} + V(\mathbf{q})\right]g(\mathbf{q},t)$$

- Interpretation
  - $g(\mathbf{q},t)$ is probability amplitude to be at point **q** at time t
  - Related probability current
  - Flux of probability current through scission line gives yields

J.-F. Berger, M. Girod, D. Gogny, CPC **63**, 365 (1991); H. Goutte, J.-F. Berger, P. Casoli, D. Gogny, PRC **71** 024316 (2005); D. Regnier, N. Dubray, N. Schunck, and M. Verrière, PRC **93**, 054611 (2016); D. Regnier, M. Verriere, N. Dubray, and N. Schunck, CPC **200**, 350 (2016)

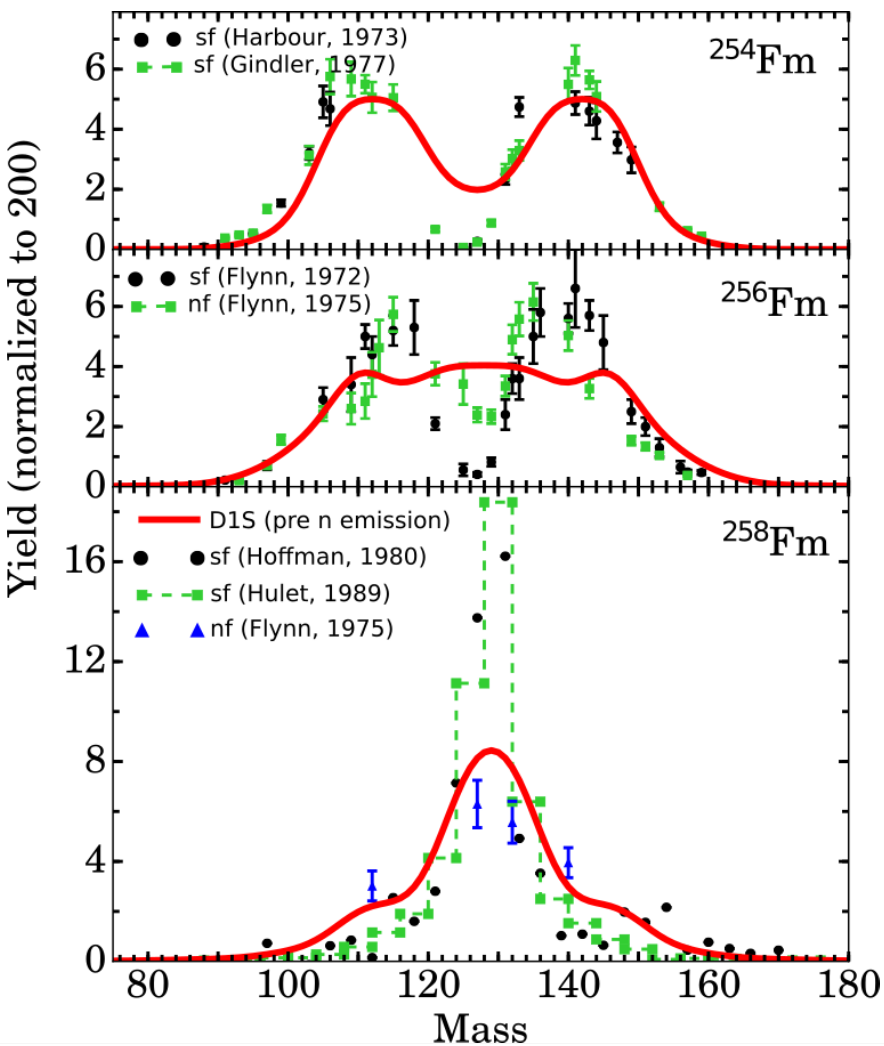
Quantum Dynamics - TDGCM (2/3)

