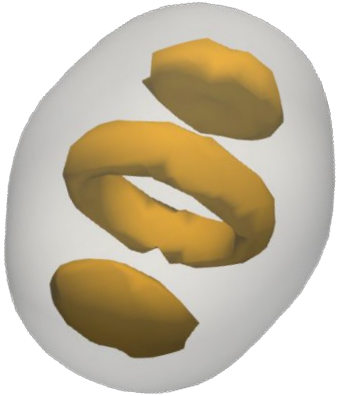
Motivations and Opportunities In Heavy-Ion Dynamics

Kyle Godbey



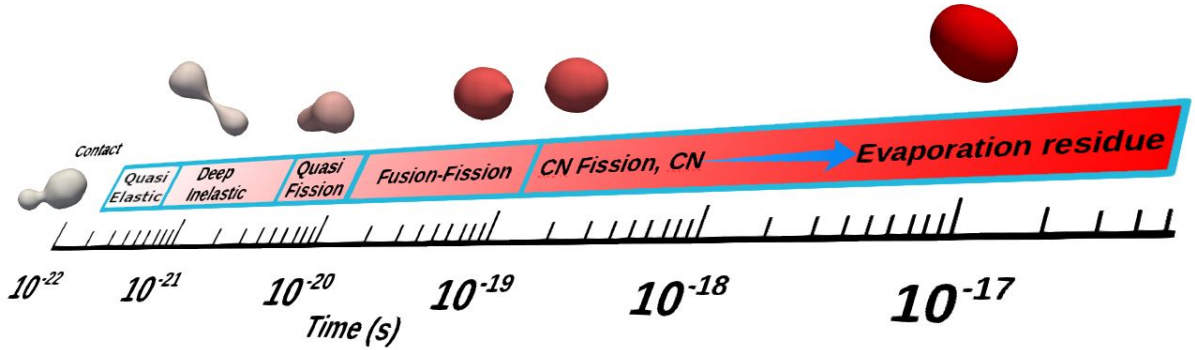
Slides with videos:
https://docs.google.com/presentation/d/1wl6KKh4Kp76M8PZOxWX61ZpD9NAhcc_PYovyz8Kj5Ig/edit?usp=sharing



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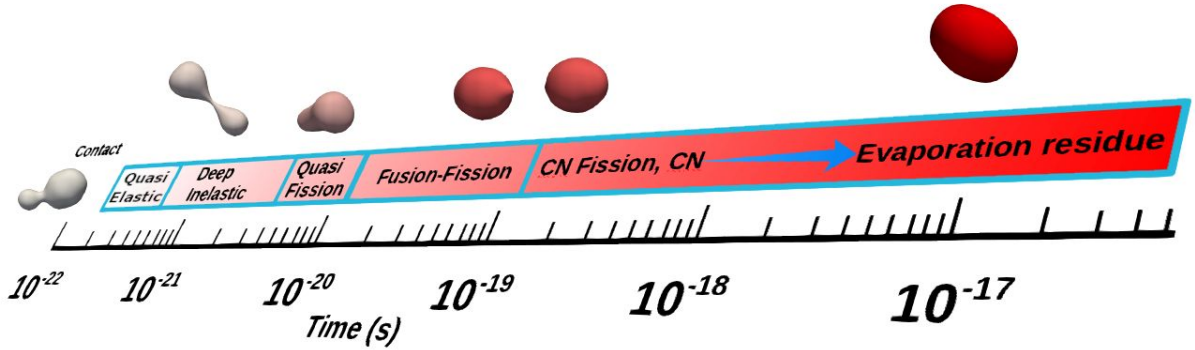


Heavy-Ion Dynamics

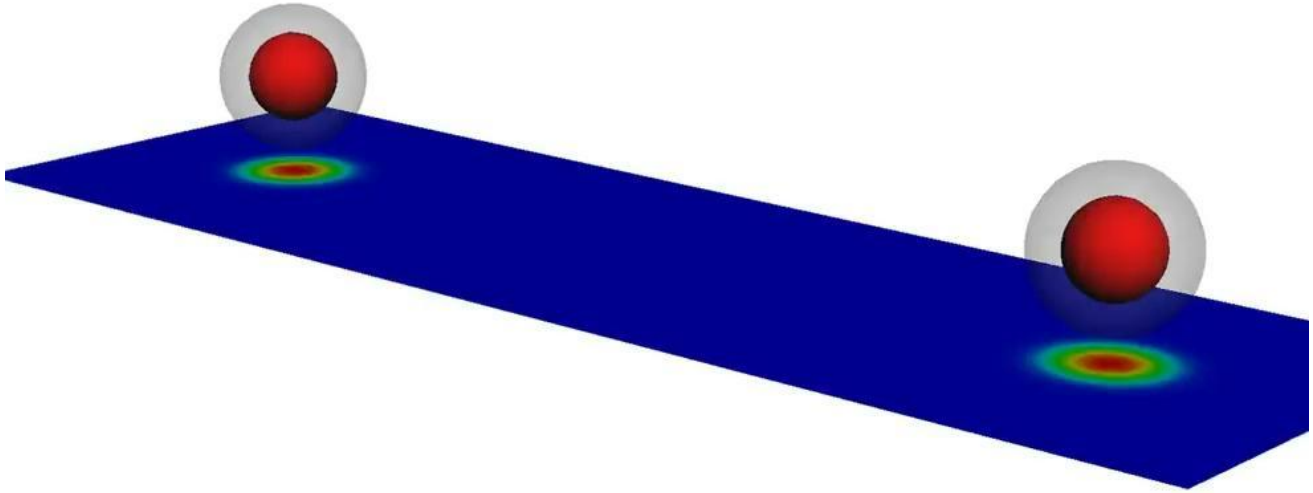


The US is well positioned to lead this area through the capabilities provided by ARUNA, ATLAS, and FRIB

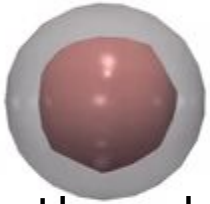
Real-Time Dynamics



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



K. Godbey, C Simenel, and A. S. Umar, Absence of hindrance in microscopic 12C + 12C fusion study, Phys. Rev. C 100, 024619 (2019)





