Towards a Langevin Model for the Stochastic Dynamics of Nuclear Fission

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Overview

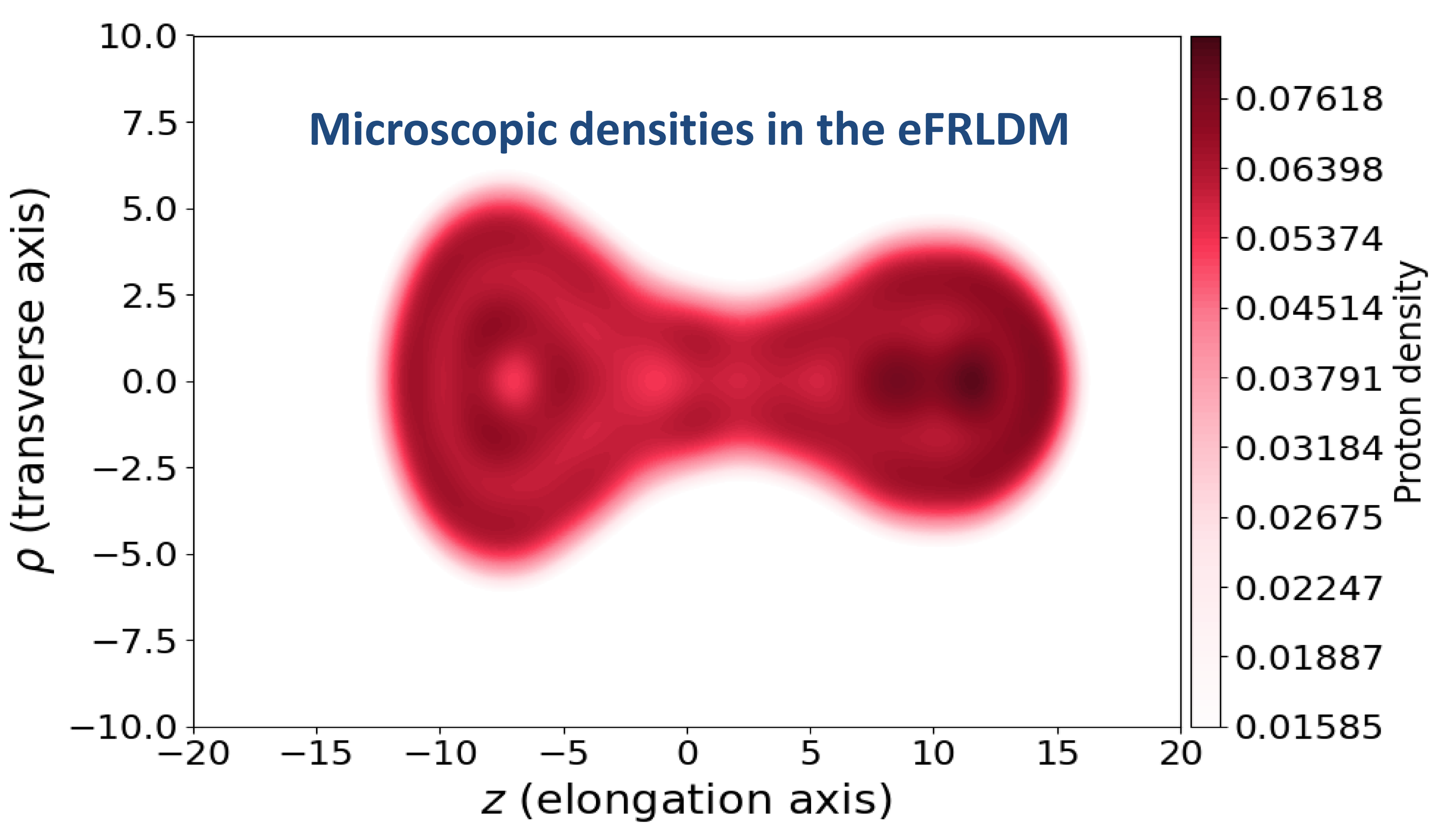
In this ongoing work, we are exploring different approaches to modelling the stochastic process of nuclear fission processes, from an initially excited state to scission and beyond. While the Langevin equations of motion provide, perhaps, the most detailed description of shape evolution dynamics throughout the fission process, different degrees of approximations can be applied that greatly simplify such simulations, thereby offering a solution to difficult numerical errors that otherwise arise in the full Langevin solution.

In the sections below, we outline the computational/theoretical framework from which we compute the quantities needed for the full Langevin solution to this problem (as well as its various approximations), and we present preliminary results that suggest promising improvements in model predictions when more advanced treatments of the stochastic dynamics are considered.

