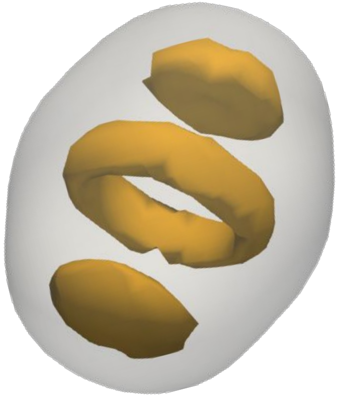
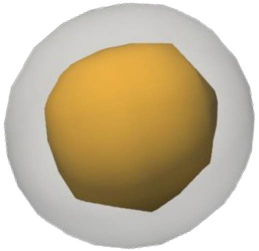
Uncertainty quantification for low-energy heavy-ion reactions

Kyle Godbey





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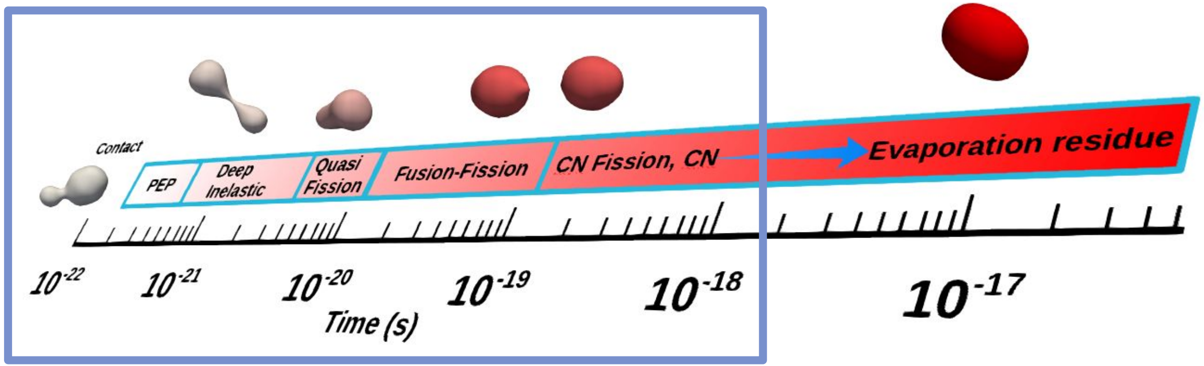
Our lens? Real-Time Dynamics

Time-dependent, microscopic theories offer a rich depiction of the many complicated things nuclei might do during a reaction