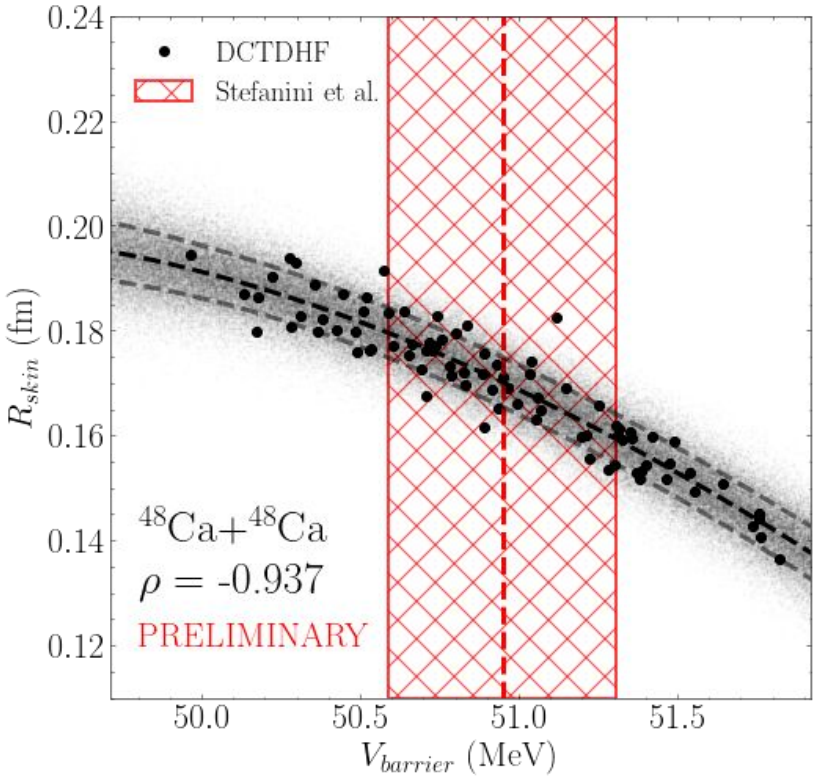
Nuclei are more than blobs!

-> Neutron skins
-> Intrinsic deformations
-> Clustering effects

Correlations Between Structure and Reactions

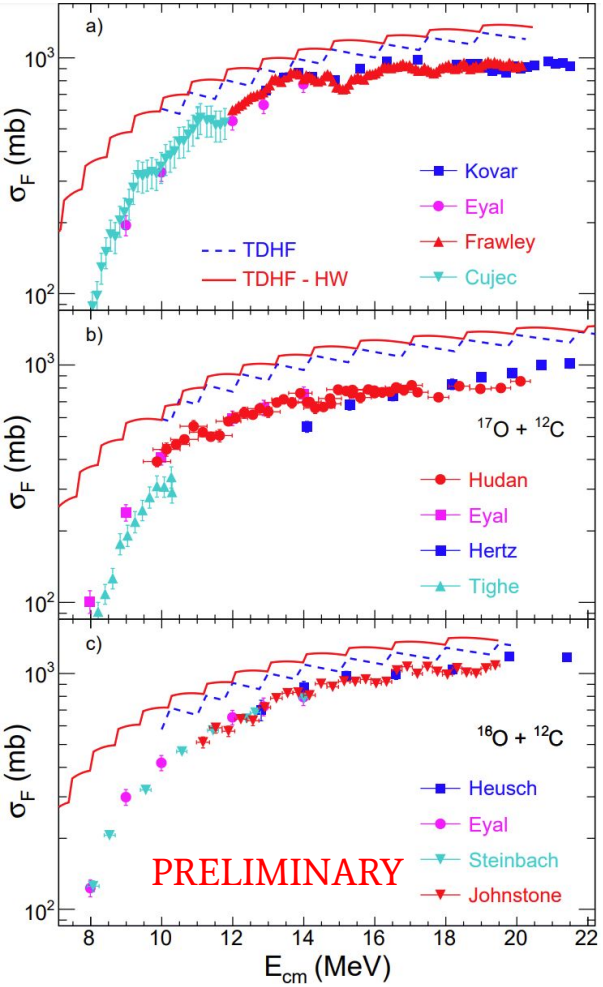
$V_{barrier}$ is a quantity extracted from fusion cross sections

Nothing precludes a comparison to cross sections directly

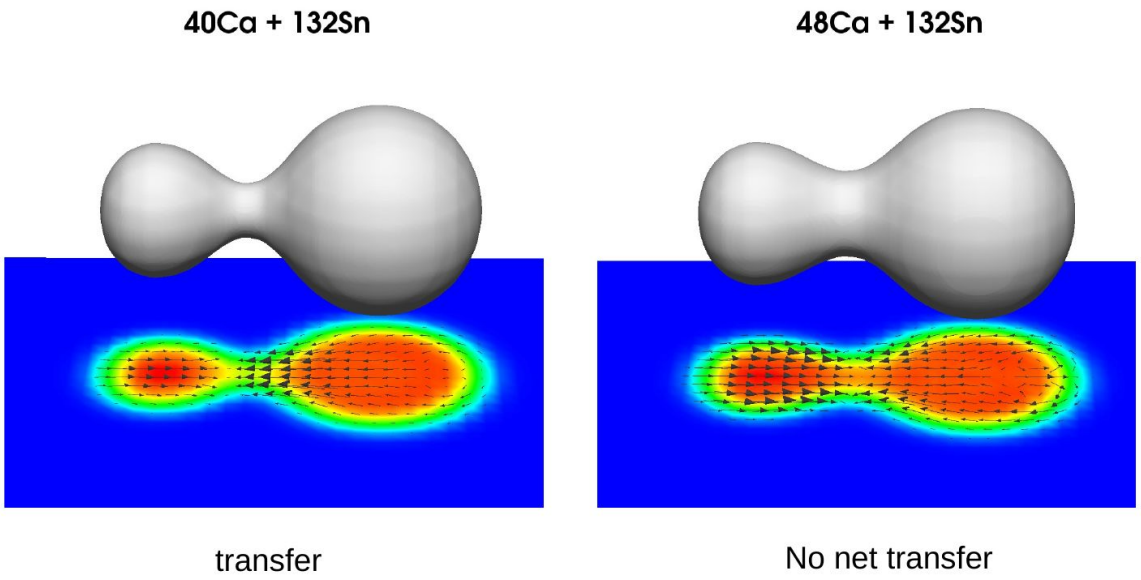


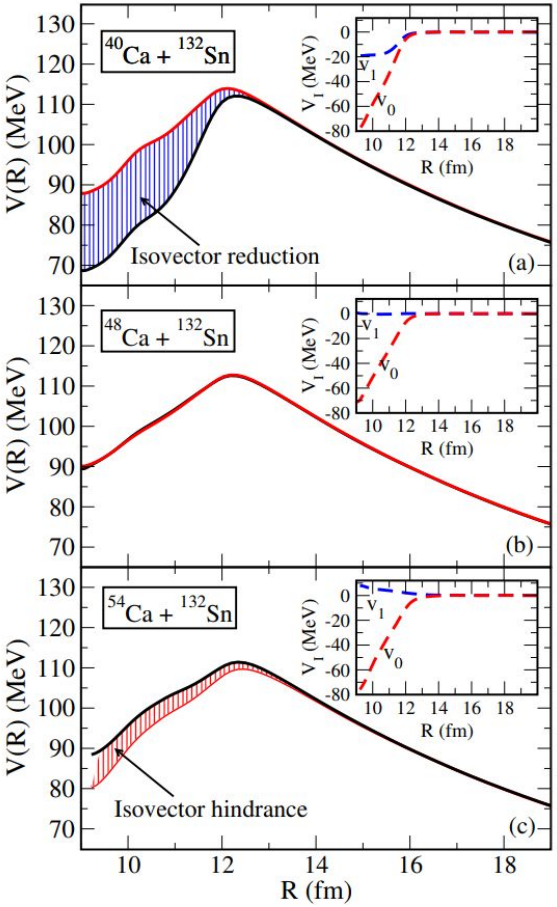
Structures in Reaction Data

L-wave ratcheting is present in both the theory and experiment, but other features are missing