Potential Energy Surface

The nuclear potential energy surface provides the starting point for our fission dynamics simulations by providing important information to calculate the energetics along individual trajectories of a nucleus from initial state to scission.

Here, we employ the enhanced Finite Range Liquid Drop Model (eFRLDM) to evaluate nuclear potential energies over a grid of ~25 million points in a five dimensional space roughly described by neck radius, left/right deformation, quadrupole moment, and mass asymmetry coordinates.



Stochastic Equations of Motion

The equations of motion for a nucleus moving along shape degrees of freedom are closely related to the traditional equations of motion for a classical particle subject to forces, moments of inertia, etc., whether derived from a Newtonian, Hamiltonion, or Lagrangian framework.

Unique considerations to the fission dynamics explored in this work include the inertia and dissipation tensors (relating "velocities" and "accelerations" in generalized coordinates to nuclear and friction forces, respectively), as well as a fluctuation force which provides for the stochasticity inherent to the overall problem.

Simplifications to the fundamental (Langevin) equations of motion result in the Smoluchowski and Brownian shape dynamics equations of motion. Smoluchowski accommodates dissipative effects in the dynamics, while Brownian derives from the potential energy surface alone.

$$\mathbf{q} = (q_1, q_2, \ldots, q_n)$$
$$\dot{\mathbf{q}} = (\dot{q}_1, \dot{q}_2, \ldots, \dot{q}_n)$$

Dissipation Tensor; Nuclear Potential

$$\mathbf{F}_{nuc} = -\nabla_{\mathbf{q}}\, U$$
$$\mathbf{F}_{diss.} = -\mathbf{D}\cdot\dot{\mathbf{q}}$$
$$\mathbf{F}_{fluc.} = \sqrt{\frac{2k_BT}{\Delta t}}\left(\mathbf{D}^{1/2}\cdot\mathbf{R}(t)\right)$$

Nuclear Temperature; Random Normal Distribution

$$\dot{\mathbf{q}} = \mathbf{u}$$
$$\dot{\mathbf{u}} = \mathbf{M}^{-1}\cdot(\mathbf{F}_{nuc.} + \mathbf{F}_{diss.} + \mathbf{F}_{fluc.})$$

Inertia Tensor

$$\mathbf{F}_{nuc.} + \mathbf{F}_{diss.} + \mathbf{F}_{fluc.} := 0$$

$$\mathbf{D}\cdot\dot{\mathbf{q}} = \sqrt{\frac{2k_BT}{\Delta t}}\left(\mathbf{D}^{-1/2}\cdot\mathbf{R}(t)\right) - \nabla_{\mathbf{q}}\, U$$
$$\dot{\mathbf{q}} = \sqrt{\frac{2k_BT}{\Delta t}}\left(\mathbf{D}^{-1/2}\cdot\mathbf{R}(t)\right) - \mathbf{D}^{-1}\cdot\nabla_{\mathbf{q}}\, U$$

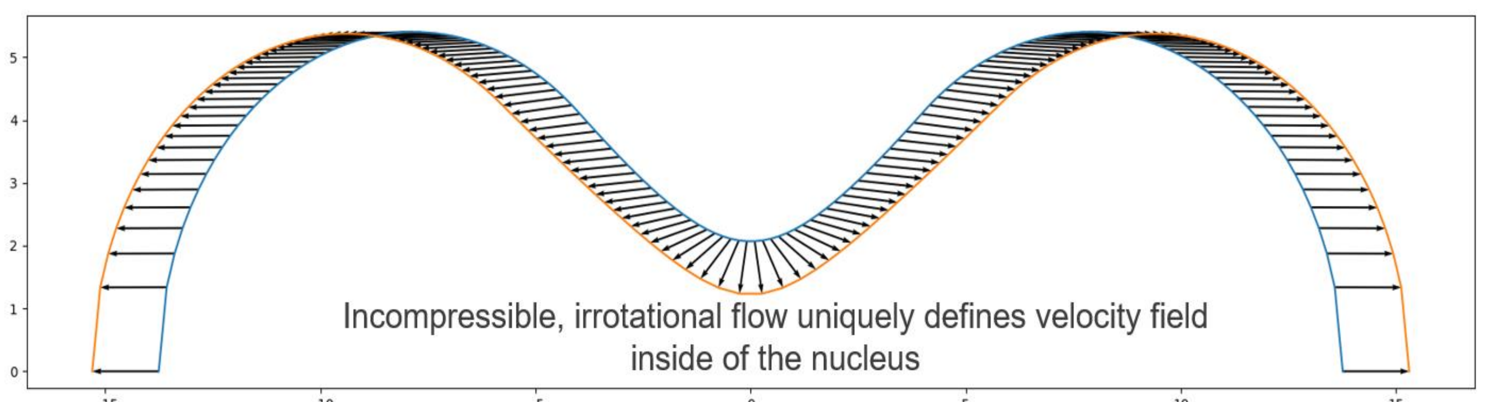
Smoluchowski

Brownian

$$\mathcal{P}(\mathbf{q}_i \to \mathbf{q}_{i+1}) = \exp\left(\frac{U(\mathbf{q}_i) - U(\mathbf{q}_{i+1})}{k_BT}\right)$$