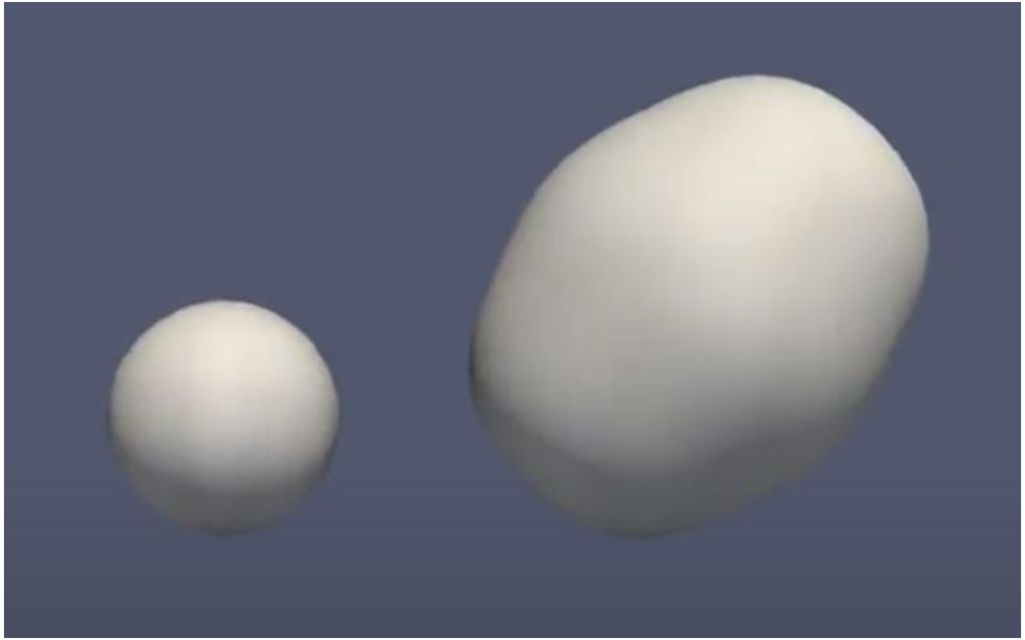


The framework: Density Functional Theory

'Microscopic' method optimized for description of one-body observables

Fantastically extensible framework to go beyond base assumptions

Features of DFT: Structure



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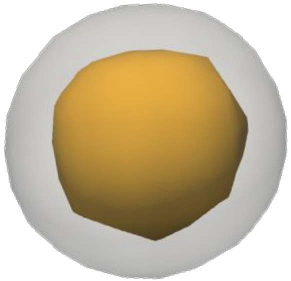
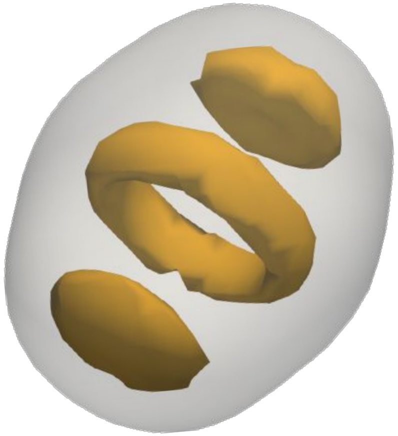
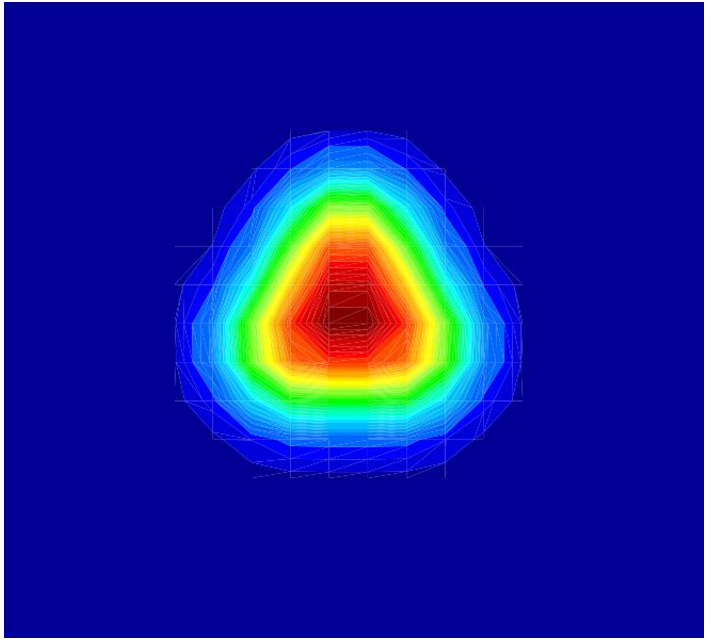
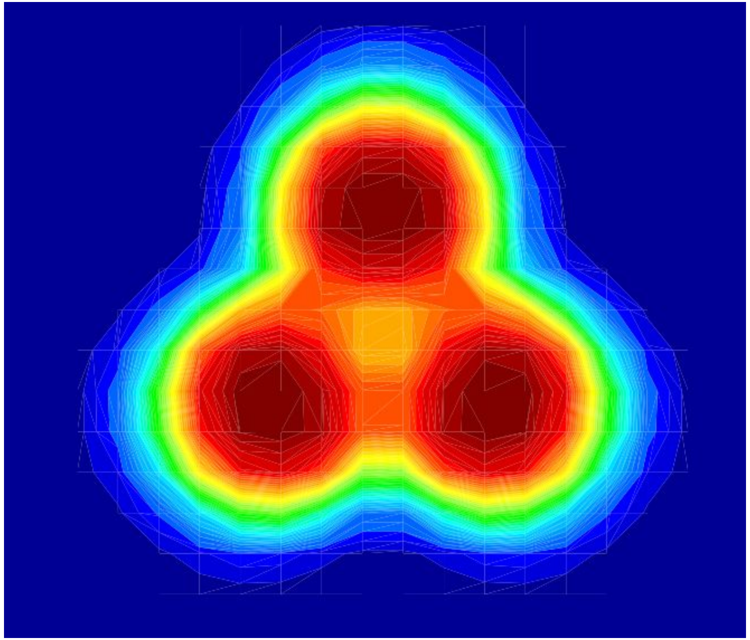