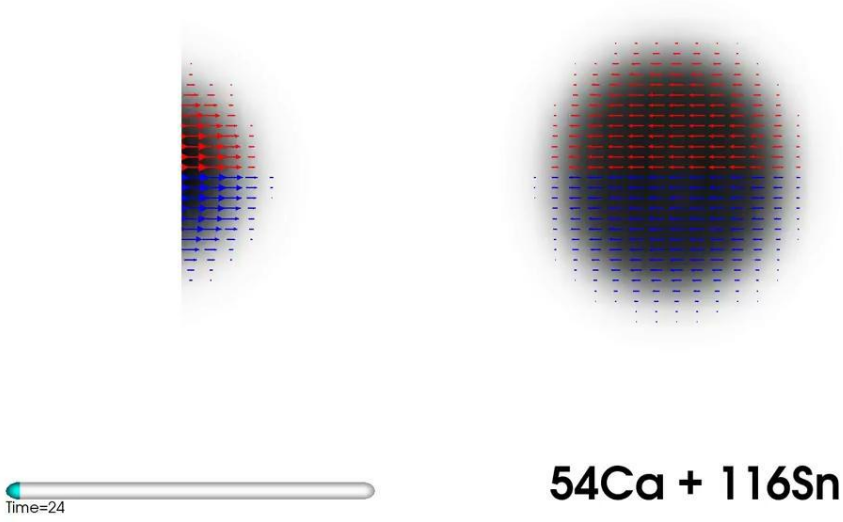
Transfer and Equilibration too!



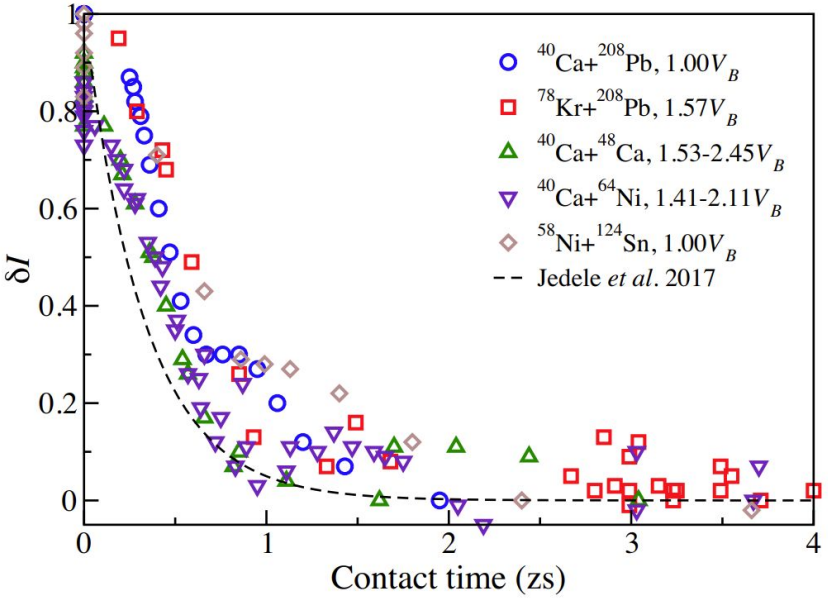


K. Godbey, A. S. Umar, and C. Simenel, "Dependence of fusion on isospin dynamics", Phys. Rev. C 95, 011601 (Rapid Communication) (2017).

Transfer and Equilibration too!



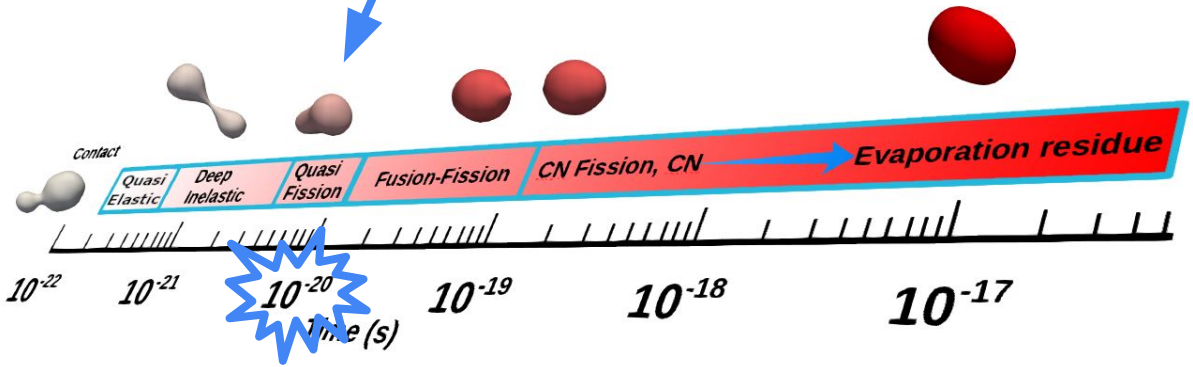
54Ca + 116Sn



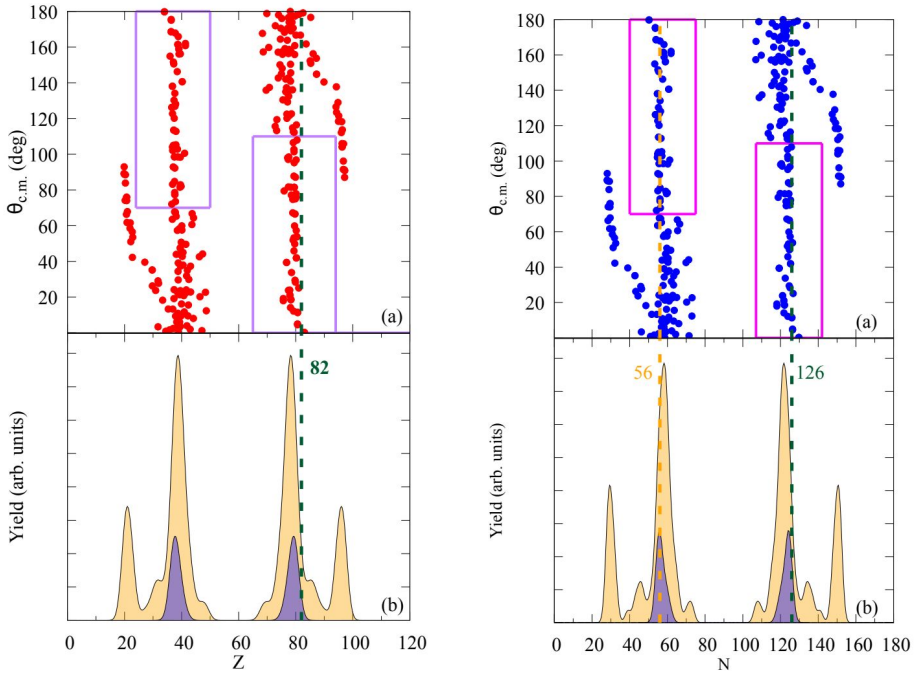
C. Simenel, K. Godbey, and A. S. Umar, Timescales of Quantum Equilibration, Dissipation Fluctuation in Nuclear Collisions, Phys. Rev. Lett. 124, 212504 (2020)

