Computing Atomic Nuclei

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12th symposium on Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences

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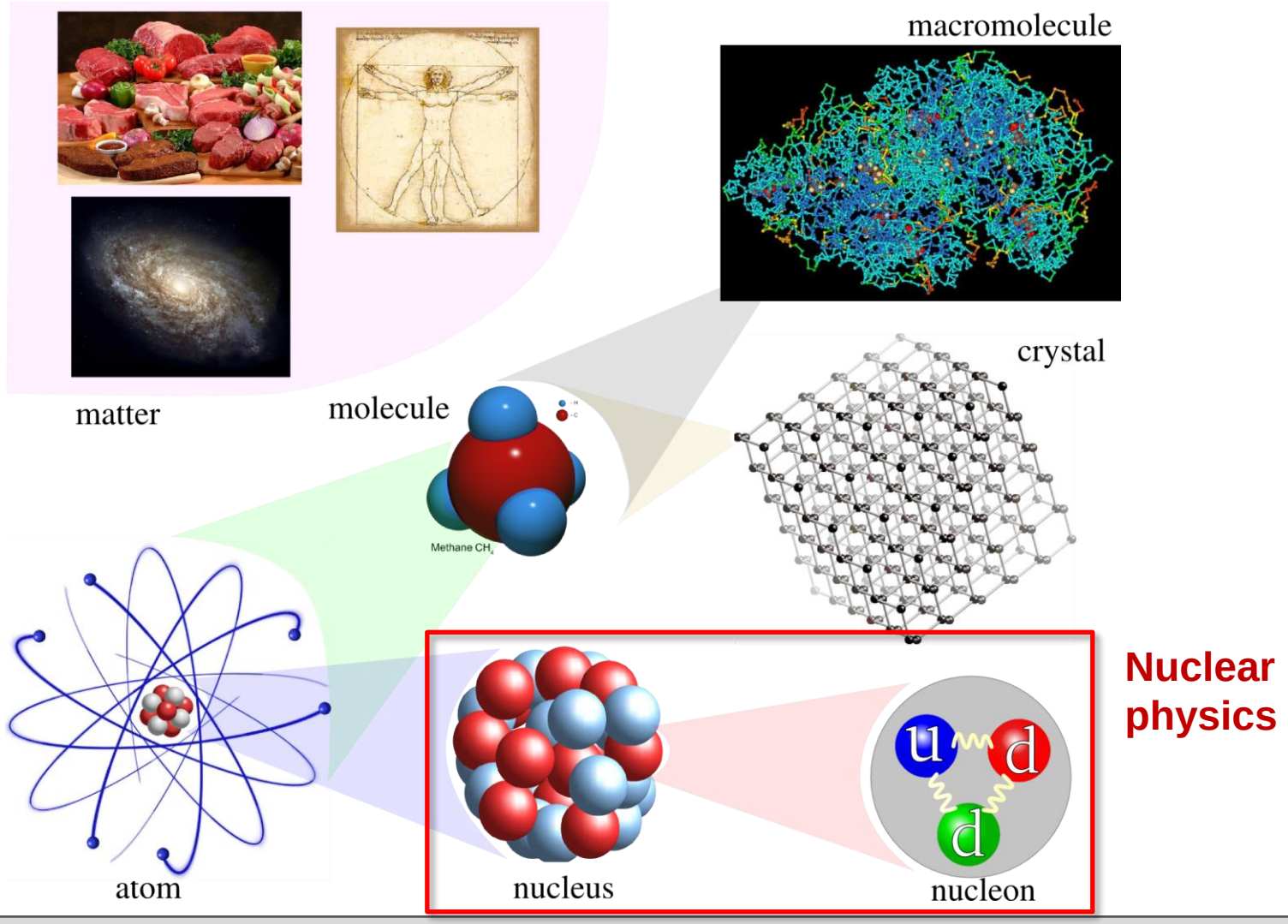
Nuclear Science

Nuclear physics is the branch of physics that studies the properties, reactions and structure of atomic nuclei



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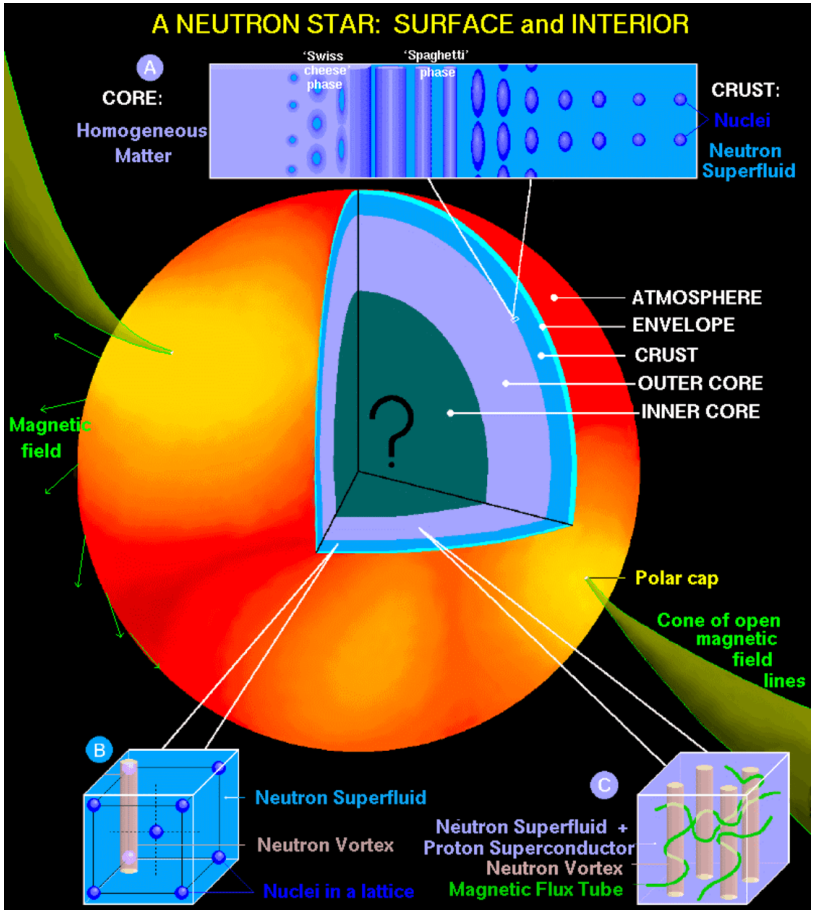
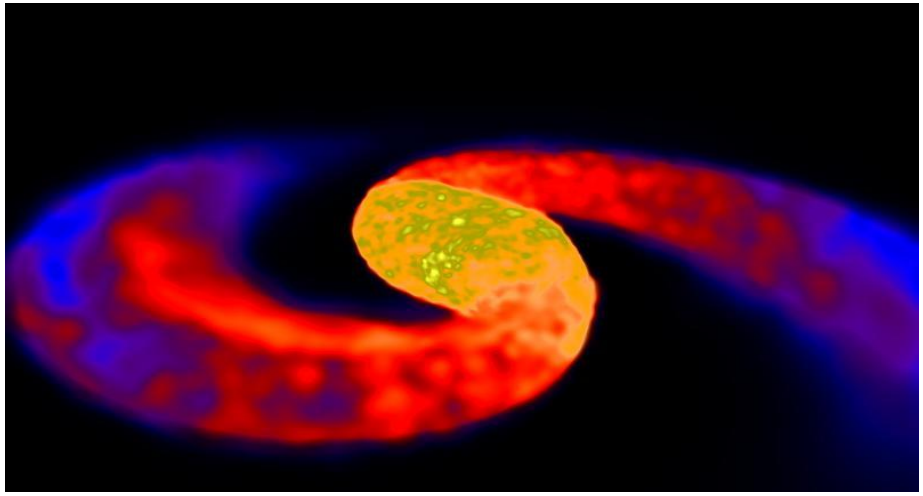
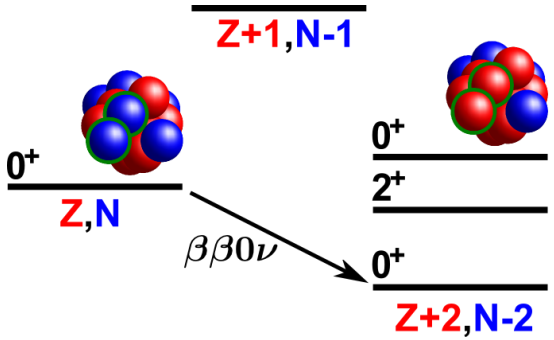
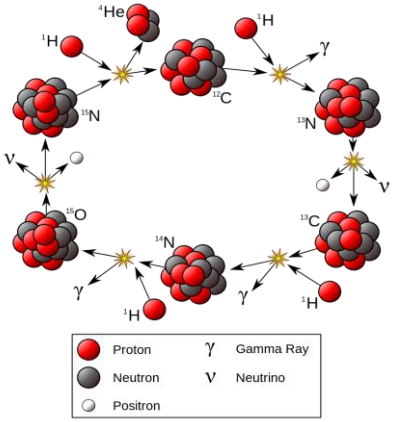
Fundamental Science

