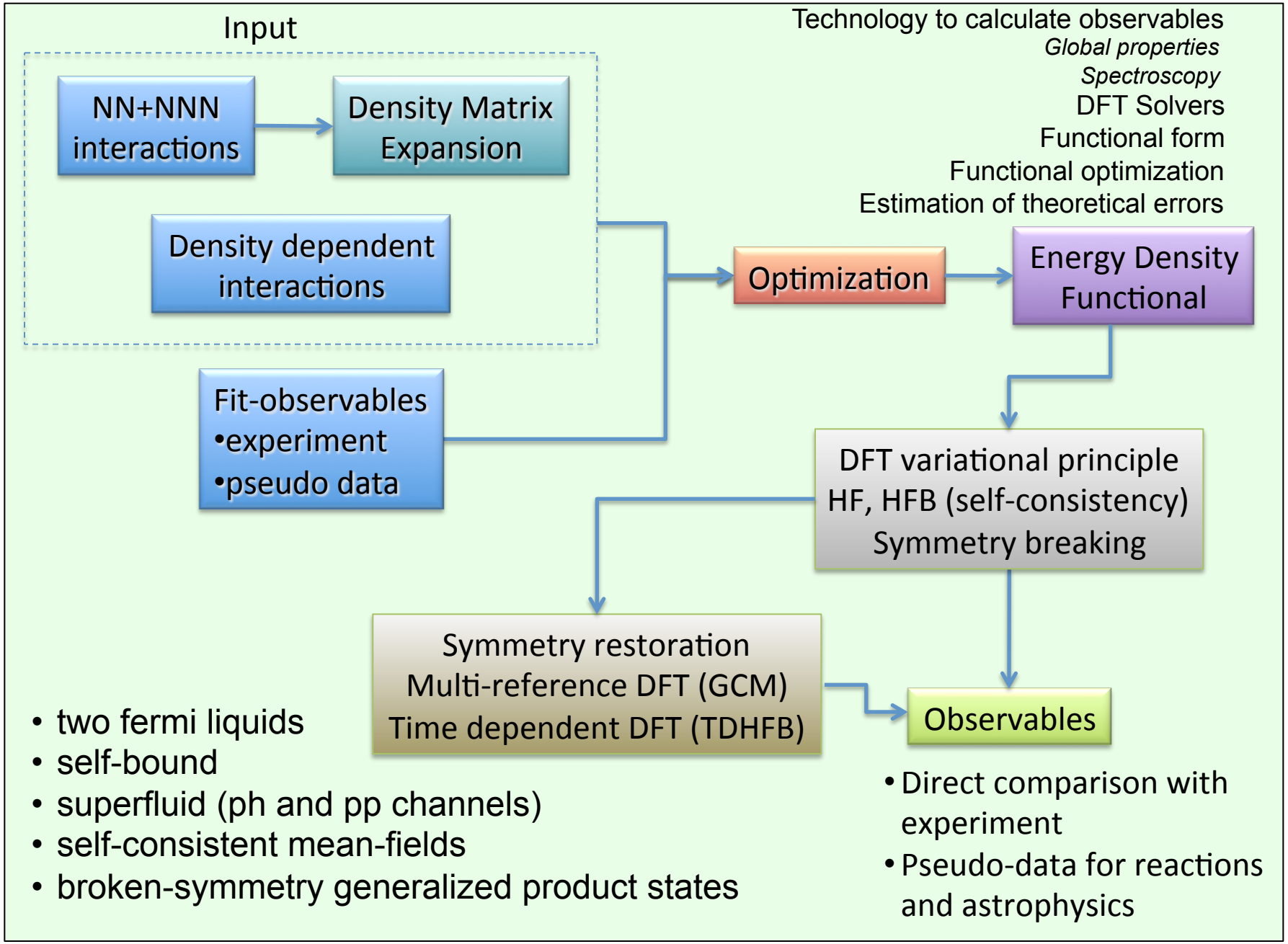
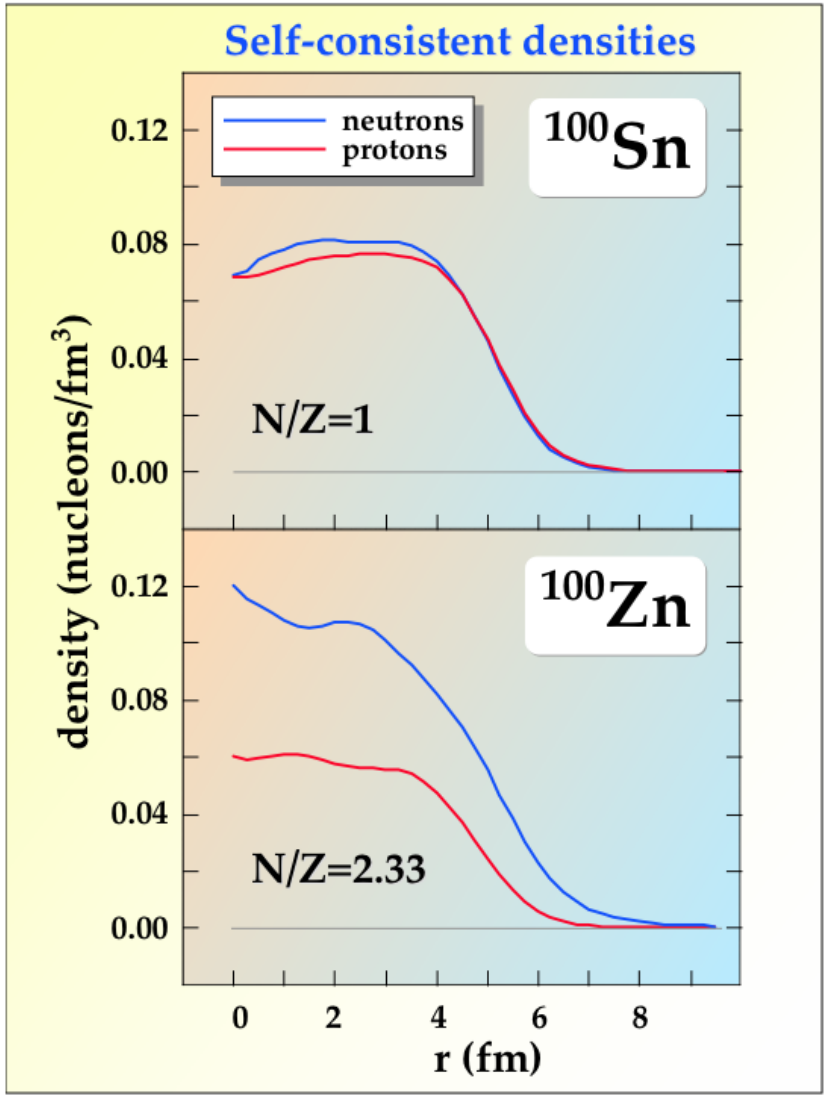
Nuclear Density Functional Theory and Extensions