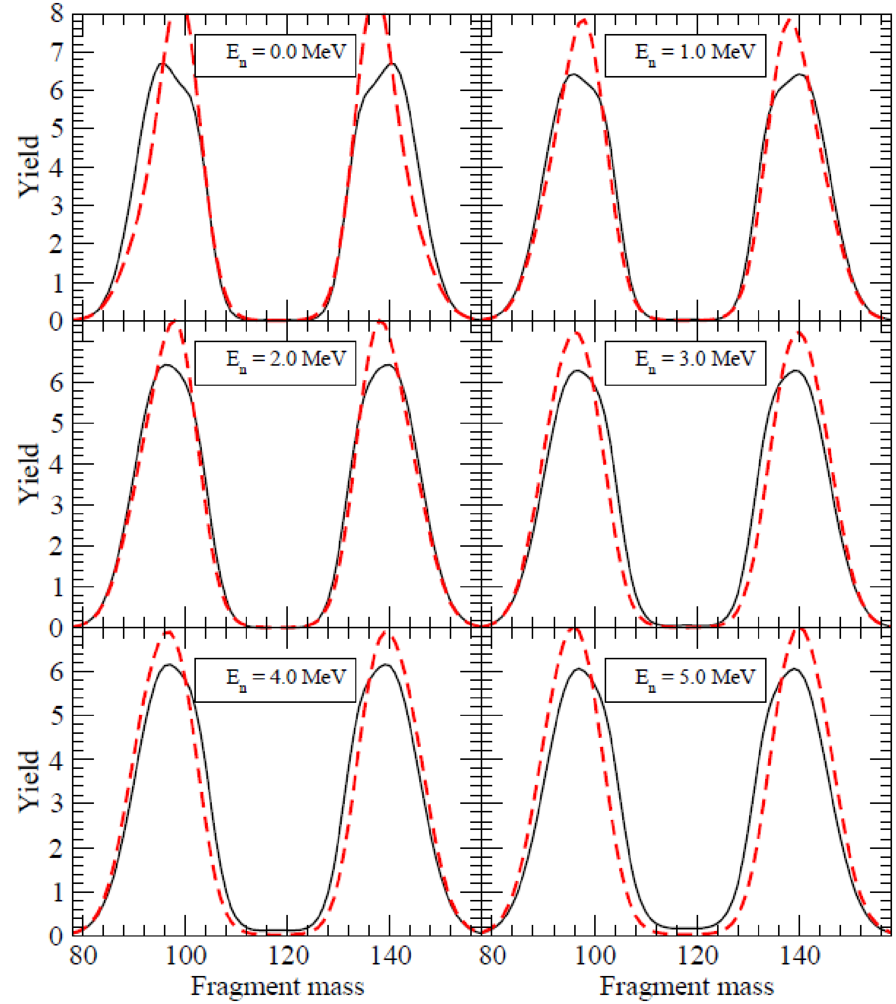
Example: TDGCM Evolution



Quantum Dynamics – TDGCM (3/3)

Examples: Fission Product Yield Calculations





Quantum Dynamics – TDDFT (1/3)

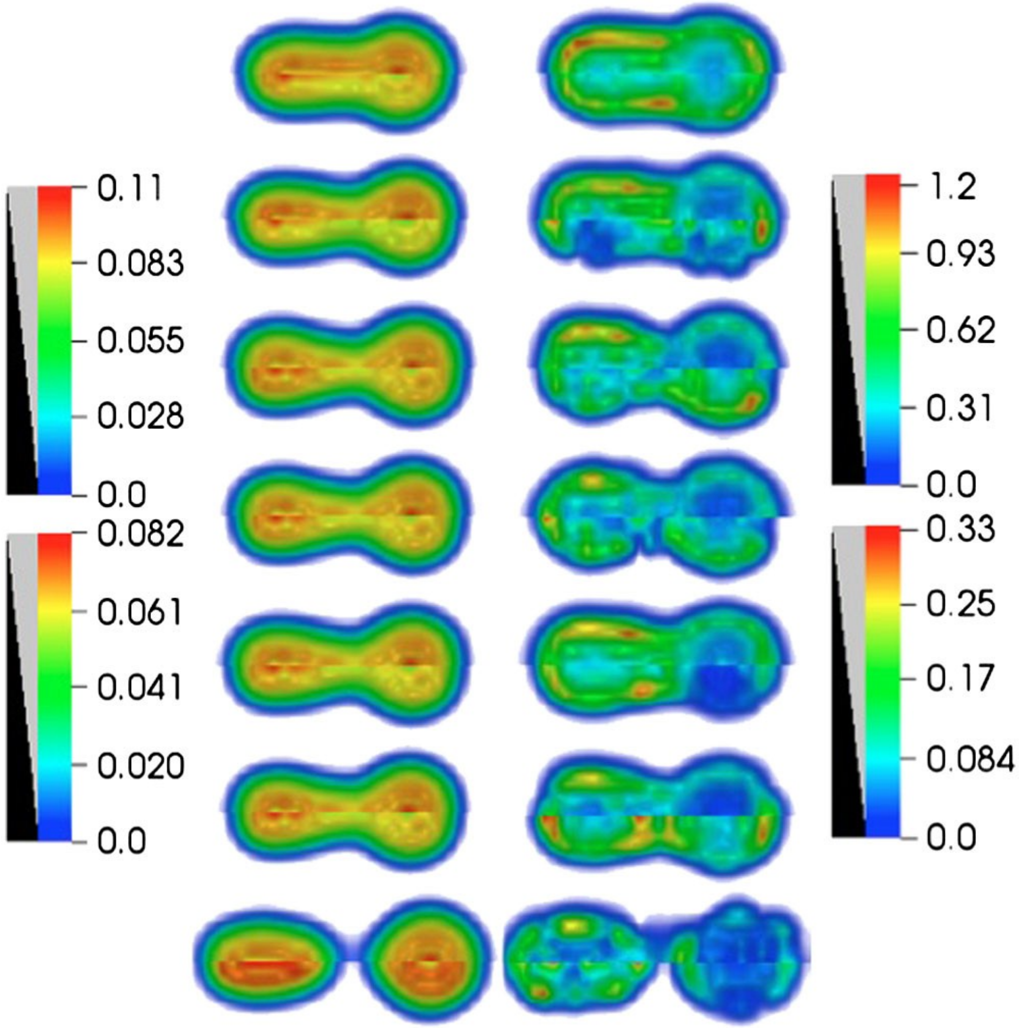
TDDFT simulates a single fission even in real time