Properties of atomic nuclei play a key role in understanding the formation of elements in the universe or the fundamental symmetries of nature









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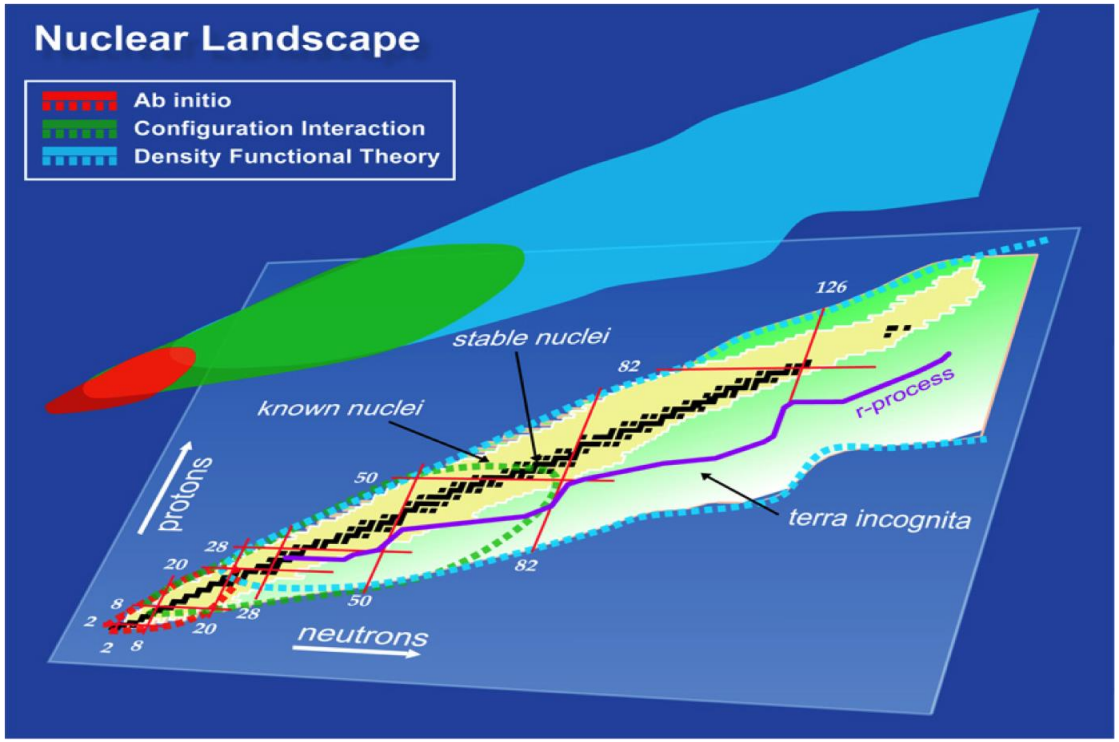
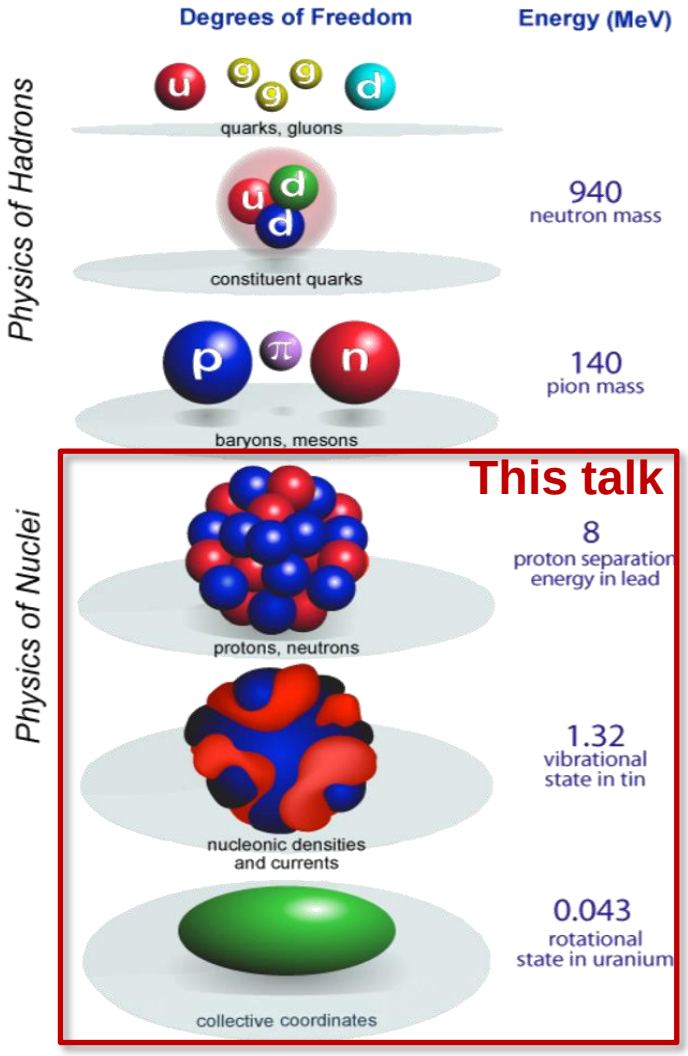
Theoretical Nuclear Physics

Different energy scales require different degrees of freedom and theoretical approaches – each with its computational challenges

- Many-body methods:
  - Ab initio approaches
  - Configuration interaction (CI)
- Density functional theory (DFT)





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Basics of Nuclear Theory

The goal of low-energy nuclear theory is to describe the structure and reactions of nuclei as strongly-interacting, quantum many-body systems

- Quantum-mechanical, many-body system
  - Entirely characterized by wave functions $\Psi_\alpha(\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_A\sigma_A)$ where r_k is the position of particle k, and $\sigma_k = \pm 1$ is the spin of that particle
  - Wave functions are eigenvectors of Hamiltonian operator, which determines the dynamics of the system

$$\hat{H} = -\sum_{k=1}^{A} \frac{\boldsymbol{\nabla}^2}{2m_k} + \frac{1}{2}\sum_{k,l=1}^{A} \hat{V}_{NN}(\boldsymbol{r}_k\sigma_k, \boldsymbol{r}_l\sigma_l) + \frac{1}{6}\sum_{k,l,m=1}^{A} \hat{V}_{3N}(\boldsymbol{r}_k\sigma_k, \boldsymbol{r}_l\sigma_l, \boldsymbol{r}_m\sigma_m) + \cdots$$

- Observables are obtained from multi-dimensional integrals, e.g.,

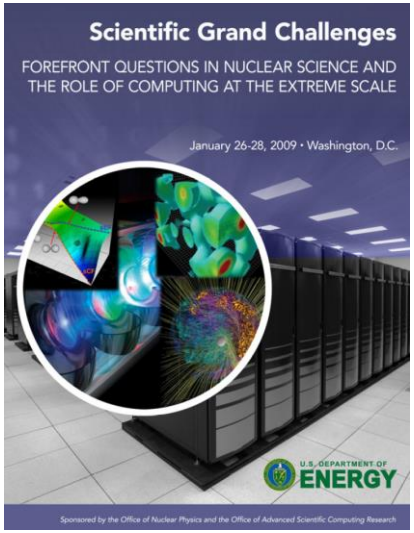
$$E_\alpha = \sum_{\text{spins}} \int d^3\boldsymbol{r}_1 \ldots \int d^3\boldsymbol{r}_A \Psi_\alpha^*(\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_A\sigma_A)\hat{H}\Psi_\alpha(\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_A\sigma_A)$$