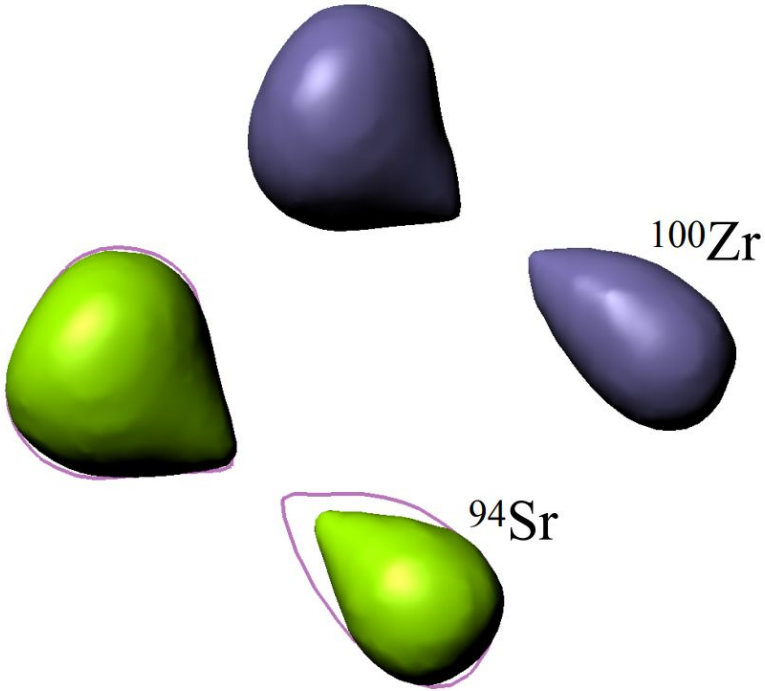
Introducing Quasifission

That's 10s of zeptoseconds!



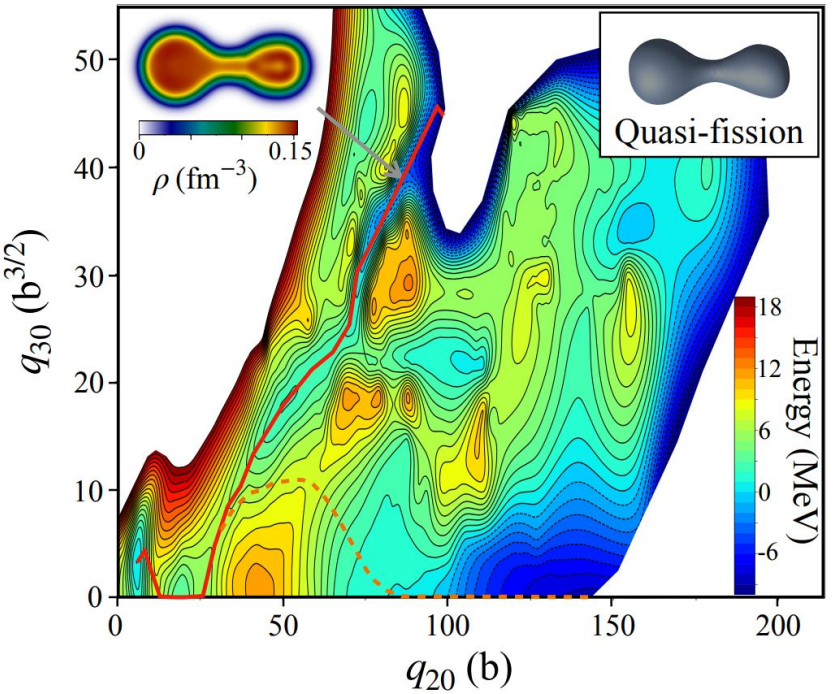
Deformed Shell Effects in Quasifission





K. Godbey, A. S. Umar, and C. Simenel, “Deformed shell effects in 48Ca+249Bk quasifission fragments”, Phys. Rev. C 100, 024610 (2019).

Quasifission as a Probe for Fission



Very similar shapes and dynamics are indeed seen in QF and fission, but to what extent?

Two excellent candidate systems to test/explore this:

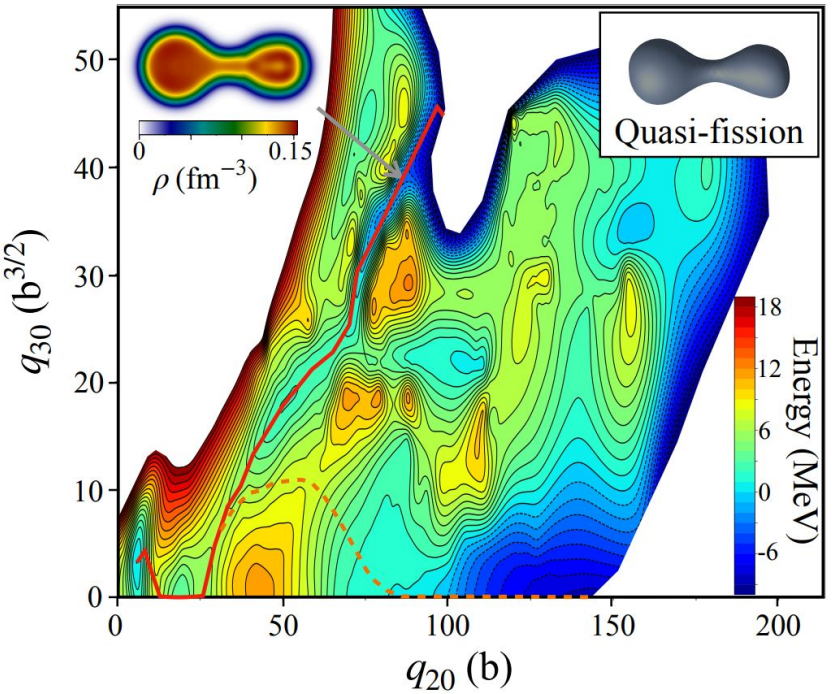
^{48,49,50}Ca + ^{176}Yb -> Some QF

^{16,17,18}O + ^{208}Pb -> No QF

C. Simenel, P. McGlynn, A. S. Umar, and K. Godbey, "Comparison of fission and quasi-fission modes", Physics Letters B 822, 136648 (2021).

Quasifission as a Probe for Fission

Quasifission as a surrogate for fission can be instrumental near the dripline, particularly in heavy nuclei



C. Simenel, P. McGlynn, A. S. Umar, and K. Godbey, "Comparison of fission and quasi-fission modes", Physics Letters B 822, 136648 (2021).