- Main limitation of Langevin and TDGCM: adiabaticity is built-in
  - Need to precompute potential energy surfaces (costly)
  - Invoke arbitrary criteria for scission
  - Phenomenological models of dissipation = exchange between intrinsic (=single-particle) and collective degrees of freedom
- Solution: Generalize DFT to time-dependent processes
  - No adiabaticity: excited fragments, dynamical excitations at scission, clear definition of TKE, etc.
  - Enormous computational cost
- Scope
  - Best for fission fragment properties (E*, TKE, angular momentum)
  - Needs extensions for FPY to include dissipation mechanisms

C. Simenel, PRL **105** 192701 (2010); C. Simenel, A. Umar, PRC(R) **89** 031601 (2014); C. Scamps, C. Simenel, D. Lacroix, PRC **92** 011602 (2015); A. Bulgac, P. Magierksi, K. Roche, I. Stetcu, PRL **116** 122504 (2016); Y. Tanimura, D. Lacroix, S. Ayik, PRL **118** 152501 (2017)

Quantum Dynamics – TDDFT (2/3)

Examples



A. Bulgac, P. Magierksi, K. Roche, I. Stetcu, PRL **116** 122504 (2016)

Quantum Dynamics – TDDFT (3/3)

Early results in ^{240}Pu show we can estimate energy sharing

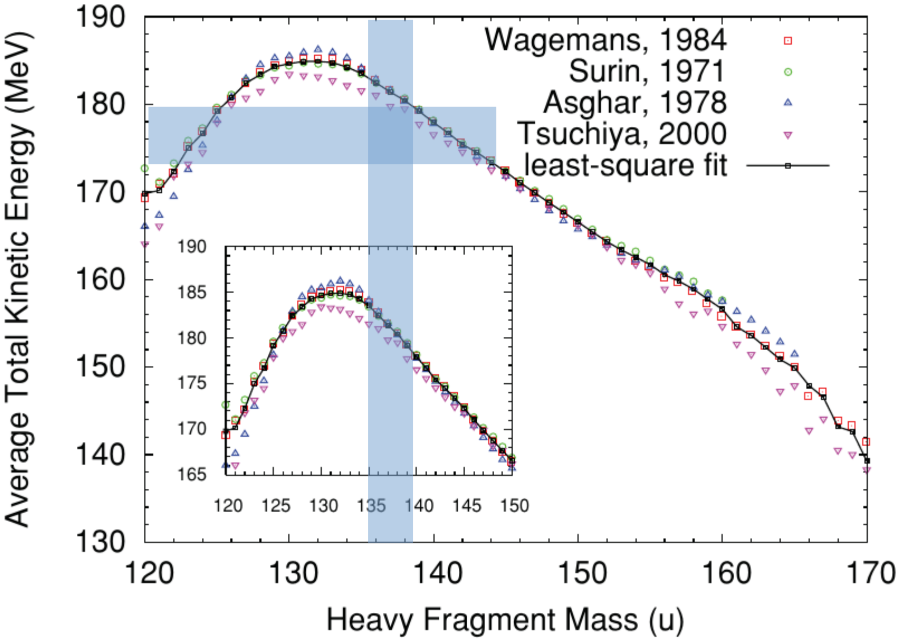
Label	E_{ini}	TKE	N_H	Z_H	N_L	Z_L	E^*_H	E^*_L	TXE	TKE+TXE
SeaLL1-1	-1808.0 ± 2.4	177.8 ± 2.8	83.5 ± 0.4	53.2 ± 0.4	62.8 ± 0.5	41.1 ± 0.4	17.0 ± 2.4	20.1 ± 2.0	37.1 ± 2.7	214.9 ± 2.4
SeaLL1-2	-1813.9 ± 1.1	178.0 ± 2.3	82.9 ± 0.4	52.9 ± 0.2	63.3 ± 0.5	41.5 ± 0.3	19.5 ± 3.8	14.0 ± 1.9	33.5 ± 5.1	211.5 ± 3.3
SkM*-a	-1780.5 ± 2.2	174.5 ± 2.5	84.1 ± 0.9	53.0 ± 0.5	61.8 ± 0.9	40.9 ± 0.5	16.6 ± 3.1	14.9 ± 2.3	31.5 ± 3.8	206.0 ± 2.4
SkM*-s	-1780.2	149.0	73.4	47.2	72.6	46.7	29.4	28.5	57.9	206.9