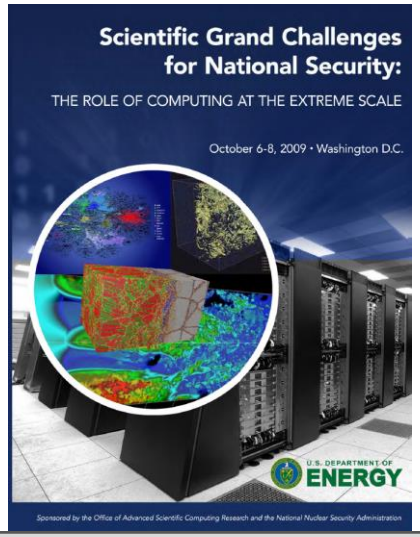
- Computational grand challenge:
  - 3A continuous degrees of freedom + A discrete ones
  - Spin alone: 2^A combinations…

Nuclear Models

The size of the computational challenge imposes different approaches tailored to specific system sizes and needs

- Two main approaches to the nuclear many-body problem
  - Many-body methods : In some suitable basis, find eigenvalues and eigenvectors of nuclear Hamiltonian
    - By direct diagonalization (no-core shell model)
    - By approximation schemes (coupled-cluster, quantum Monte-Carlo, in-medium similarity renormalization group, etc.)
  - Density functional theory (DFT): Find surrogate many-body wave functions that approximate experimental observables well
- No unique theory = no unique computational implementation





Many-body Methods

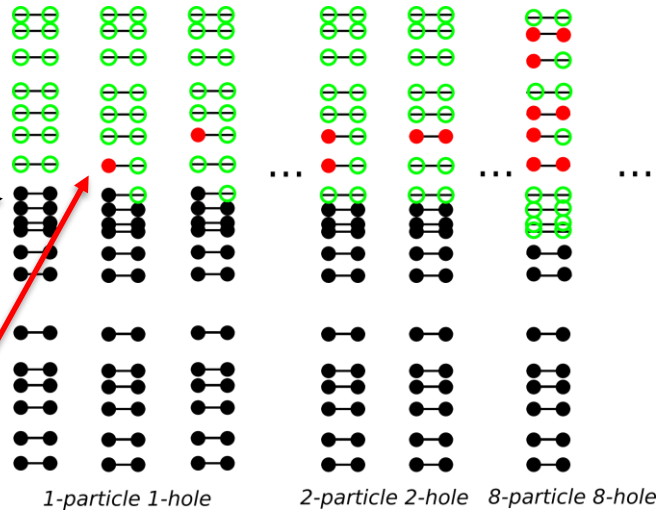
The algorithmic and computational building blocks of many-body methods are tensor contractions and (sparse) linear algebra at very large scale

- Choose single-particle basis of $\mathcal{L}^2(\mathbb{C})$ made of eigenfunctions $\phi_n(\boldsymbol{r})$ of some operator. Ex.: $\left(-\frac{\nabla^2}{2m}+\frac{1}{2}m\omega^2 r^2\right)\phi_n = \varepsilon_n\phi_n$
- Build many-body states by taking product states of the ϕ_n
- Compute matrix of Hamiltonian operator (>100 GB…) ⇒ tensor contractions
- Diagonalize / evolve ⇒ very large-scale linear algebra, often sparse

$$\Phi_1(\boldsymbol{r}_1\sigma_1,\ldots,\boldsymbol{r}_A\sigma_A) = \begin{vmatrix} \phi_1(\boldsymbol{r}_1\sigma_1) & \cdots & \phi_1(\boldsymbol{r}_A\sigma_A) \\ \vdots & \ddots & \vdots \\ \phi_A(\boldsymbol{r}_1\sigma_1) & \cdots & \phi_A(\boldsymbol{r}_A\sigma_A) \end{vmatrix}$$

$$\vdots$$

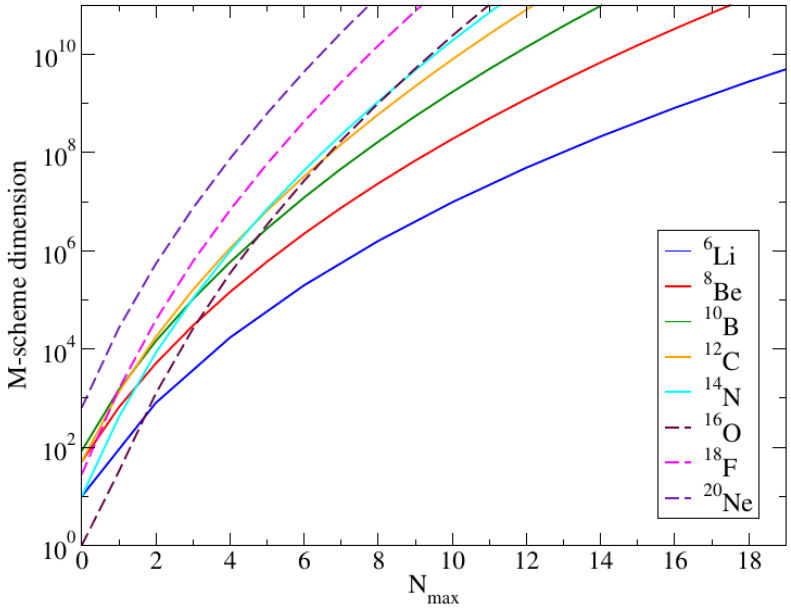
$$\Phi_2(\boldsymbol{r}_1\sigma_1,\ldots,\boldsymbol{r}_A\sigma_A) = \begin{vmatrix} \phi_1(\boldsymbol{r}_1\sigma_1) & \cdots & \phi_1(\boldsymbol{r}_A\sigma_A) \\ \vdots & \ddots & \vdots \\ \phi_A(\boldsymbol{r}_1\sigma_1) & \cdots & \phi_{A+1}(\boldsymbol{r}_A\sigma_A) \end{vmatrix}$$

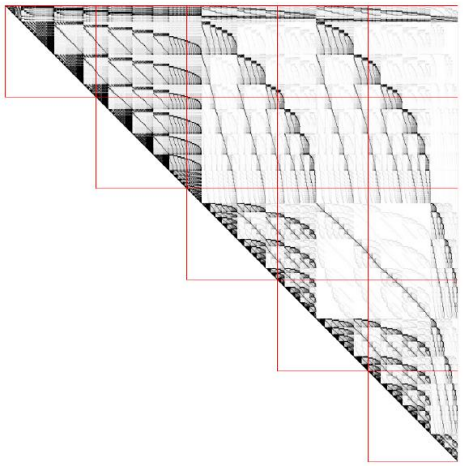


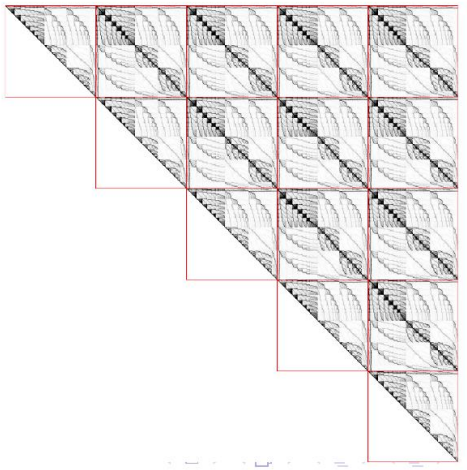
Limitations

Ab initio methods provide the most accurate and precise data on structure and reactions, but are inapplicable beyond the lightest nuclei (memory-bound)

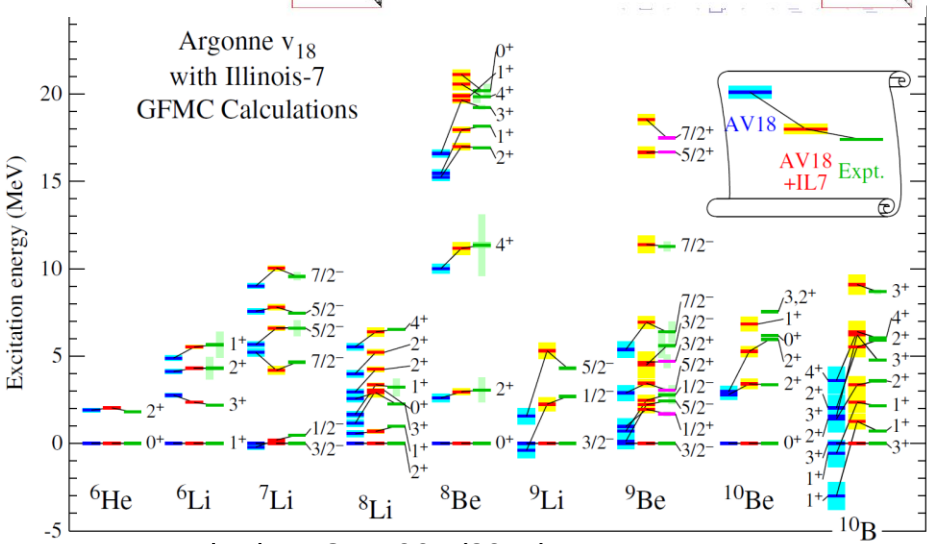
Comput. Phys. Commun. **222**, 1 (2018)