Features of DFT: Structure

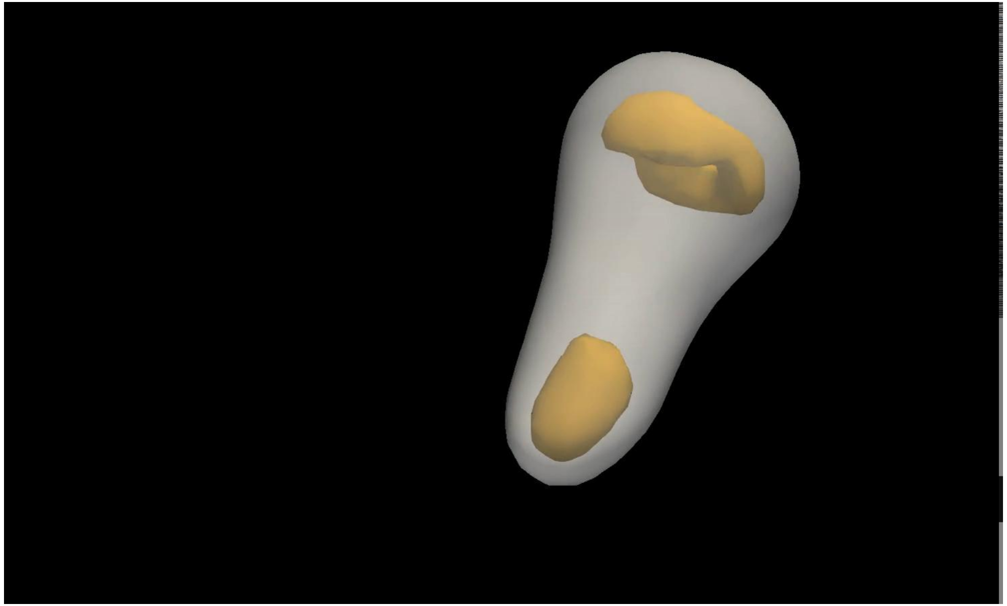


Density, $\varrho(r)$

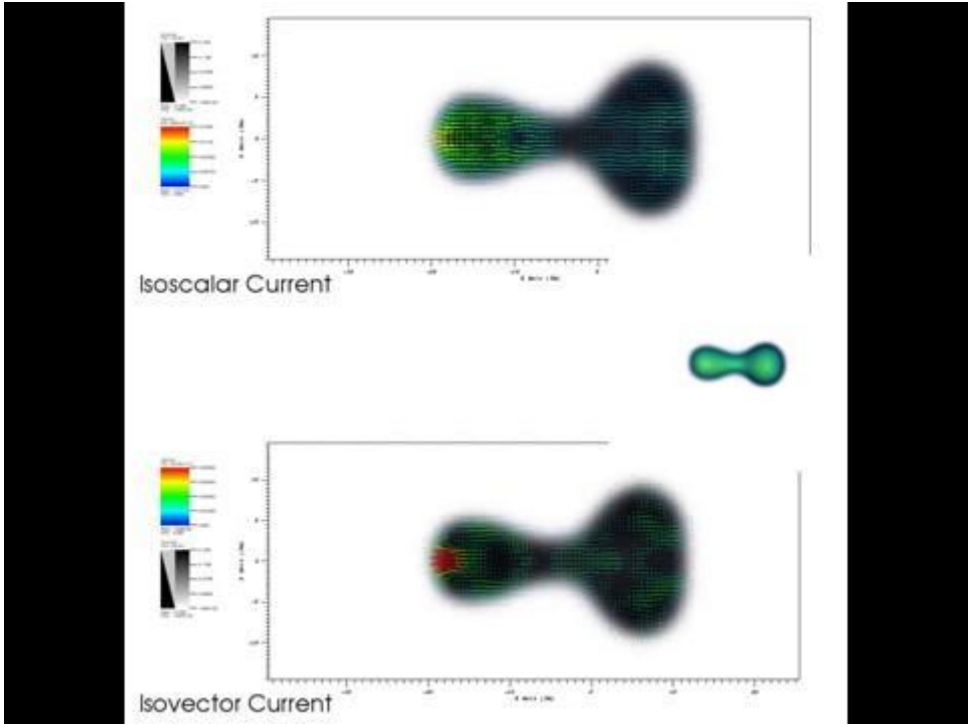


Nucleon localization function

Features of DFT: Dynamics



Features of DFT: Dynamics



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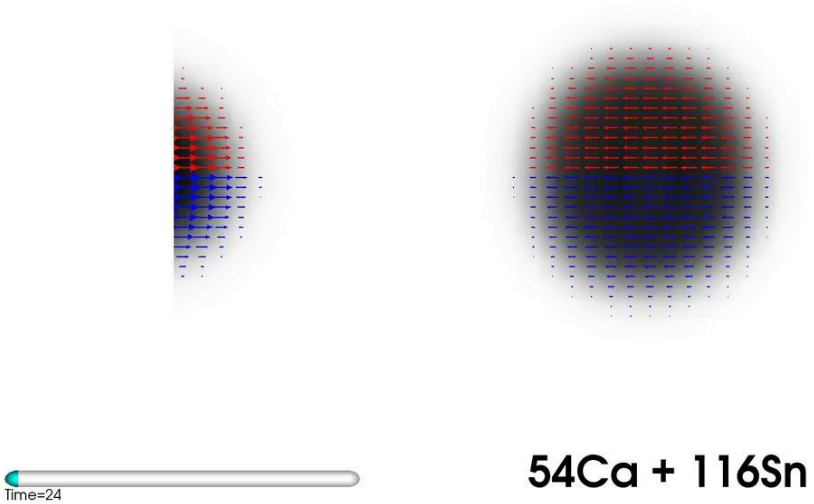
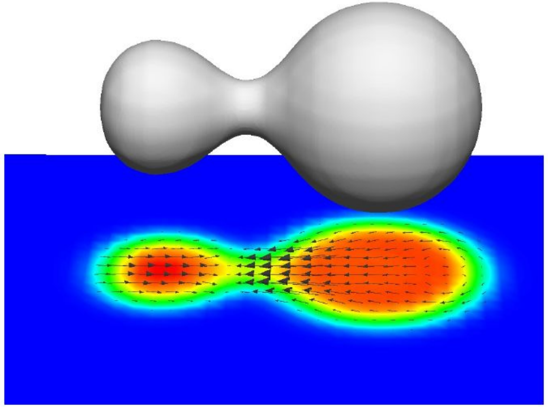


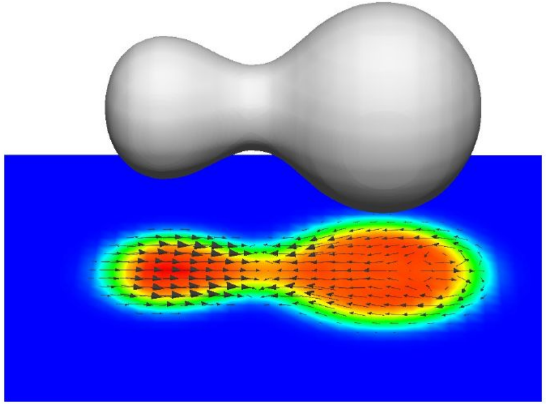
Features of DFT: Dynamics

40Ca + 132Sn



transfer

48Ca + 132Sn



No net transfer

What Drives the Dynamics (and Structure)?

The energy density functional! A functional of various densities and currents that defines the system

e.g.

$$\mathscr{H}_{\mathrm{I}}(\mathbf{r}) = C_{\mathrm{I}}^{\rho}\rho_{\mathrm{I}}^{2} + C_{\mathrm{I}}^{s}\mathbf{s}_{\mathrm{I}}^{2} + C_{\mathrm{I}}^{\Delta\rho}\rho_{\mathrm{I}}\Delta\rho_{\mathrm{I}} + C_{\mathrm{I}}^{\Delta s}\mathbf{s}_{\mathrm{I}}\cdot\Delta\mathbf{s}_{\mathrm{I}} + C_{\mathrm{I}}^{\tau}\left(\rho_{\mathrm{I}}\tau_{\mathrm{I}} - \mathbf{j}_{\mathrm{I}}^{2}\right) + C_{\mathrm{I}}^{T}\left(\mathbf{s}_{\mathrm{I}}\cdot\mathbf{T}_{\mathrm{I}} - \overleftrightarrow{J}_{\mathrm{I}}^{2}\right) + C_{\mathrm{I}}^{\nabla J}\left(\rho_{\mathrm{I}}\nabla\cdot\mathbf{J}_{\mathrm{I}} + \mathbf{s}_{\mathrm{I}}\cdot(\nabla\times\mathbf{j}_{\mathrm{I}})\right)$$