- Total energy conserved in TDDFT

  ⇒ Total kinetic energy can be computed explicitly

- Total energy of fragment give their excitation energy

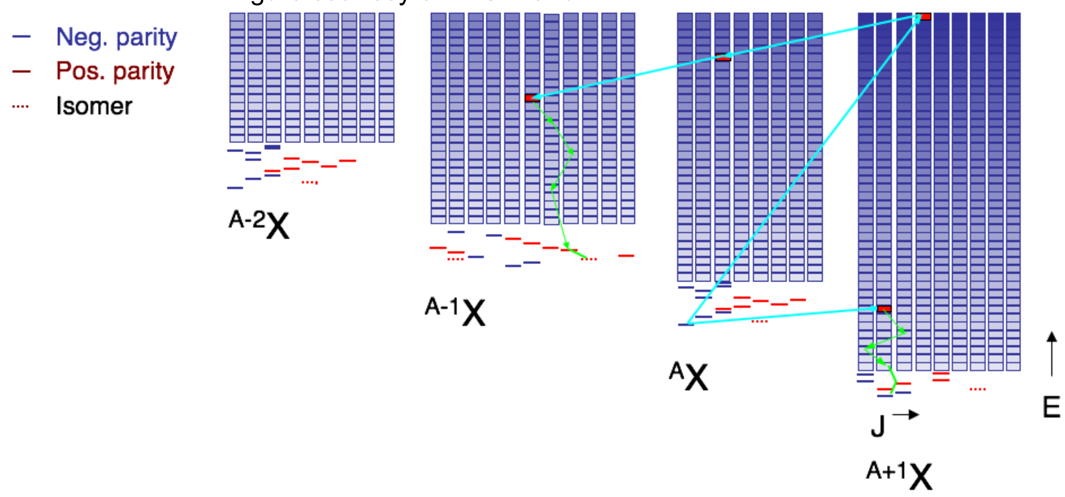
  ⇒ TDDFT gives prescription to determine sharing of excitation energy at scission