- Direct ab initio approaches not applicable beyond A ~ 16
- Other many-body methods scale up only near ^{40}Ca, ^{48}Ca, ^{100}Sn, ^{132}Sn, ^{208}Pb



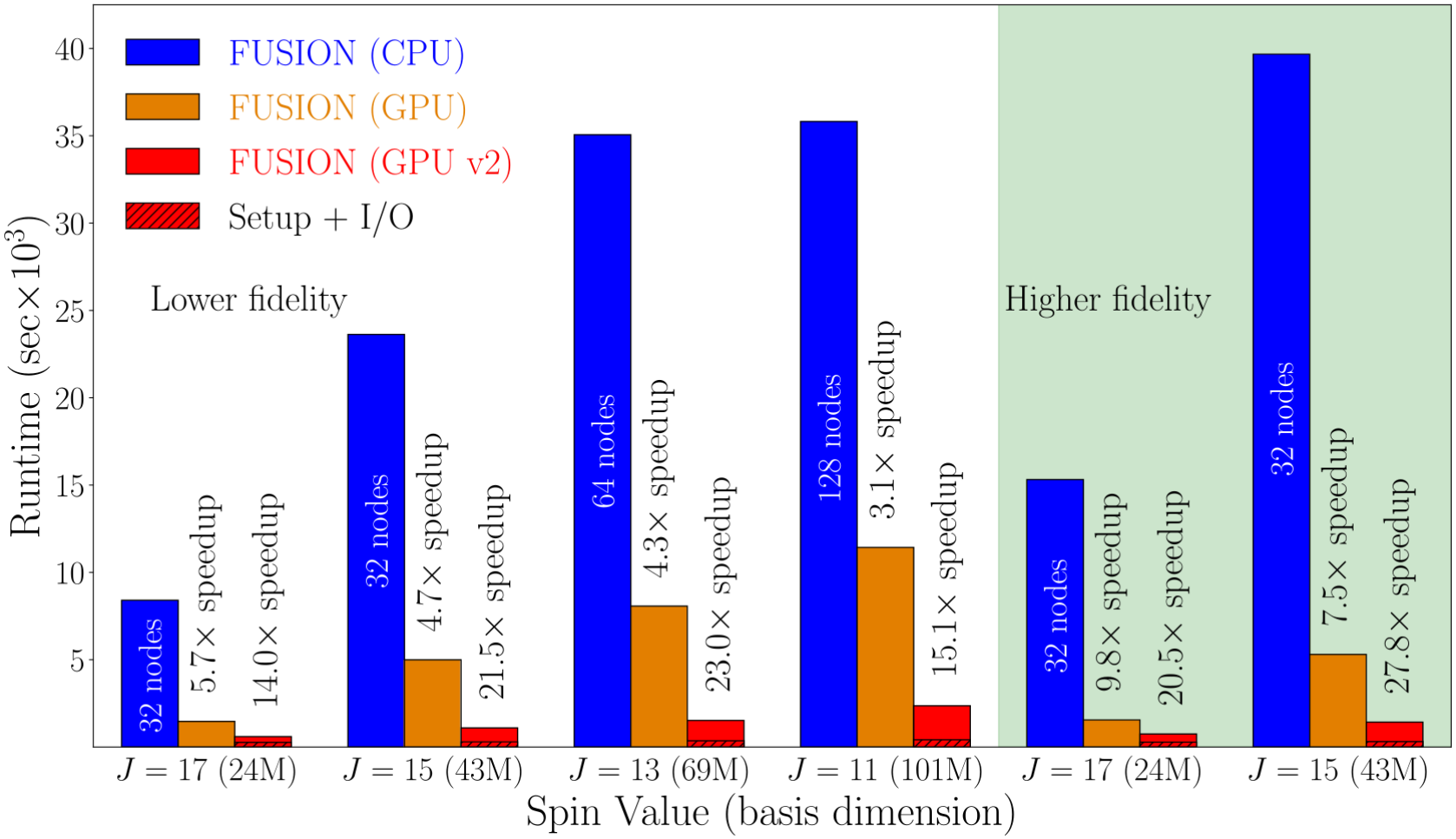
Rev. Mod. Phys. **87**, 1067 (2015)

Benefits of New Architectures

New architectures based on GPU open new avenues of research – but often require considerable code refactoring and important human investment

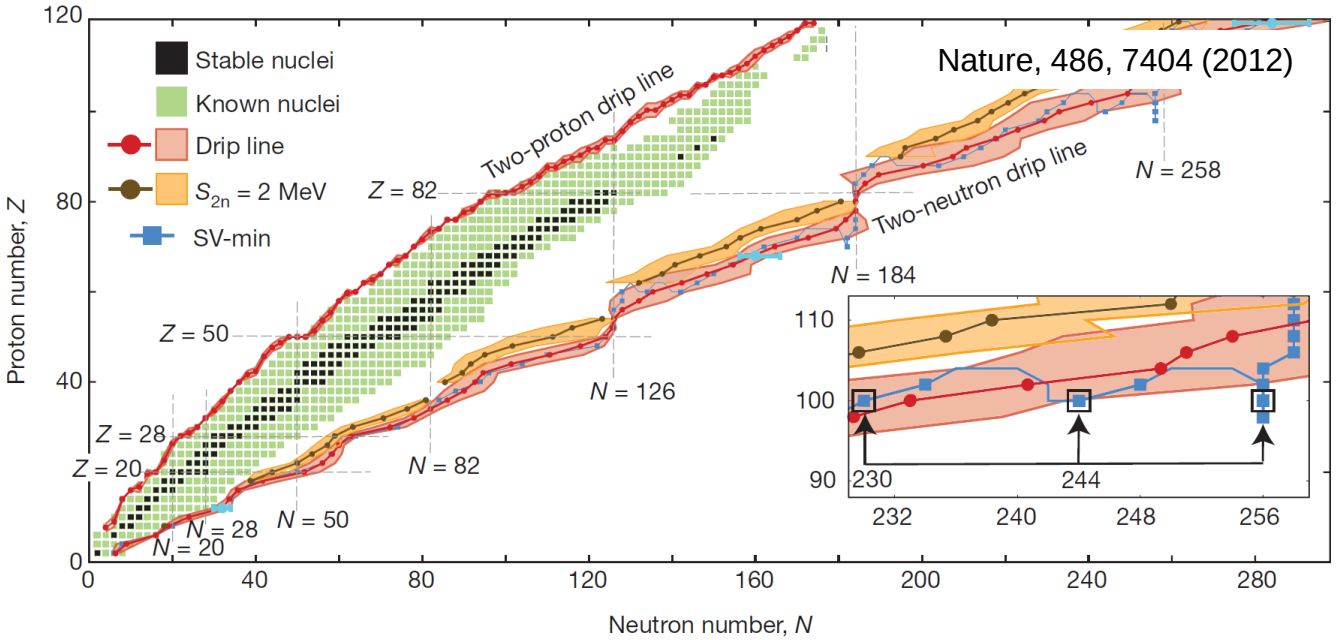
PRC **102**, 024616 (2020)

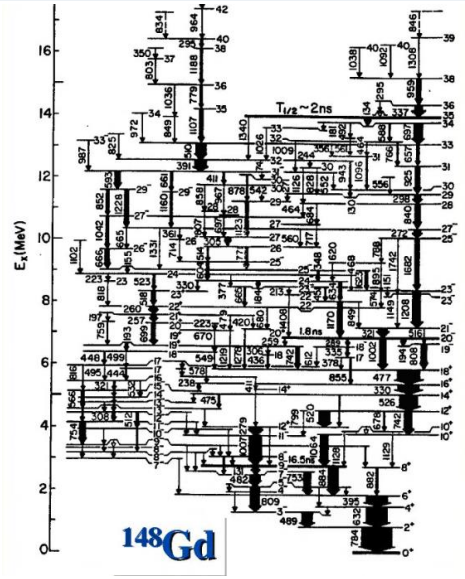
Work by K. Kravvaris, S Quaglioni (LLNL)



Density Functional Theory

DFT is the only quantum many-body method that can scale up to the entire table of isotopes and provide structure and decay properties