Enabling Progress

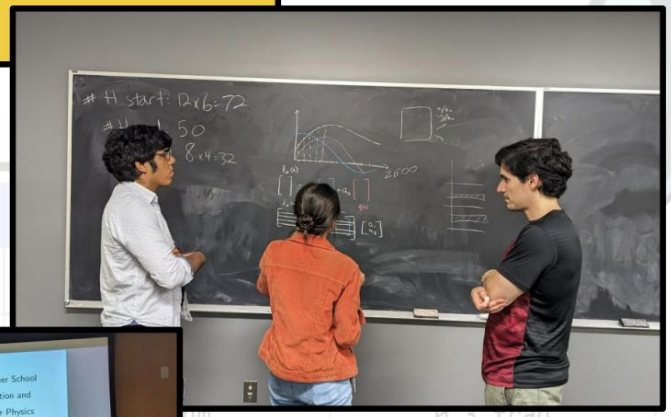
Explosion of interest in principled uncertainty quantification across nuclear physics in recent years

Now we can leverage that interest in collaboration with applied mathematicians, statisticians, and computer scientists

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics











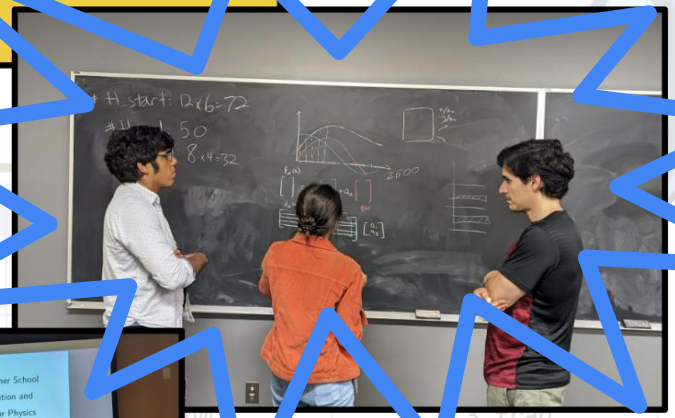
~60 participants spanning a wide audience

Slide from Pablo Giuliani

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

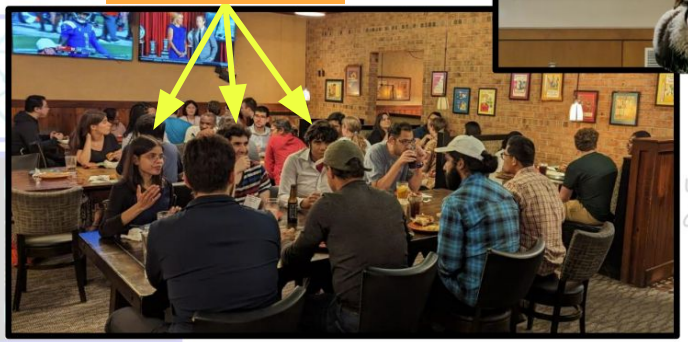
FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics





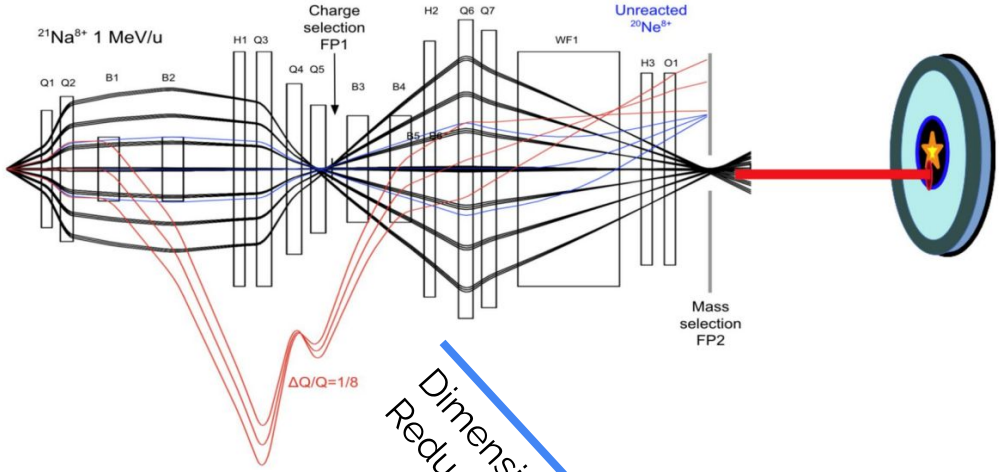


Social, too!





Slide from Pablo Giuliani



Dimensionality Reduction

PRELIMINARY

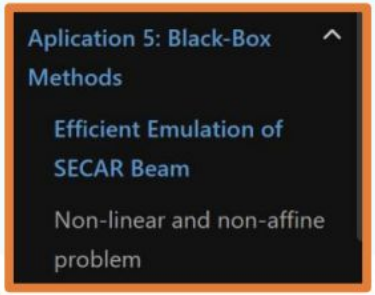
# of Bases	Emulation Time (to FP1)	Max Position Error (x)	Max angular Error (ax)
3	(9.7 ± 0.3) ms*	1 μm	1 nrad
10	(10.9 ± 0.6) ms*	0.01 μm	7.5 prad
15	(12.1 ± 0.2) ms*	0.7 nm	0.3 frad

Fast

Accurate

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN





Always accepting new examples!

https://dr.ascsn.net

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

Introduction to Dimensionality Reduction in Nuclear Physics
Introduction
Application 1: The Quantum Harmonic Oscillator
Application 2: Two body single channel nuclear scattering
Application 3: The Empirical Interpolation Method
Application 4: Time Dependent Systems (evolution in the reduced space)
Aplication 5: Black-Box Methods
Contributors

Path(s) Forward

Low-energy, heavy ion reactions are very likely to be informative for questions across the FRIB community

Continued developments in time-dependent microscopic many-body theory are vital

Immense Gratitude to All Collaborators!



Funding

DOE NNSA Grant No. DE-NA0004074
DOE Grant Nos. DE-SC0013365, DE-SC0023175
NSF CSSI Program No. 2004601

Computing Resources

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

Bayesian Mass Explorer
βeta!



1 | 2 | +

Dimension: Landscape

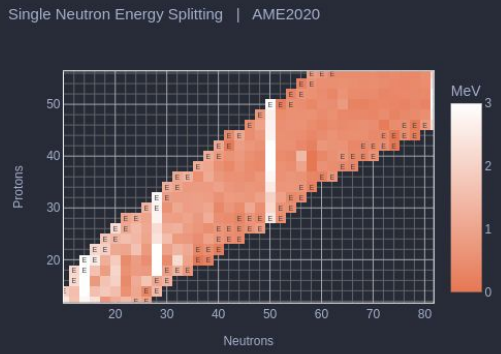
Select Quantity: Single-Neutron Energy Splitting

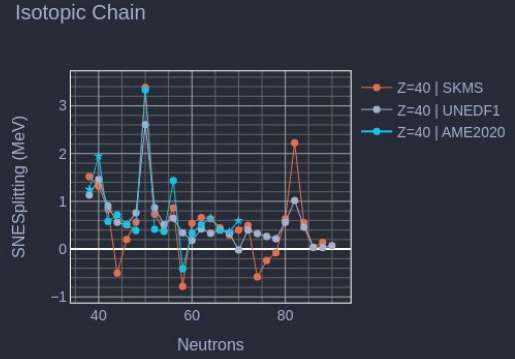
Select Dataset: AME2020

Wigner Adjustment: Wigner (2)