Transport Tensors

From the changing shape of the nuclear surface, one may immediately derive the velocity field everywhere on the interior of the nucleus by assuming incompressible and irrotational flow and, in turn, solving a Laplace equation.



Once the velocity on the surface (and, in turn, the interior) of the nucleus is known, it is possible to solve for kinetic energy and dissipated energy for arbitrary velocities in the generalized coordinates. Projecting these functions onto quadratic forms immediately produces the inertia and friction tensors, respectively, as needed for Langevin and/or Smoluchowski simulations of fission.

$$T = \frac{1}{2}\rho\int_{\Omega}\mathbf{v}(\mathbf{x})\cdot\mathbf{v}(\mathbf{x})\; d\mathbf{x}$$

$$\mathbf{v}(\mathbf{x}) = -\nabla\;\phi(\mathbf{x})$$
$$\Delta\phi = 0$$
$$T = \frac{1}{2}\rho\int_{\partial\Omega}-\phi\;\mathbf{v}\cdot d\mathbf{A}$$

$$T(\dot{\mathbf{q}}) = \frac{1}{2}\sum_{i,j}\dot{q}_i M_{i,j}\dot{q}_j$$
$$M_{i,i} = 2\cdot T(\dot{\mathbf{q}} = \dot{q}_i)/\dot{q}_i^2$$
$$M_{i,j\neq i} = \left\{2\cdot T(\dot{\mathbf{q}} = (\dot{q}_i, \dot{q}_j)) - M_{i,i}\dot{q}_i^2 - M_{j,j}\dot{q}_j^2\right\}/\left(2\cdot\dot{q}_i\dot{q}_j\right)$$

Inertia Tensor

Friction Tensor

$$W_{diss.} := \frac{dE_{diss.}}{dt} \propto \int_{\partial\Omega} v_{normal}^2\; dA$$

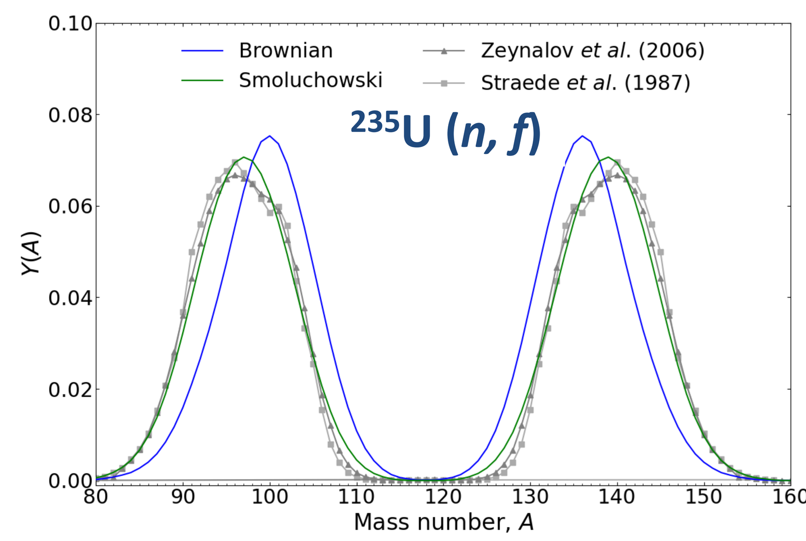
$$W_{diss.}(\dot{\mathbf{q}}) = \frac{1}{2}\sum_{i,j}\dot{q}_i D_{i,j}\dot{q}_j$$
$$D_{i,i} = 2\cdot W_{diss.}(\dot{\mathbf{q}} = \dot{q}_i)/\dot{q}_i^2$$
$$D_{i,j\neq i} = \left\{2\cdot W_{diss.}(\dot{\mathbf{q}} = (\dot{q}_i, \dot{q}_j)) - D_{i,i}\dot{q}_i^2 - D_{j,j}\dot{q}_j^2\right\}/\left(2\cdot\dot{q}_i\dot{q}_j\right)$$