- About 2,500 nuclei predicted to be stable, from Hydrogen to (currently) $^{294}_{196}Og_{118}$
  - Variety of excitation mechanisms: collective rotations, vibrations, nucleonic excitations, et.
  - Decay modes: α-particle emission, β-radioactivity, γ-ray emission, cluster emission, fission

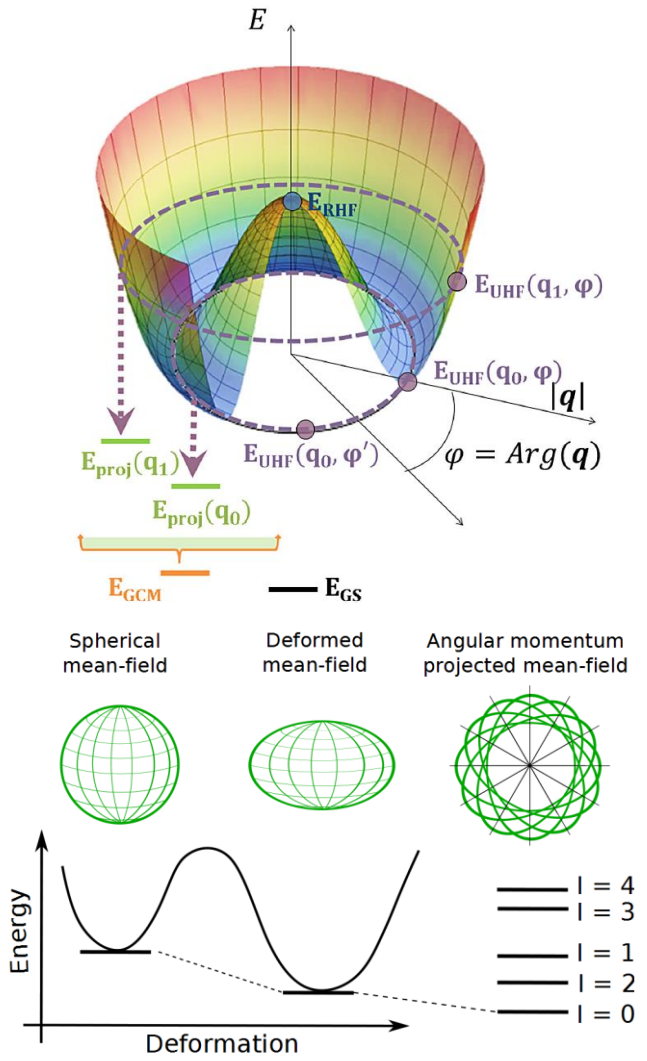
Basic Concepts of DFT

Density functional theory is based on remapping the original A-body problems into an effective 1-body problem

- Energy is a functional (to be determined from physics argument) of the density of particles, e.g.

$$E[\rho(\boldsymbol{r})] = C^{\rho\rho}\rho^2 + C^{\rho\Delta\rho}\rho\Delta\rho + \cdots$$

- Actual density is determined by minimizing the energy ⇒ Kohn-Sham equation
  - The density of particles does not conserve the same symmetries as the nuclear Hamiltonian
  - Justification for the concepts of nuclear deformation and nuclear pairing
- Constraints on, e.g., the nuclear shape or the total spin, allow building in more correlations



Computational Implementation

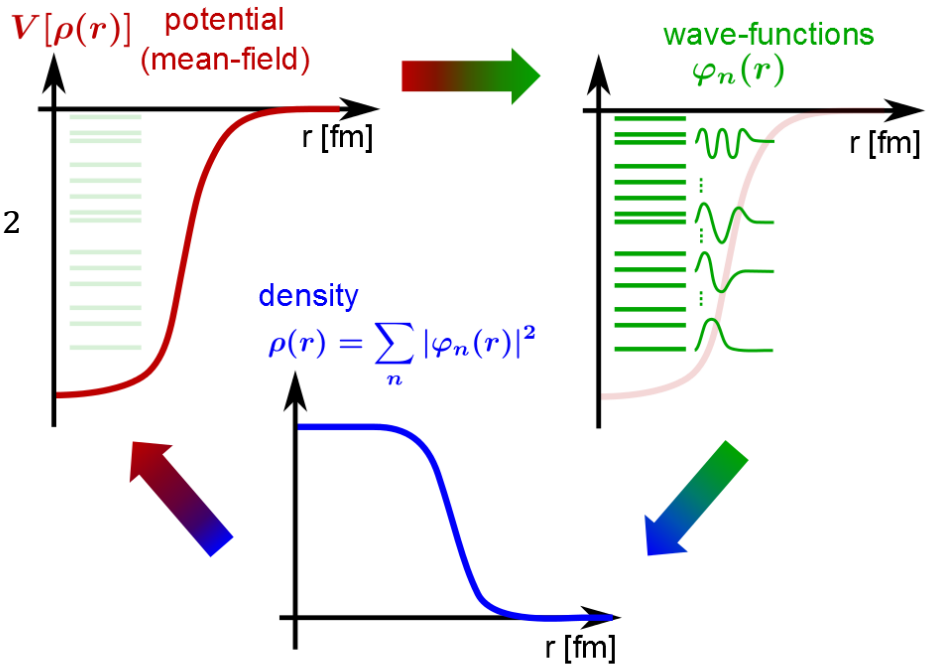
The Kohn-Sham equation involves a self-consistent loop that is solved by an iterative procedure until convergence

- Kohn Sham equation:

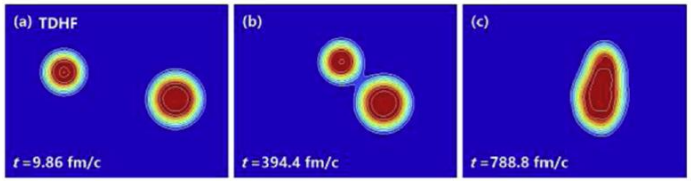
$$\hat{h}\varphi_k(\boldsymbol{r}) = e_k\varphi_k(\boldsymbol{r})$$

$$\hat{h} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \hat{V}[\rho(\boldsymbol{r})] \qquad \rho(\boldsymbol{r}) = \sum_{k=1}^{A}|\varphi_k(\boldsymbol{r})|^2$$

- Linear algebra (structure)
  - Differential operators in Hilbert spaces
  - Define basis of vectors $\phi_1, \ldots, \phi_n$
  - Diagonalize matrix h_{ij} in that basis
- PDE on a lattice (reactions)
  - Mesh discretization, e.g., Lagrange
  - Integrate PDE with boundary conditions



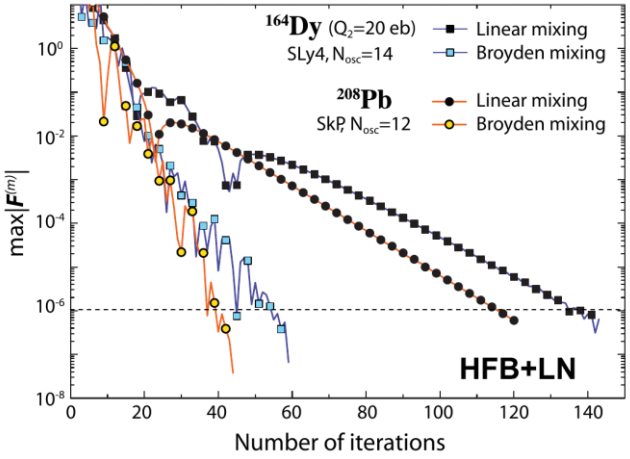
Self-consistent mean-field theory



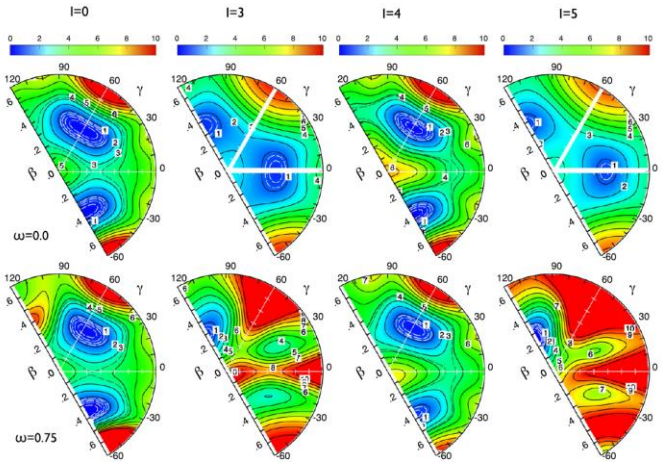
Computational Challenges

Computational challenges come from non-linearity of self-consistent loop and number of configurations required to reach given accuracy