Parameter Determination

One method is, given an EDF, fit the constants to some experimental data

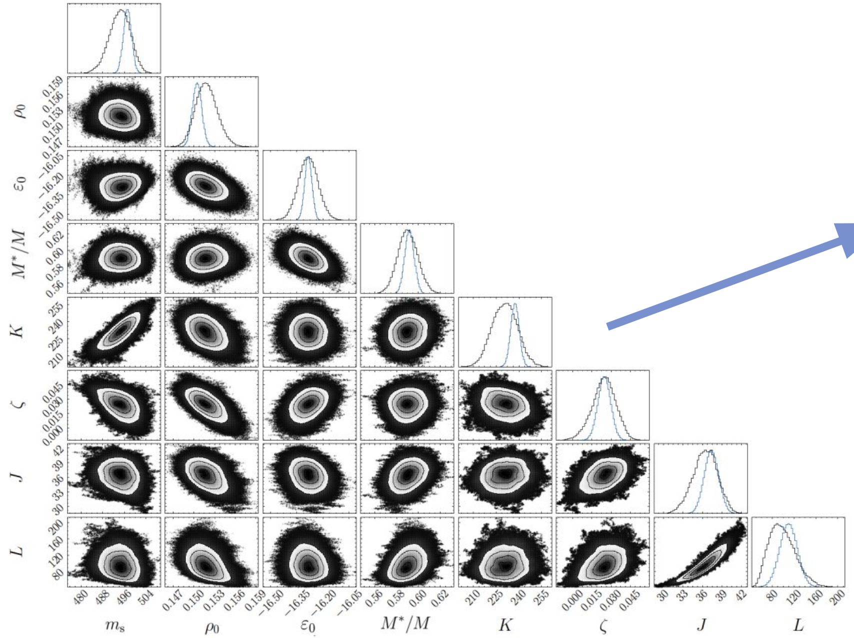
The result? Many, many, many ‘forces’ for a given functional. Some fave Skyrme-types include SkM*, SLy4d, SLy5t, SV-Min, UNEDF1, etc.

Parameter Determination

But.. nobody is perfect, sorry SLy4d. Given a certain set of data there is some uncertainty on what the optimal parameters are

So why do we even need optimal parameters? Instead we can define our physical model as a distribution of reasonable parameters

“Doing UQ”



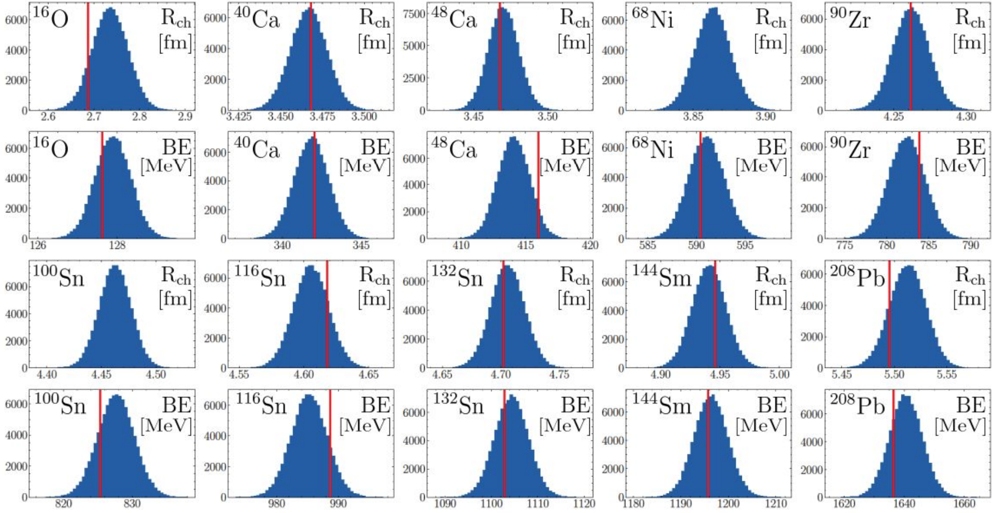
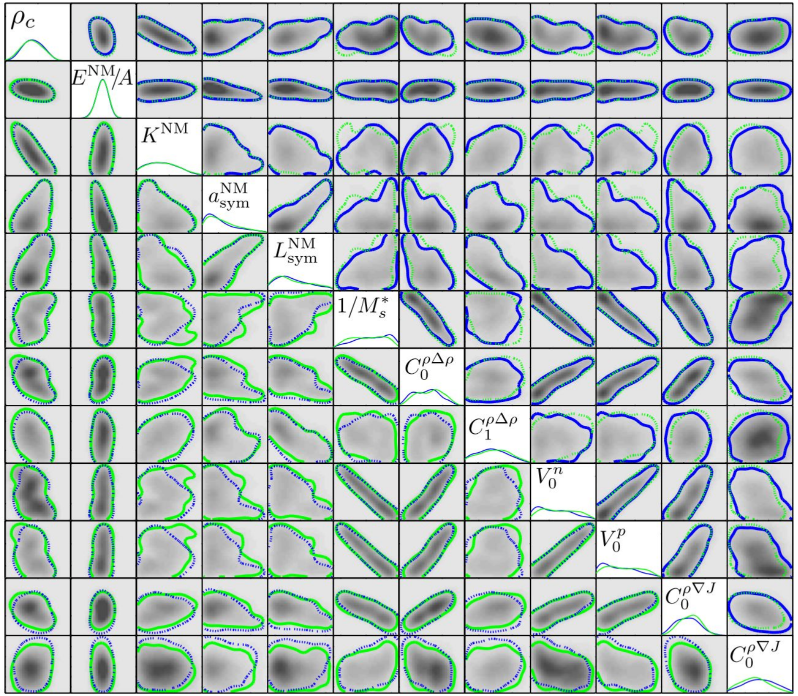


Image Credit:
P Giuliani, **K Godbey,** E Bonilla, F Viens, J Piekarewicz, Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method

“Doing UQ”