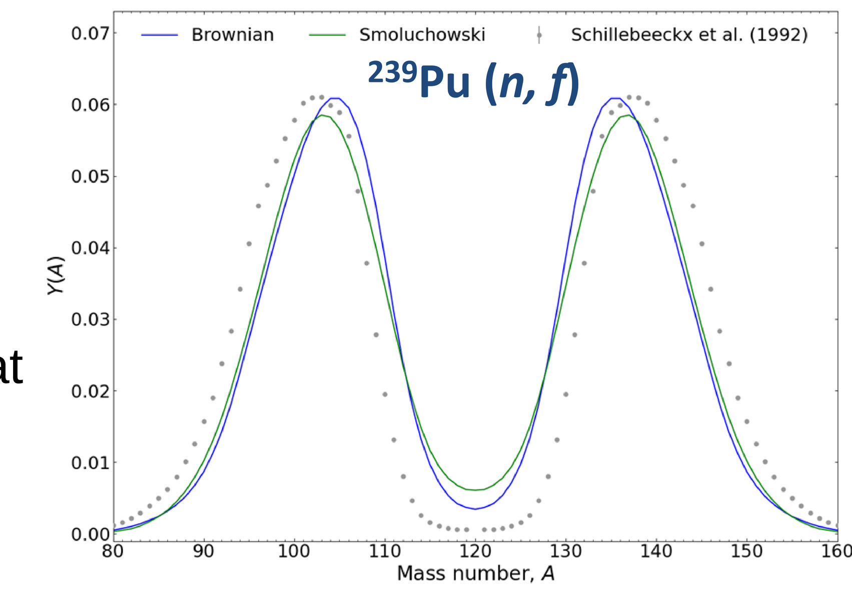
Results

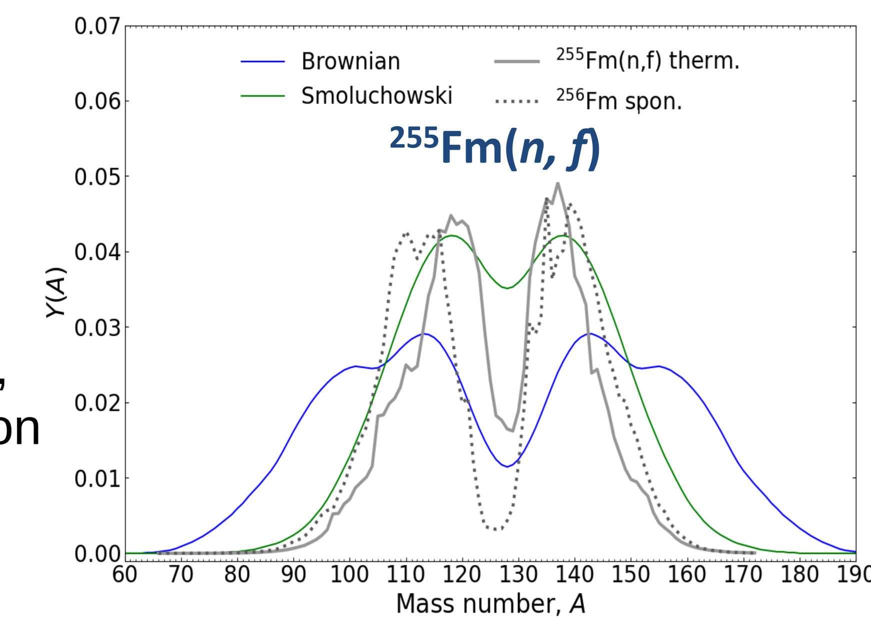
We currently have the capacity to calculate potential energies and transport coefficients, as well as solve the stochastic equations of motion at varying levels of approximation, within a single theoretical/computational framework.

For preliminary calculations carried out for select nuclei, the introduction of Smoluchowski dynamics (relative to Brownian) predicts isotopic fission yields that are more consistent with experiment, especially with regards to peak shape, height, and location.

Early calculations based on a Langevin treatment (not plotted) produce fission yields nearly indistinguishable from our Smoluchowski results. However, higher-order numerical integration may be especially critical for the Langevin case, which we are currently investigating.







This work was supported by the US Department of Energy through the Los Alamos National Laboratory (LANL). LANL is operated by Triad National Security, LLC, for the National Nuclear Security Administration of US Department of Energy (Contract No. 89233218CNA000001). T.M.S. and M.R.M were partly supported by the Fission In R-process Elements (FIRE) topical collaboration of the US Department of Energy. T.M.S, M.R.M., and I.S. were further supported by the LANL Laboratory Directed Research and Development Exploratory Research Project titled "Low-energy fission dynamics" (Project No. LDRD-20200384ER).