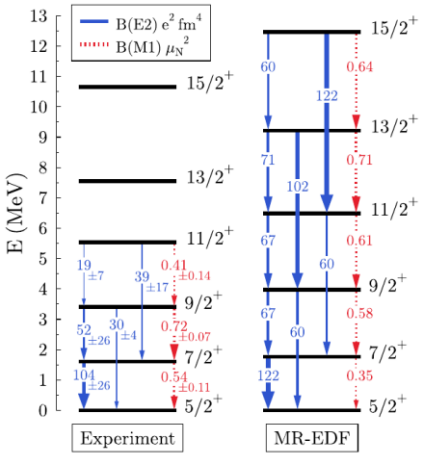
PRC **78**, 014318 (2008)



Phys. Scr. **91**, 073003 (2016)



PRL **113**, 162501 (2014)

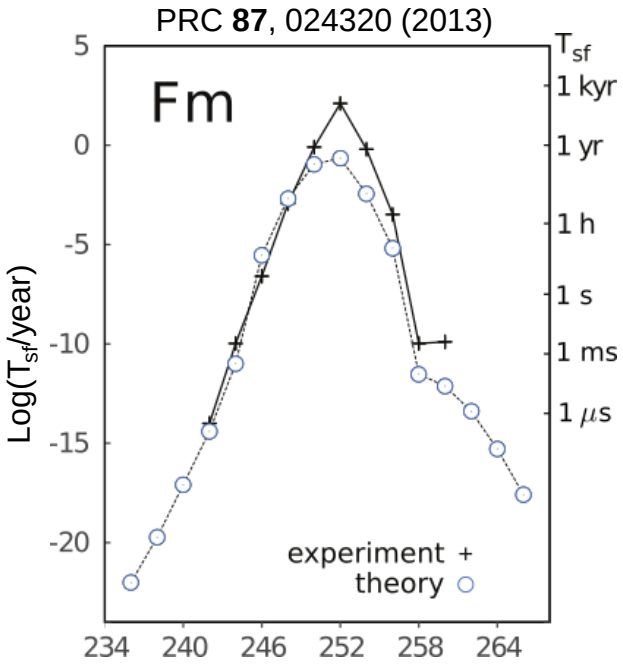


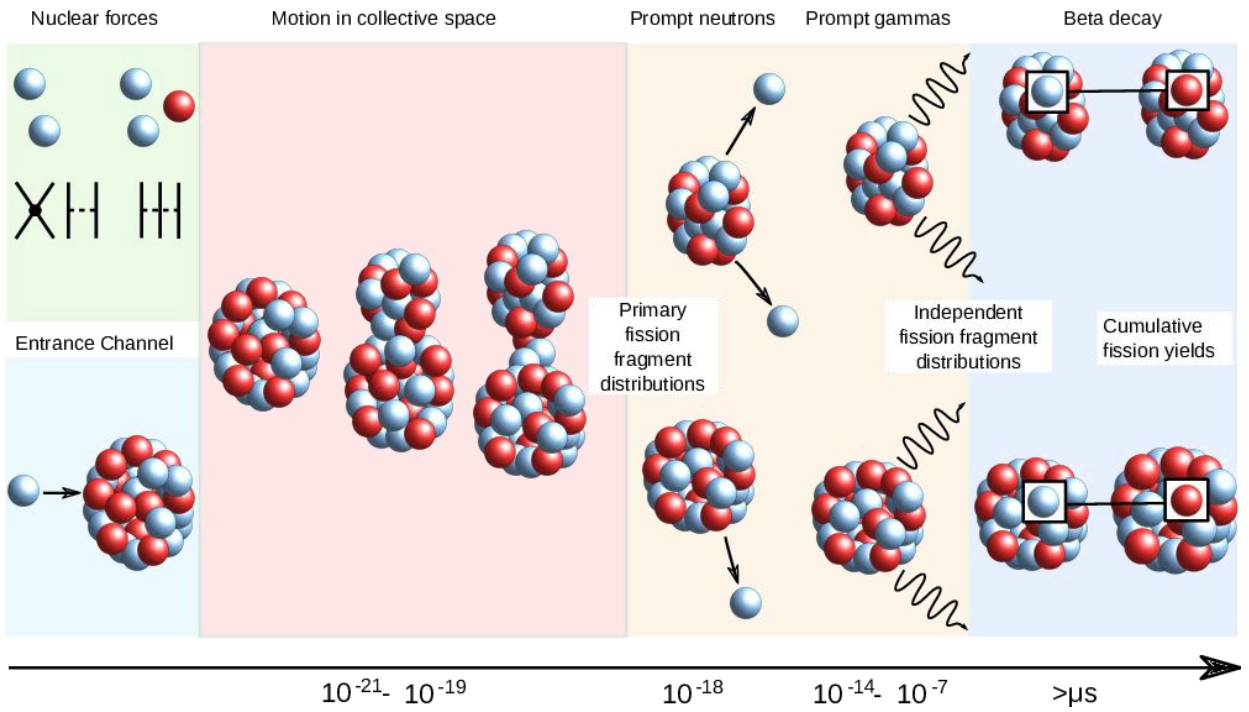
- Variational principle of DFT only gives lowest solution
- Improve model by quantum mixing of different configurations
  - Configurations obtained with constraints on Kohn-Sham solutions
  - Thousands/millions of different calculations (=ensemble runs)
  - 1 iteration of KS loop = up to a few minutes on 4-8 threads
  - Convergence may require 100+ iterations

Application: Theory of Nuclear Fission

A predictive theory of fission built on quantum many-body methods such as DFT remains a formidable computational challenge

- Fission = extreme application of DFT
  - Both collective and intrinsic degrees of freedom relevant
  - Time-evolution of a quantum many-body system
  - Sensitivity of observables on details of model





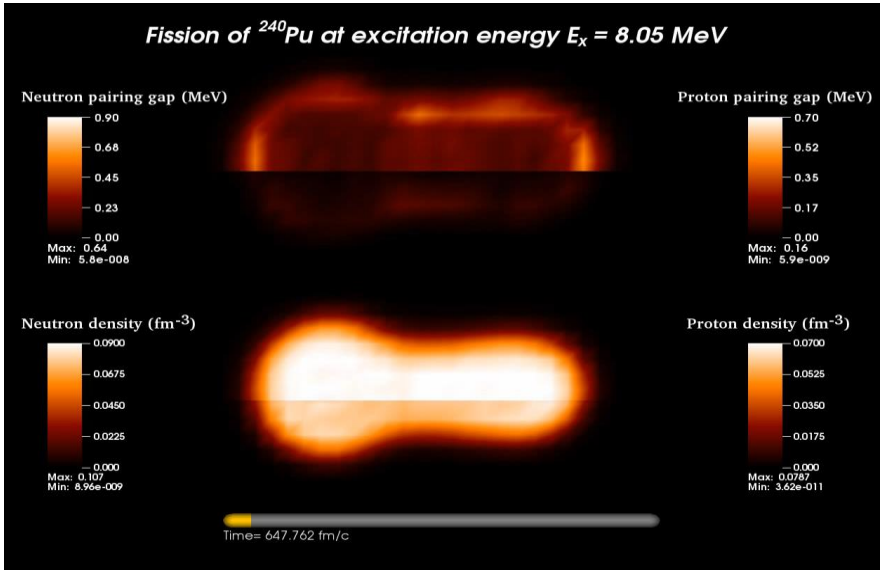
Real-Time Fission Dynamics

Time-dependent density functional theory for fusion or fission is based on solving hundreds of thousands coupled PDE

PRC **100**, 034615 (2019)

Code	CUs	Computer	PDEs	Lattice	Cost (sec.)
Sky3D [18]	128	Titan	1,024	$18^2 \times 30$	3.86×10^{-6}
U&S [19]	16	Linux cluster	714	$40^2 \times 70$	8.72×10^{-5}
TDSLDA	514	Titan	442,368	$24^2 \times 48$	4.35×10^{-8}
TDSLDA	256	Piz Daint	442,368	$24^2 \times 48$	1.26×10^{-8}
TDSLDA	240	Summit	442,368	$24^2 \times 48$	1.05×10^{-8}
TDSLDA-simp	2	Titan	684	$20^2 \times 60$	7.55×10^{-8}

PRL **116**, 122504 (2016)