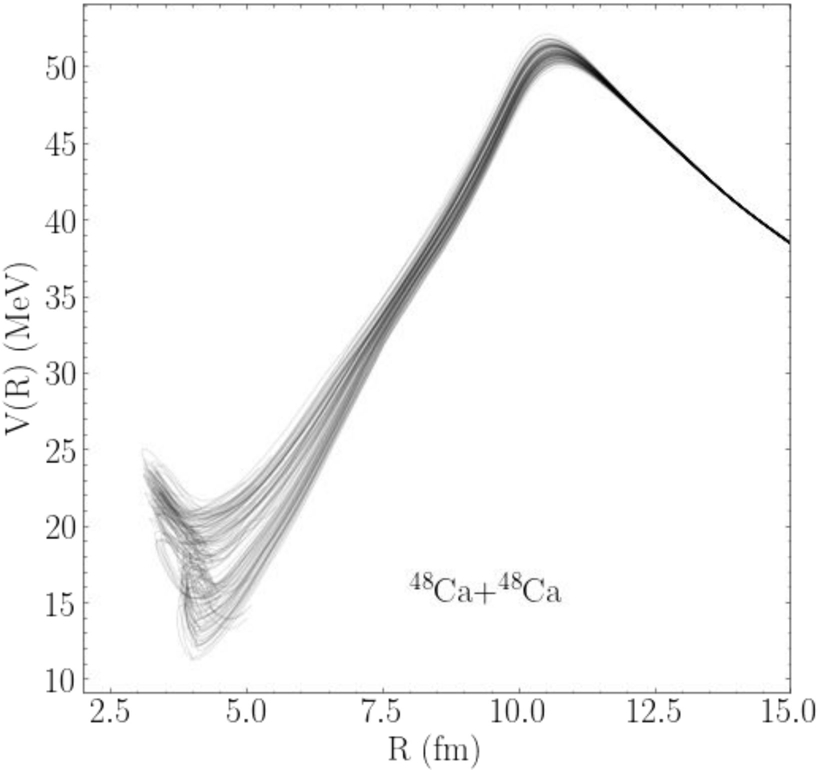
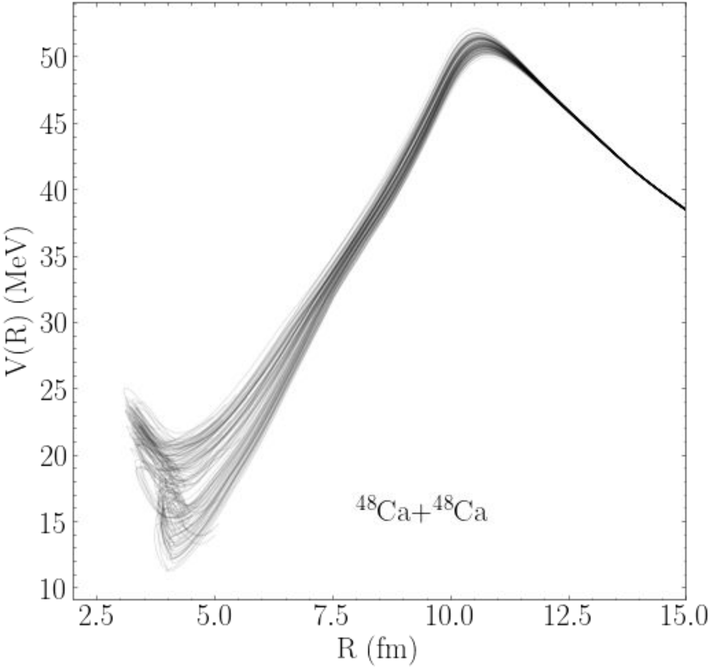
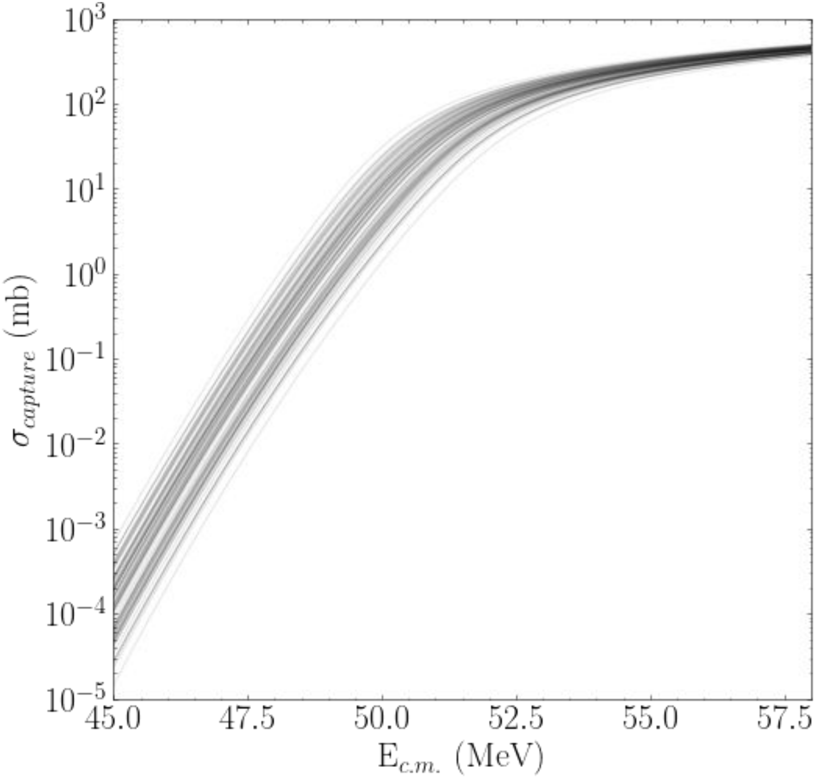


Image Credit:
J. D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz, Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements, Phys. Rev. Lett.114, 122501 (2015).