Colorbar Style: Monochrome

Colorbar Range: min | 3





Share View

EXPORT PUB. PDFS

LINK VIEWS 1 2

Even-Even Nuclei

RESCALE COLORBAR

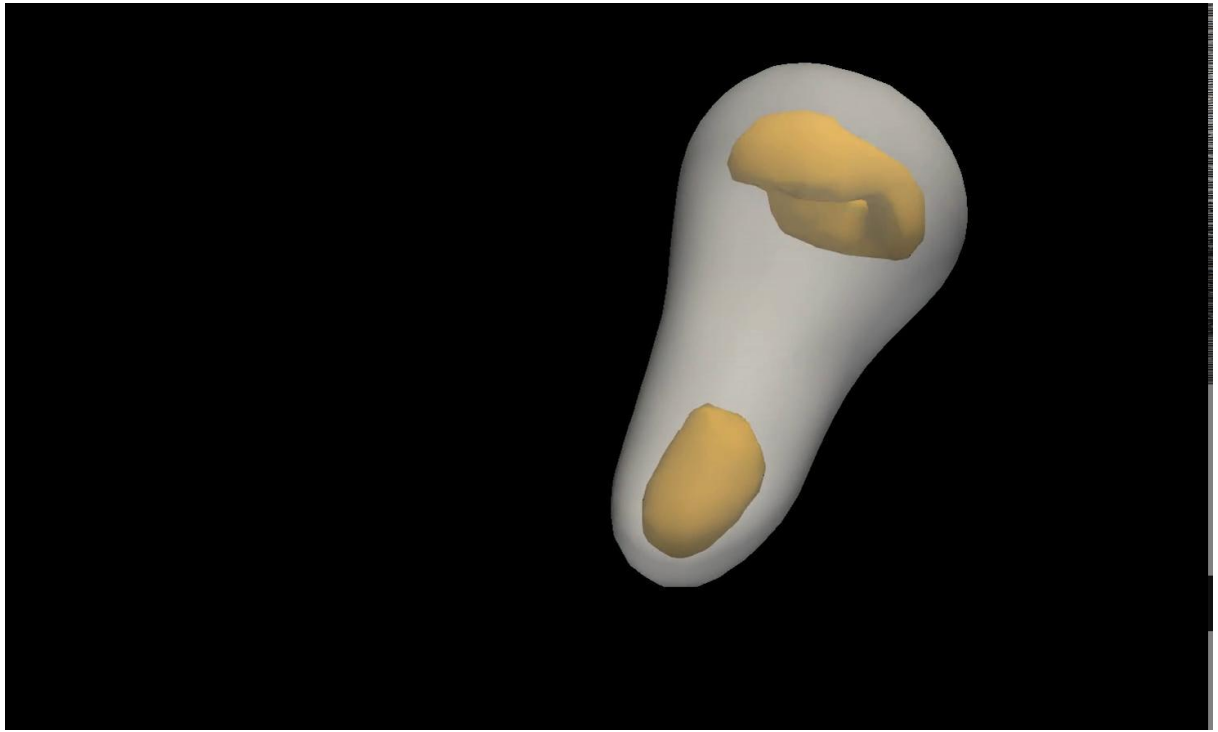
RESET PAGE



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Challenges in UQ



Challenges in UQ

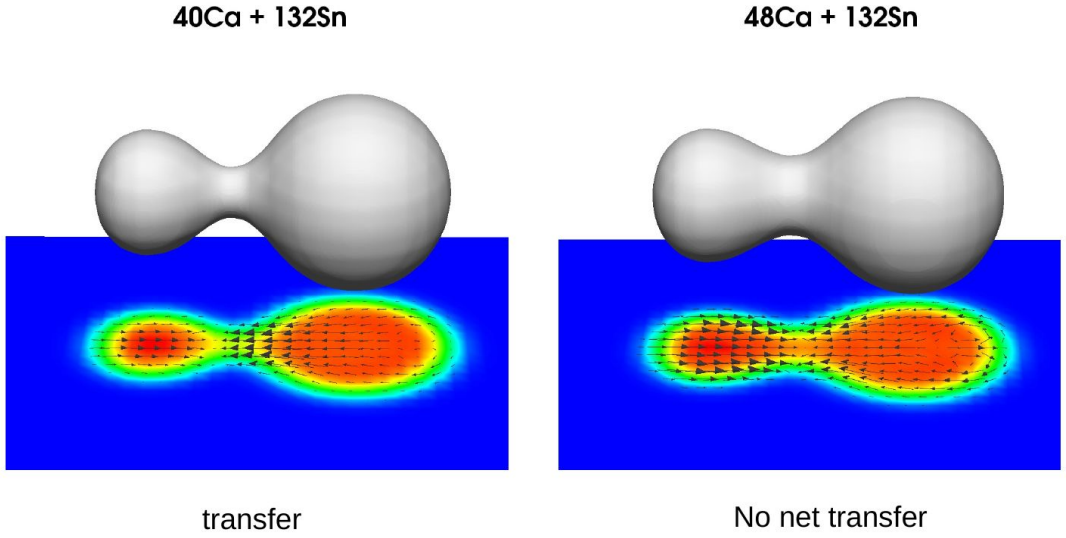
In statistics:

a)This expense motivates investing in methods that give us high quality UQ with as few samples of our parameters as possible

b)Our parameter space isn't huge — currently order of 10-15 model parameters

Case Study: Heavy-Ion Fusion

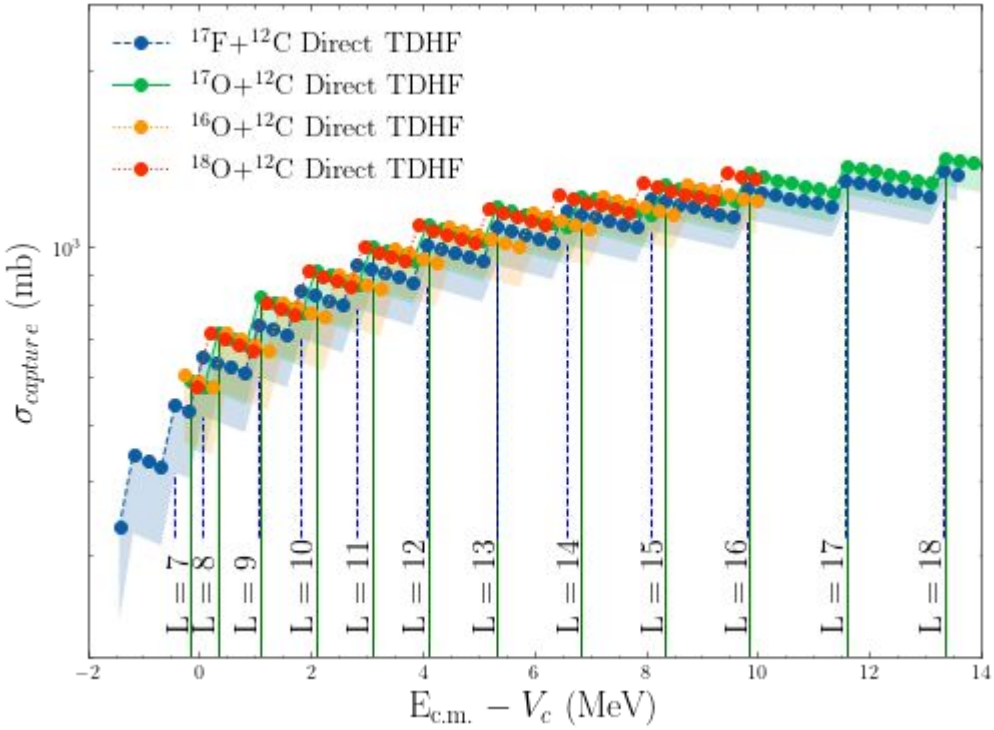
Near-barrier fusion reactions are filled with insights into the structure and dynamics of the systems of interest