- State-of-the-art simulations on advanced architectures

$$\hat{h} := \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \hat{V}[\rho(\boldsymbol{r})] \right)$$

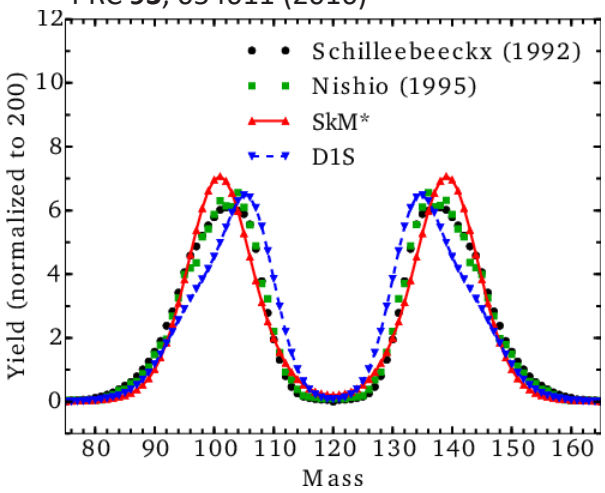
$$\rho(\boldsymbol{r}) = \sum_{\mu} \left[V_{\mu\uparrow}(\boldsymbol{r},t)V_{\mu\uparrow}(\boldsymbol{r},t) + V_{\mu\downarrow}(\boldsymbol{r},t)V_{\mu\downarrow}(\boldsymbol{r},t) \right]$$

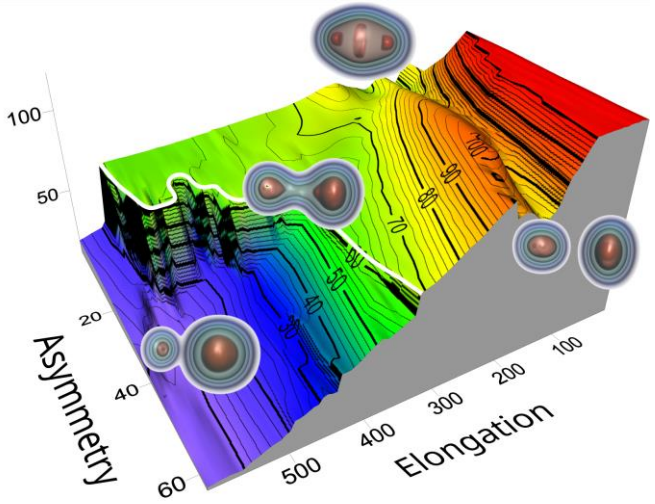
$$\hbar \frac{\partial}{\partial t} \begin{pmatrix} U_{\mu\uparrow}(\boldsymbol{r},t) \\ U_{\mu\downarrow}(\boldsymbol{r},t) \\ V_{\mu\uparrow}(\boldsymbol{r},t) \\ V_{\mu\downarrow}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow\uparrow} - \lambda & h_{\uparrow\downarrow} & 0 & \Delta \\ h_{\downarrow\uparrow} & h_{\downarrow\downarrow} - \lambda & -\Delta & 0 \\ 0 & -\Delta^* & -h_{\uparrow\uparrow}{}^* + \lambda & -h_{\uparrow\downarrow}{}^* \\ \Delta^* & 0 & -h_{\downarrow\uparrow}{}^* & -h_{\uparrow\uparrow}{}^* + \lambda \end{pmatrix} \begin{pmatrix} U_{\mu\uparrow}(\boldsymbol{r},t) \\ U_{\mu\downarrow}(\boldsymbol{r},t) \\ V_{\mu\uparrow}(\boldsymbol{r},t) \\ V_{\mu\downarrow}(\boldsymbol{r},t) \end{pmatrix}$$

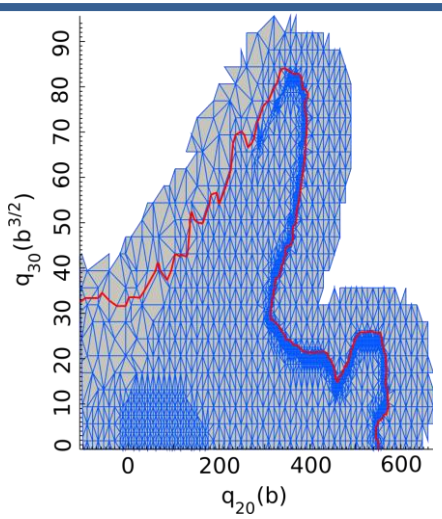
Microscopic Description of Fission

Fission can be characterized by the shape of the nucleus as it deforms: the actual phase space includes millions of different configurations

PRC **93**, 054611 (2016)



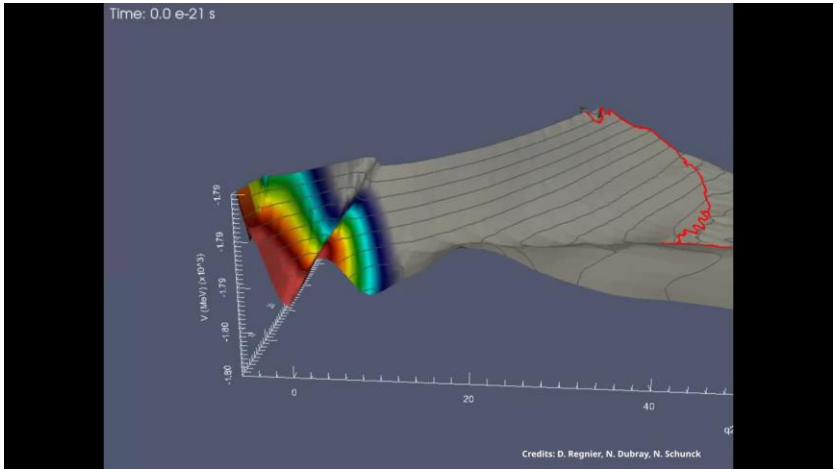




Comput. Phys. Commun. **225**, 180 (2018)

- Map fragmentations into deformations of fissioning nucleus
- Compute potential energy surface
- Compute flow of probability to extract relative yields

$$i\hbar\frac{\partial g}{\partial t}(\boldsymbol{q},t)=\left[-\frac{\hbar^2}{2}\sum_{ij}\frac{\partial}{\partial q_i}B(\boldsymbol{q})\frac{\partial}{\partial q_j}+V(\boldsymbol{q})\right]g(\boldsymbol{q},t)$$



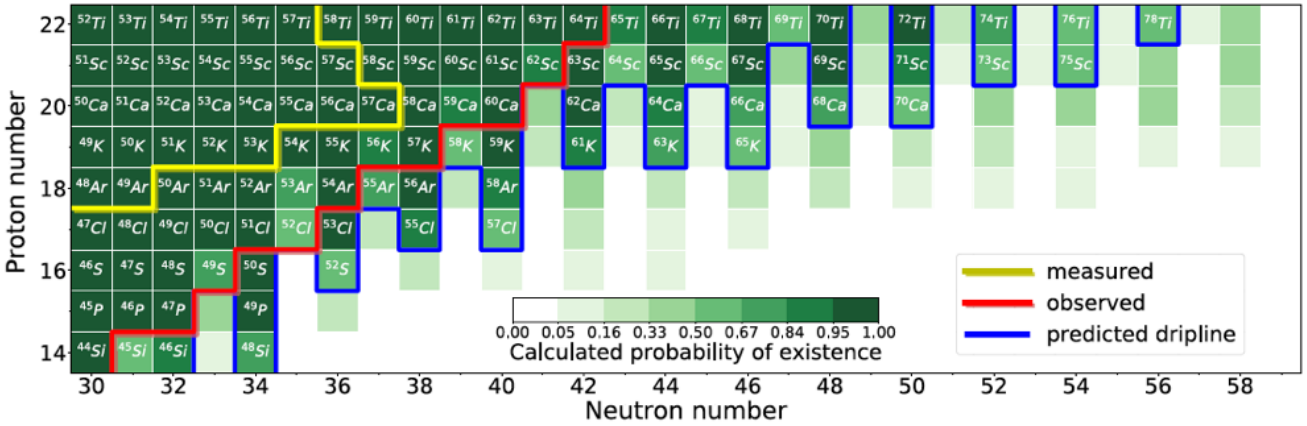
Machine Learning / AI

Nuclear theories always rely on a small number of parameters difficult to calibrate: ML/AI offer methods to quantify the related uncertainties