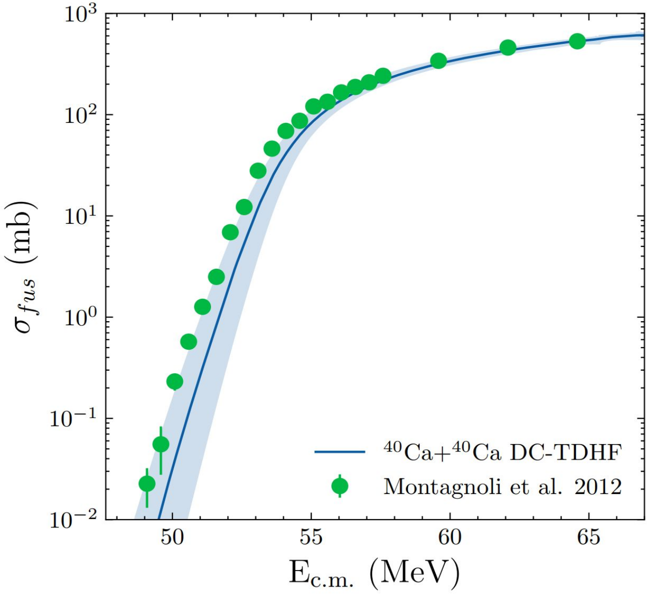
“Doing UQ”





“Doing UQ”

$^{40}Ca + ^{40}Ca$



$^{48}Ca + ^{48}Ca$

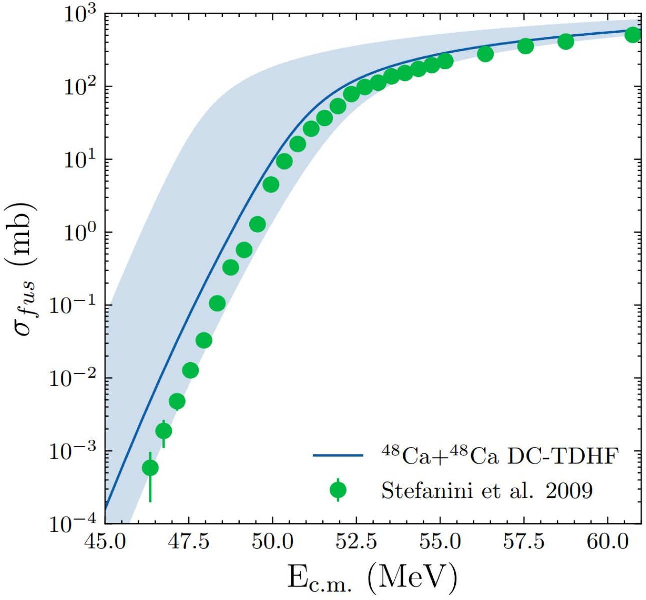


Image Credit:
K. Godbey, A. S. Umar, and C. Simenel, Uncertainty quantification in microscopic heavy-ion fusion simulations Phys. Rev. C 106, L051602 (2022) (Editors Suggestion),

Extracting Barrier Height

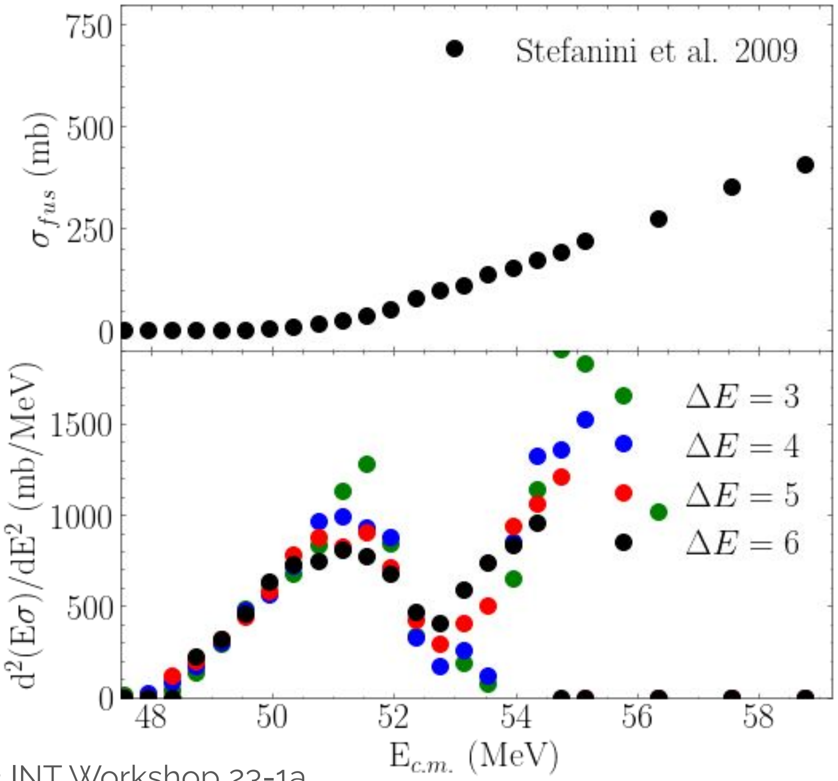
To get the barrier height from experimental data without any model dependence, we should deal only with the data

To this end, let's consider the experimental barrier distribution:

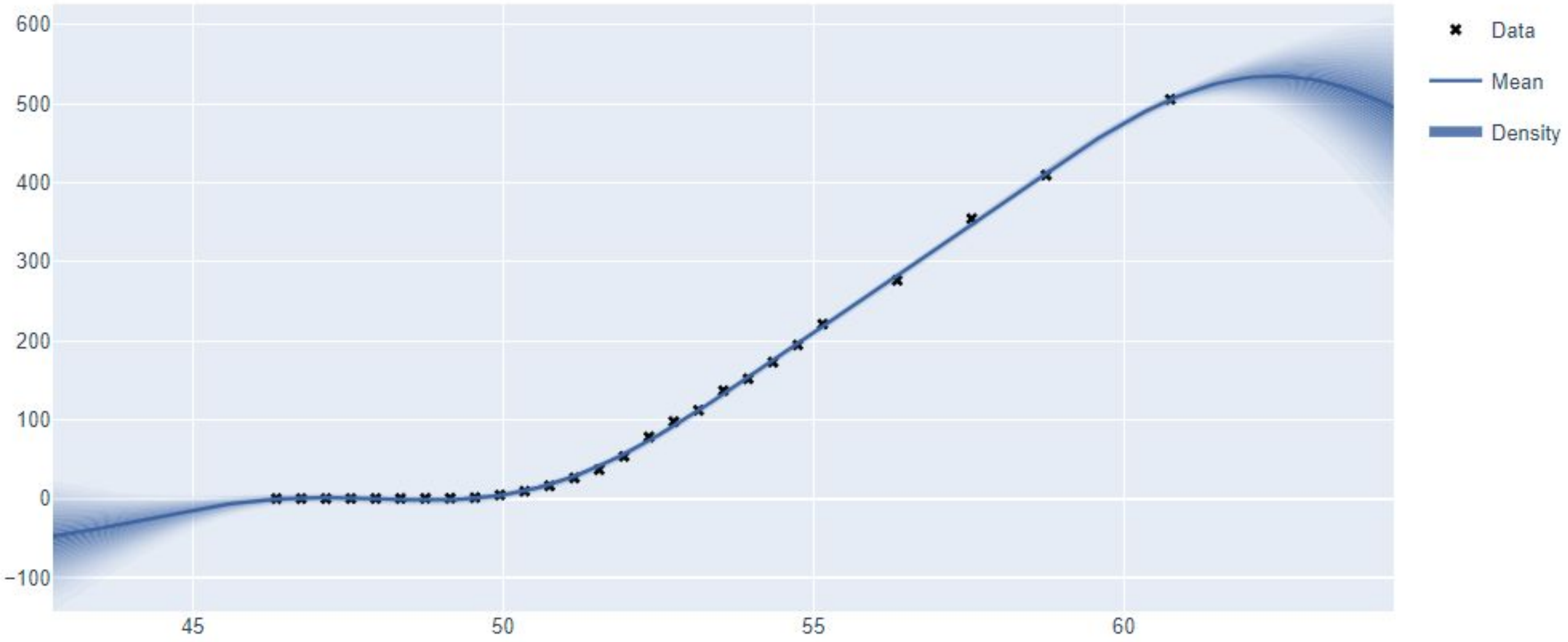
$$D_{\exp}(E) = \frac{d^2(E\sigma)}{dE^2}$$

M. Dasgupta, D. J. Hinde, N. Rowley, A. M. Stefanini, "MEASURING BARRIERS TO FUSION", Annual Review of Nuclear and Particle Science, Vol. 48:401-461 (1998)