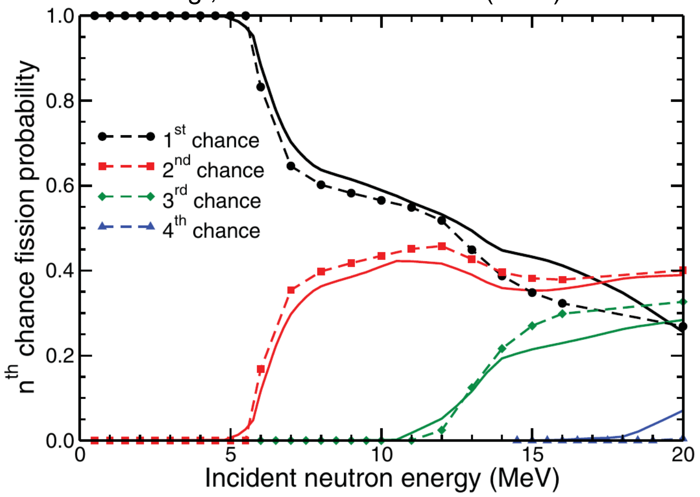
Fission Spectrum

Computing neutrons and gammas from fragment deexcitation

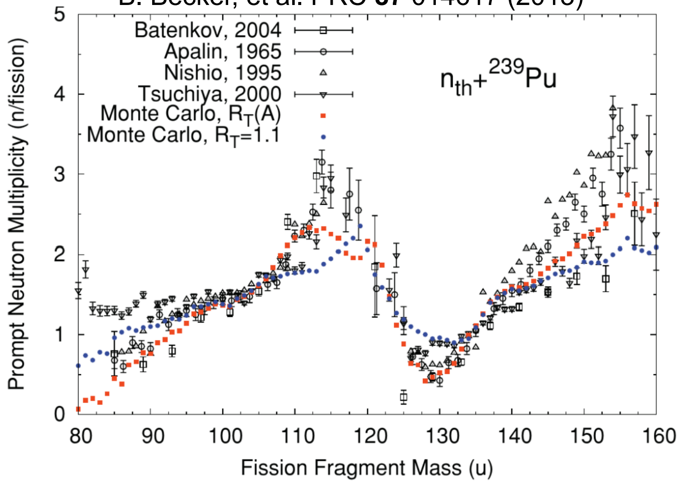
Figure courtesy of E. Ormand



R. Vogt, et al. PRC **85** 024608 (2012)



B. Becker, et al. PRC **87** 014617 (2013)



- Fission spectrum models rely on inputs such as FPY (primary), TKE, excitation energy of fragments, level densities, etc.
- Most codes (CGMF, FREYA) tuned to specific isotopes

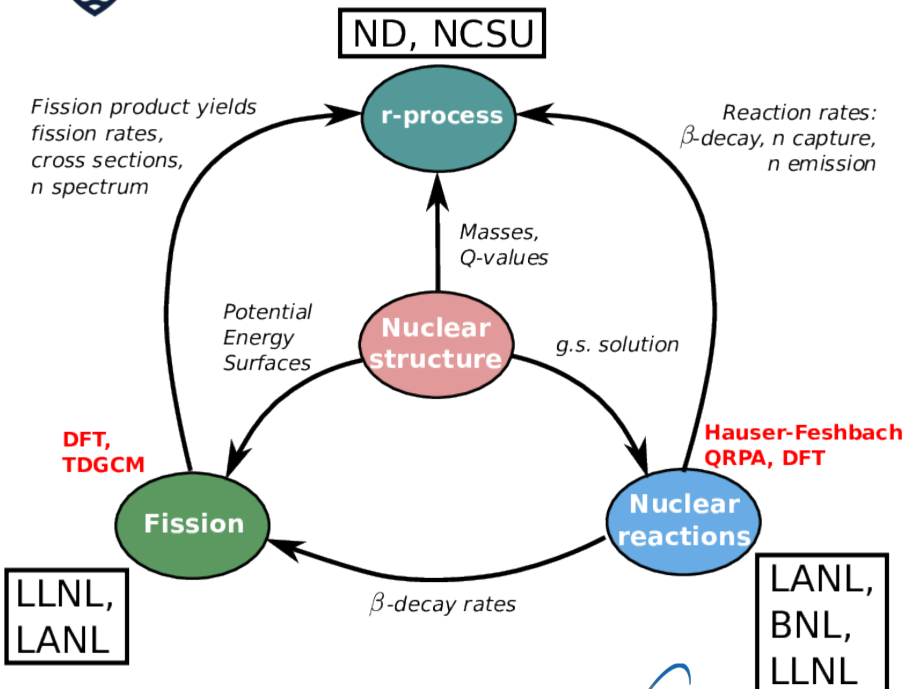
Conclusions

Fission models are predictive but expensive to use

- Two main approaches to compute global nuclear properties
  - Macroscopic-microscopic approaches
  - Nuclear density functional theory
- Realistic simulations of fission dynamics can predict
  - Spontaneous fission half-lives
  - Primary (independent) fission yields
  - Fission spectra
- Three major challenges
  - Interfacing all these models and scale up to mass-table types of calculations
  - Understanding and modeling uncertainties
  - Maintaining and expanding in-house know-how: a workforce issue

The FIRE Topical Collaboration

Bringing together experts in fission theory, nuclear data and nuclear astrophysics



- Project team
  - LLNL: N.Schunck (PI), R. Vogt
  - LANL: T. Kawano, P. Talou, A. Hayes
  - BNL: A. Sonzogni, L. McCutchan
  - Notre Dame: R. Surman
  - North Carolina State: G. McLaughlin
- Additional participants
  - 1 postdoc at LANL
  - 1 postdoc at Notre Dame
  - 1 graduate student at NCSU
  - 1 summer student at LLNL
- Jointly funded by DOE/NP, DOE/USNDP and NA221 (Non-proliferation)