Case Study: Heavy-Ion Fusion

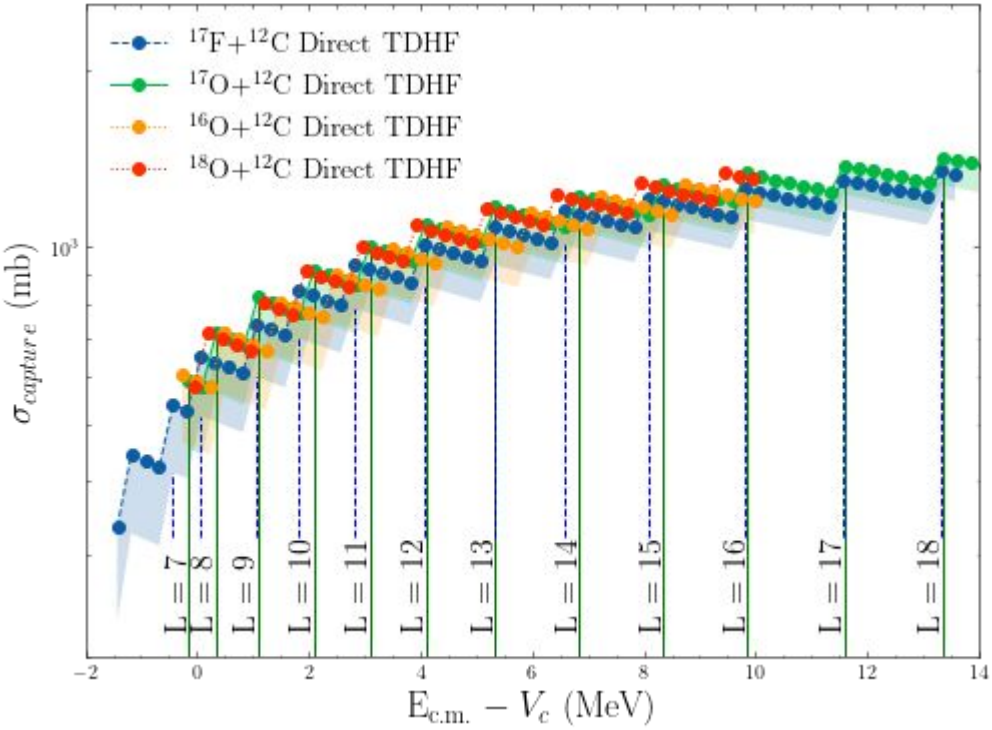
Barrier determination requires ~10s of time-dependent trajectories for each geometric configuration

Cross sections require 100s-1000s of evaluations



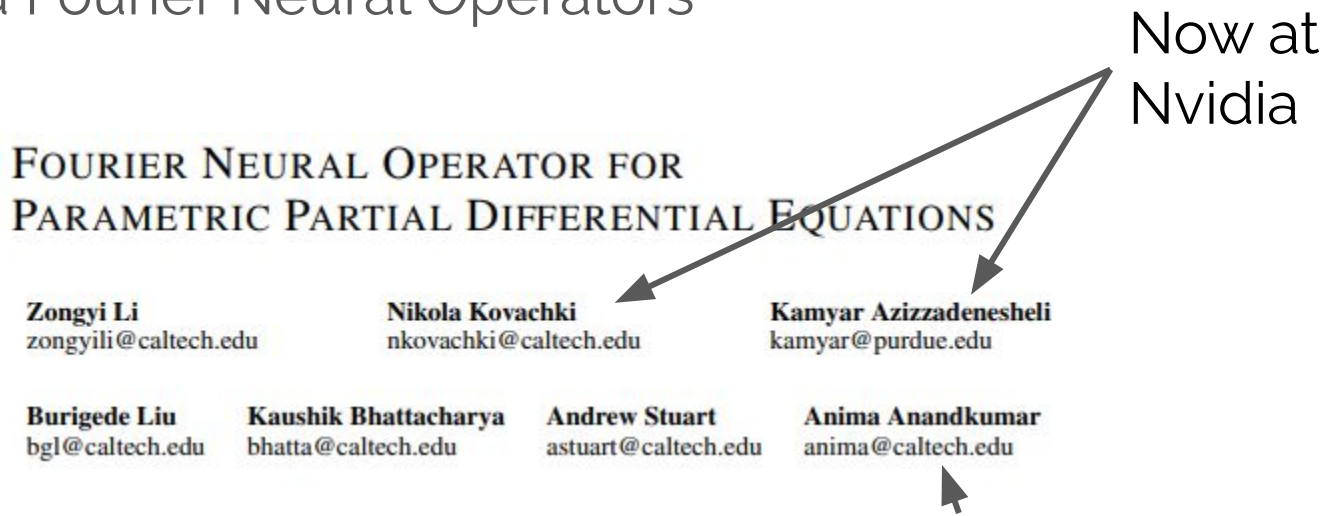
Case Study: Heavy-Ion Fusion

Simulation times vary from a few hours for light systems to a few days for heavy systems

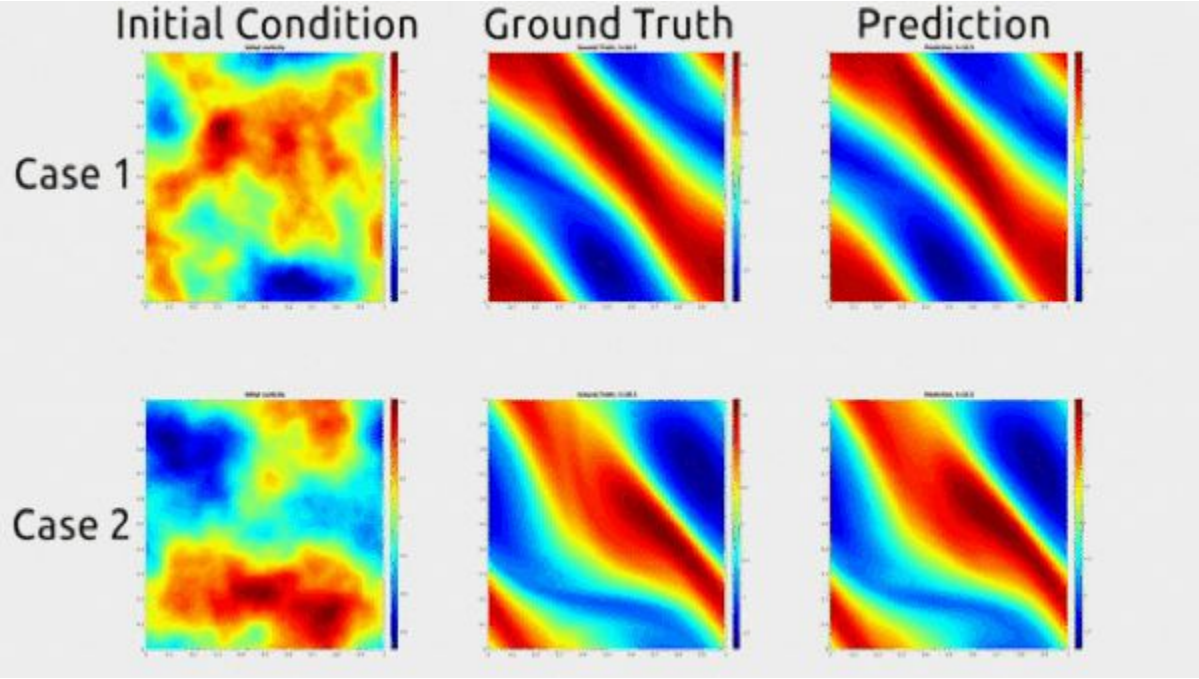


Current Ideas for Dynamics

Exploring multiple approaches, including Neural Implicit Flow and Fourier Neural Operators