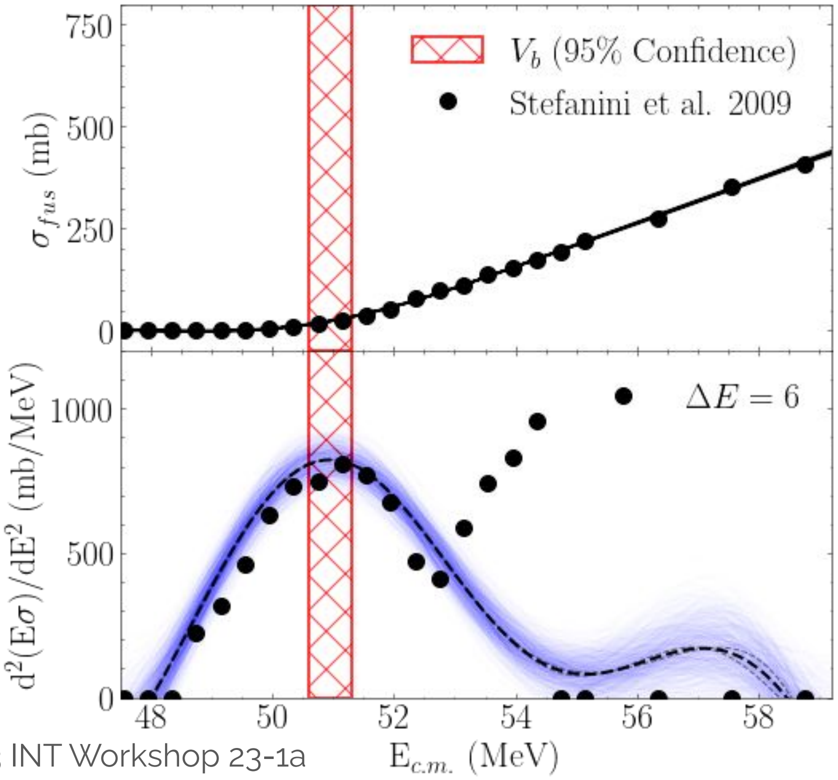
Extracting Barrier Height



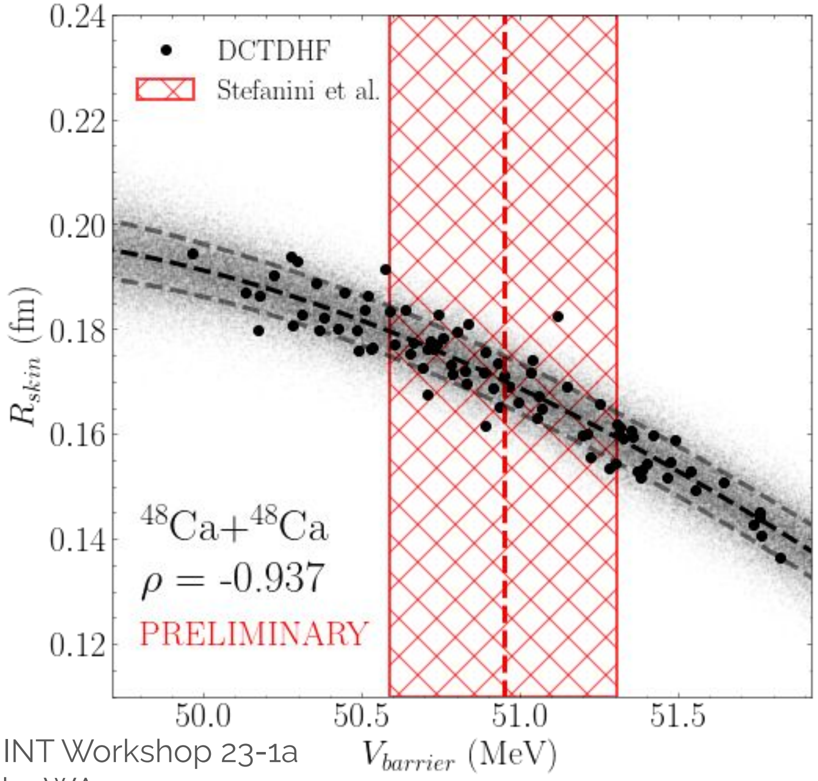
Extracting Barrier Height



Extracting Barrier Height



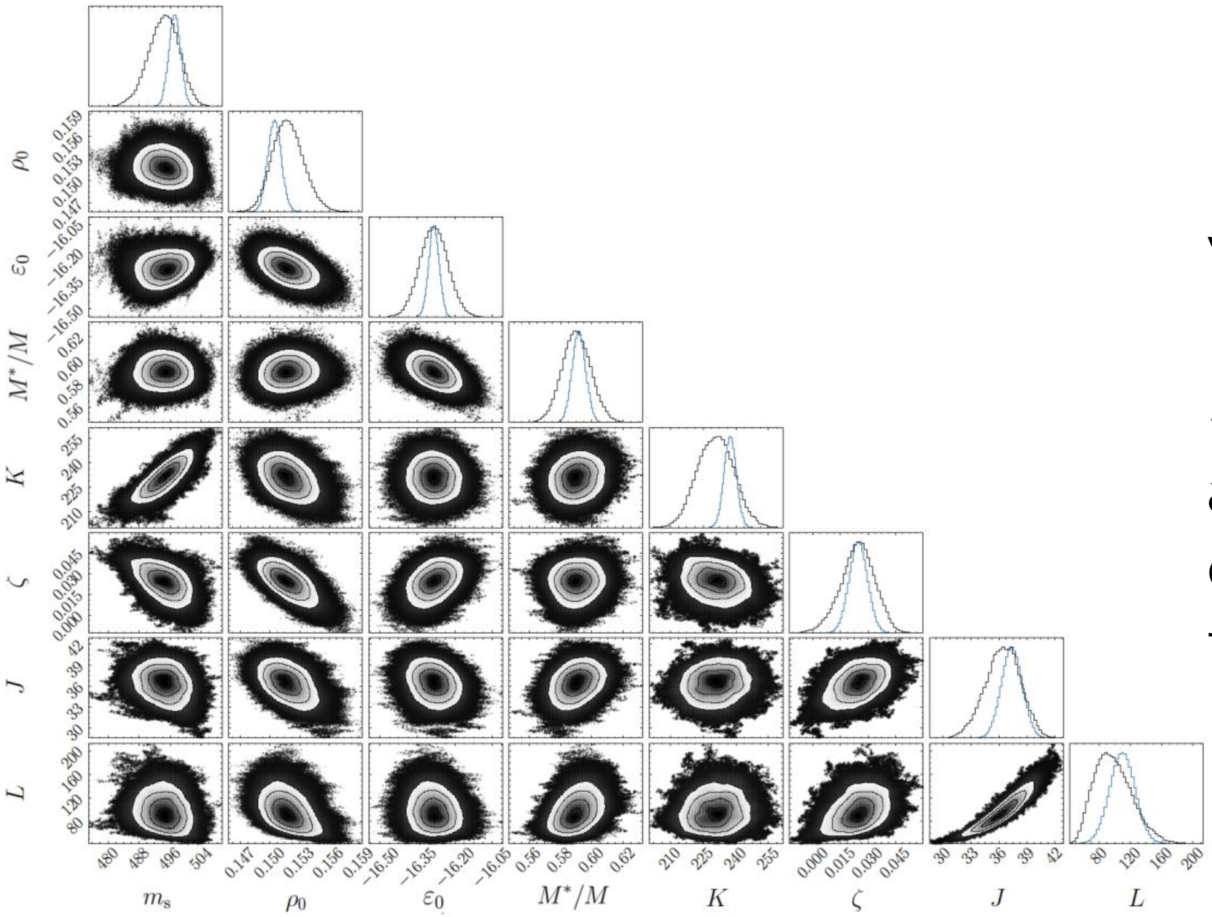
Checking Skin vs. Barrier Correlations



What Next?

A strong correlation is a strong indicator of opportunity, and this is just one system

Constraints are great, but including fusion cross sections from TDDFT in a direct Bayesian calibration is unlikely without advances in emulation



What about RBMs?

~5,000,000 samples in about a day on commodity hardware for covariant DFT

Image Credit:
P Giuliani, **K Godbey,** E Bonilla, F Viens, J Piekarewicz, Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method

Challenges

Robust calibration requires great emulators, but we're behind on time-dependent emulation

RBMs have proven great for DFT and scattering, but generally perform worse for time evolution

Thus current direction is on data-driven approaches like neural implicit flow or Fourier neural operator

Challenges

Even with powerful emulation, direct Bayes may still be out of reach

Techniques such as the polynomial chaos expansion (like an RBM for your random distribution) might be crucial to lower the total number of samples required

Conclusions

Linking structure to reactions must consider the uncertainties lurking at every step, no matter the energy scale

Nuclear structure often contains lots of intricacies and possible refinements. Each of these intricacies are affected by the model uncertainties that generated them

Immense Gratitude to All Collaborators!

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Computing Resources

Australian National Computational Infrastructure Raijin and Gadi
Oak Ridge Leadership Computing Facility Summit
Argonne Leadership Computing Facility Polaris
Texas A&M High Performance Research Computing Terra and Ada
Michigan State University HPCC