- Two major sources of uncertainties in nuclear models
  - Models for the (unknown) nuclear Hamiltonian
  - Many-body method and its computational implementation
- Quantify and propagate theoretical uncertainties (UQ)
  - Calibration of parameters of nuclear potentials
  - Truncation effects in systematic expansions
  - Extrapolation where experimental data is unavailable
- Build accurate emulators of (very) expensive computational models
  - Approximate solution at limit of infinite basis
  - Run large-scale MCMC calculations with expensive computer models

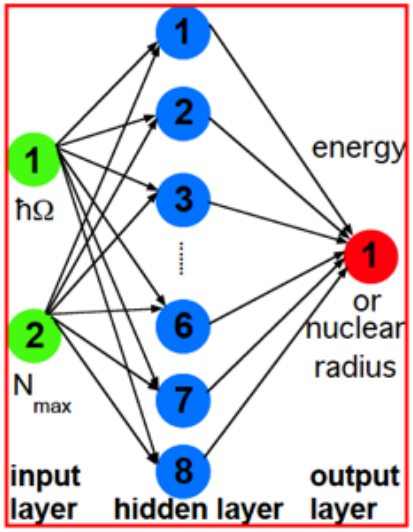
Machine Learning / AI

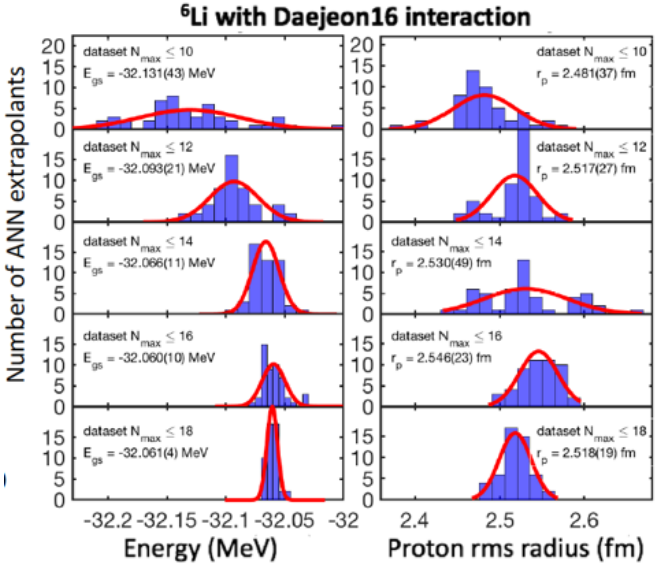
Nuclear theories always rely on a small number of parameters difficult to calibrate: ML/AI offer methods to quantify the related uncertainties



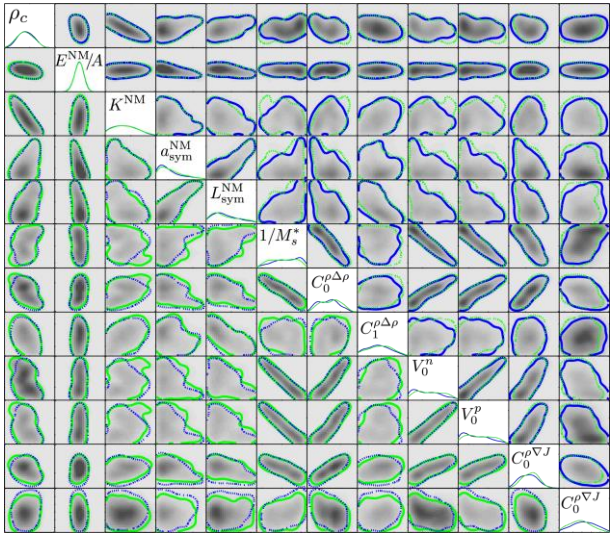
PRL **122**, 062502 (2019)

PRC **99**, 054308 (2019)





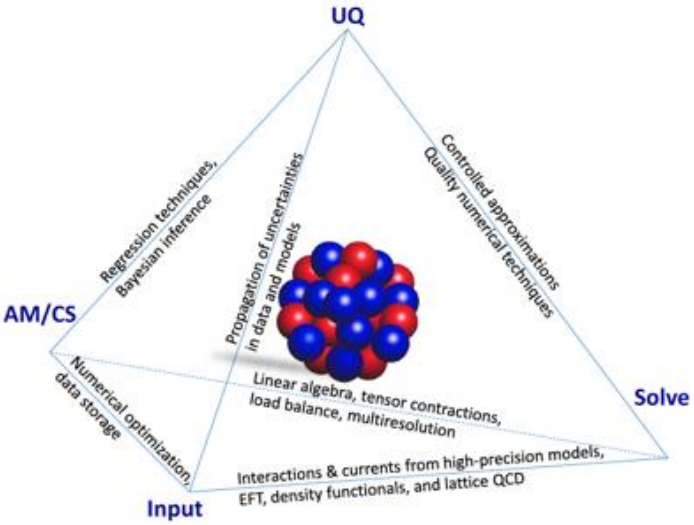
PRL **114**, 122501 (2015)



The SciDAC Project

Breakthrough can emerge from jointly-funded, multidisciplinary teams of nuclear theorists, applied mathematicians and computer scientists

http://nuclei.mps.ohio-state.edu/



Scientific Achievement

- **Parallel optimization code POUNDERS for optimizing low-energy functional**
- **Disrupted conventional manual and underoptimized approaches**

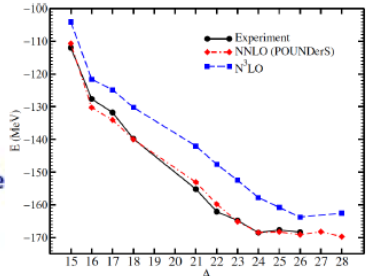
Math of complex systems: POUNDERS foundation

UNEDF SciDAC-2: UNEDF0

Derivative-free optimization method developed under ASCR math program on complex systems and ASCR + NP SciDAC partnership

UNEDF SciDAC-2: UNEDF1

Nuclear energy density optimization. Kortelainen, Lesinski, Moré, Nazarewicz, Sarich, Schunck, Stoitsov, Wild. *Phys Rev C*, 2010.



Correct neutron dripline at ^{24}O

NUCLEI SciDAC-3: N2LOopt

Nuclear energy density optimization: Large deformations. Kortelainen, McDonnell, Nazarewicz, Reinhard, Sarich, Schunck, Stoitsov, Wild. *Phys Rev C* 2012.

NUCLEI SciDAC-4

An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order. Ekström, Baardsen, Forssén, Hagen, Hjorth-Jensen, Jansen, Machleidt, Nazarewicz, Papenbrock, Sarich, Wild. *Phys Rev Lett*, 2013.

Open-source, scalable implementation available in PETSc

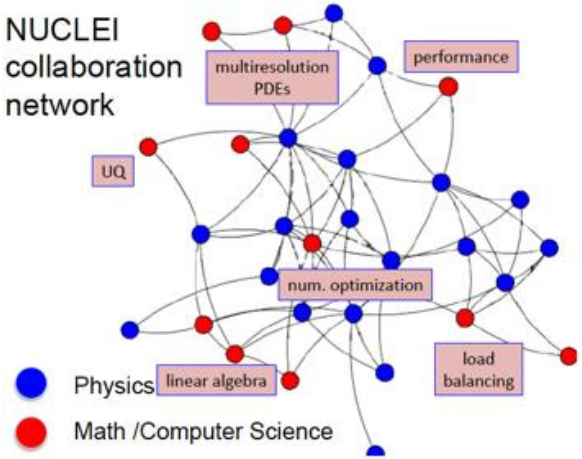
Latest developments account for correlations

mcs.anl.gov/petsc

Now Designated Essential Science Indicator Highly Cited Papers in Physics

NP researchers

ASCR researchers



- On-going effort since 2007
- Several mathematical/computational methods opened new avenues in physics
- Very effective pipeline for workforce

Conclusions

High-performance computing has been a paradigm shift for low-energy nuclear theory

- There is no "standard model" for nuclear theory: Coexistence of different theoretical approaches imply different computational strategies
  - Extreme-scale linear algebra and tensor contractions (ab initio methods)
  - Dense, complex linear algebra and very large ensemble runs (DFT)
- The two biggest challenges for computational nuclear physics
  - Physics models are not fixed but are continually evolving
  - Cost of adapting existing codes to emerging architectures is high
    - Complexity of legacy codes
    - Physics models are changing
- Nuclear theory is embracing machine leaning / AI
  - As diagnostics of approximate theories
  - For emulating/optimizing computationally expensive models
  - No substitute for better theories…