Current Ideas for Dynamics



Development of New Functionals

Complementary to efforts in UQ is the development of new energy density functionals

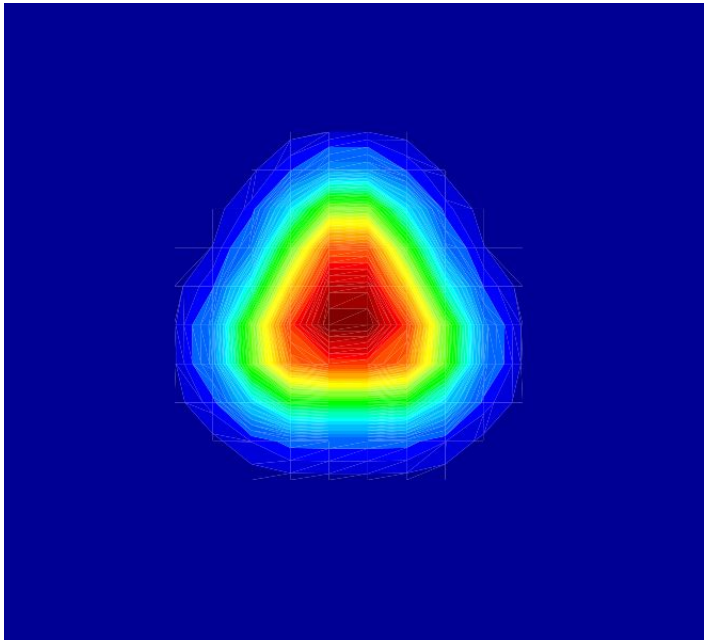
I'd classify this direction as **model discovery**

Development of New Functionals

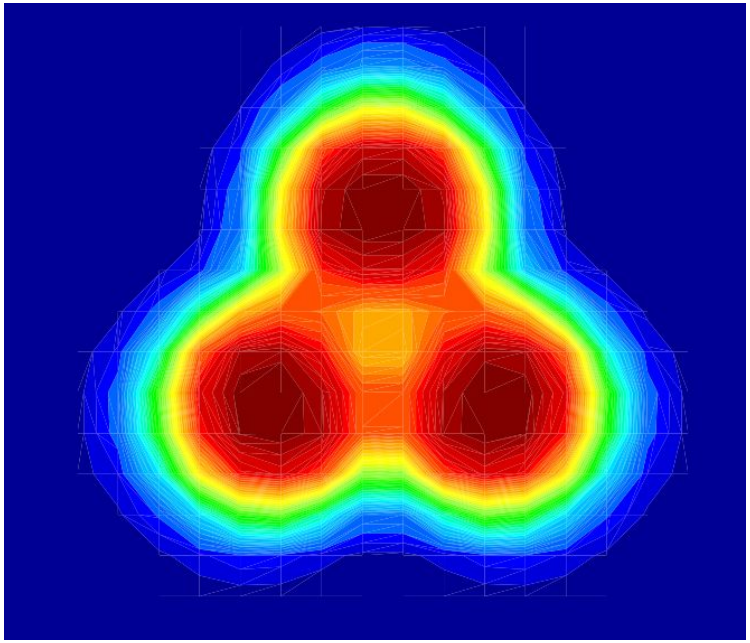
One approach to data-driven model discovery is in considering similar observables to UQ studies

The flexibility of DFT can be exploited, however, to pin down densities from ab initio methods via an inverse Kohn-Sham procedure

Development of New Functionals



Density, $\varrho(r)$



Nucleon localization function

Needs for EDF Development

On the HPC, math, and stats side:

a)Same stuff as before! But even more so now since we are considering entirely new physics models

b)Any expertise in sparse or symbolic regression is welcomed too

Needs for EDF Development

On the physics side:

a)Precision densities and currents for model discovery over a (wide) range of nuclei

Infrastructure Development

The glue that keeps the ship together:
Infrastructure!

Infrastructure impacts every aspect of the research enterprise, from software development through final data distribution

Infrastructure Development

Primary goal:

Improve data reproducibility and accessibility standards across the board

Infrastructure Development

Benefits:

Documented, repeatable pipelines saves time

Traceable results with associated data used in calibration and ML applications

Infrastructure Development

Benefits:

Increased accessibility and visibility of your results

Easier onboarding of new researchers

Infrastructure Development

Benefits:

Easier to tie into other research workflows, fostering collaboration

Easier to more rapidly deploy results for user-focused applications

Infrastructure Development

Current plan is to automate the model discovery elements of the pipeline to automatically build and test emulators for more expedient UQ

Also planned are continuous calibration runners that can agilely adapt to new experimental data

Infrastructure Development

The technology that enables this are the (relatively) cheap and abundant cloud computing resources on the market

Cloud computing is a different paradigm from traditional HPC, but it shouldn't be overlooked if you need something elastic and quickly scalable

Bayesian Mass Explorer
βeta!





What about other sources of data?



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Needs in Infrastructure

We're always seeking inspiration in terms of DevOps/MLOps and how our workflows and deployments can be made more efficient and scalable

Cloud computing applications benefit from platform flexibility, so simultaneously (and efficiently) targeting multiple architectures can pay off

Highlight | HFBFFT



Computer Physics Communications
Volume 276, July 2022, 108344

Three-dimensional Skyrme Hartree-Fock-Bogoliubov solver in coordinate-space representation ☆

Mengzhi Chen [a b], Tong Li [a b], Bastian Schuetrumpf [a], Paul-Gerhard Reinhard [c], Witold Nazarewicz [a b]

Next generation 3D coordinate space DFT software with a focus on usability, flexibility, and platform independence

Highlight | HFBFFT

Planned features include:

a) Efficient multipole constraints
b) Density constraints for the inverse Kohn-Sham problem
c) Time-dependence
d) Interface for generic EDFs

Highlight | HFBFFT

Planned features in line with thi

a) Efficient multipole c

b) Density constr se Kohn-Sham problem

c) Tin

d) eneric EDFs

Stick around for Metin's talk!

The framework: Density Functional Theory

‘Microscopic’ method optimized for description of one-body observables

Fantastically extensible framework to go beyond base assumptions