Mean-Field Theory ⇒ Density Functional Theory

Degrees of freedom: nucleonic densities



Nuclear DFT

- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.

Nuclear Energy Density Functional

isoscalar (T=0) density $\left(\rho_0 = \rho_n + \rho_p\right)$

isovector (T=1) density $\left(\rho_1 = \rho_n - \rho_p\right)$

+isoscalar and isovector densities:
spin, current, spin-current tensor, kinetic, and kinetic-spin
+ pairing densities

$$E = \int \mathcal{H}(r) d^3 r$$

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0(r) + \sum_{t=0,1} \left(\chi_t(r) + \breve{\chi}_t(r)\right)$$

p-h density p-p density (pairing functional)

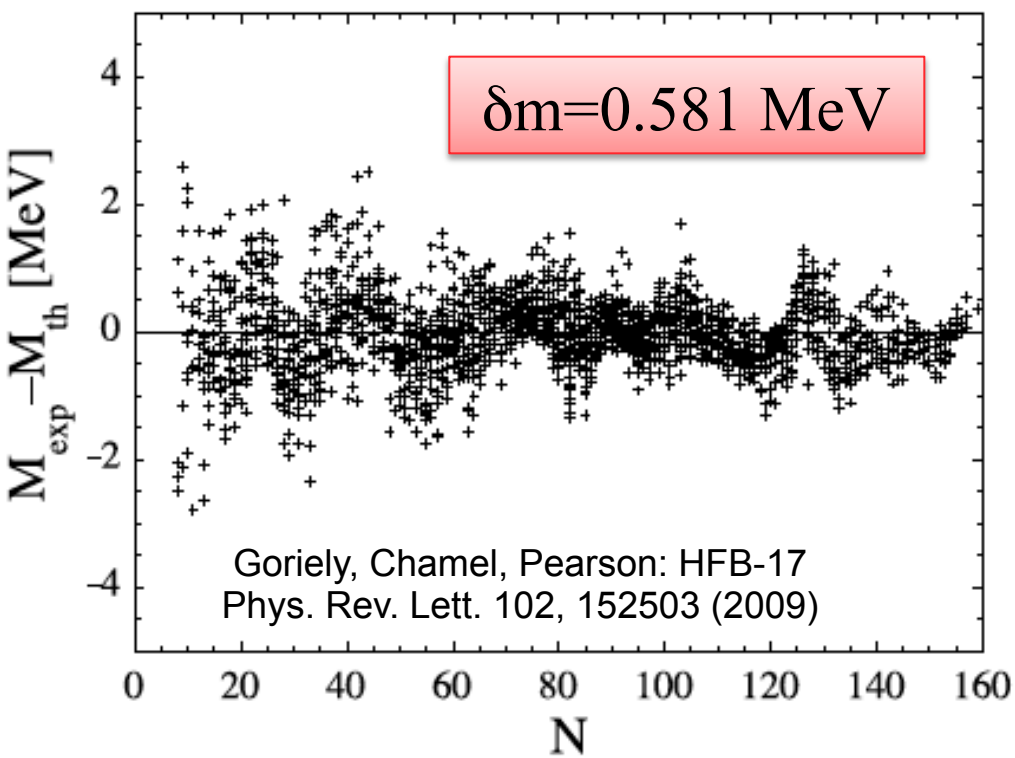
Expansion in densities and their derivatives

- Constrained by microscopic theory: ab-initio functionals provide quasi-data!
- Not all terms are equally important. Usually ~12 terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active.
- Becomes very simple in limiting cases (e.g., unitary limit)
- Can be extended into multi-reference DFT (GCM) and projected DFT

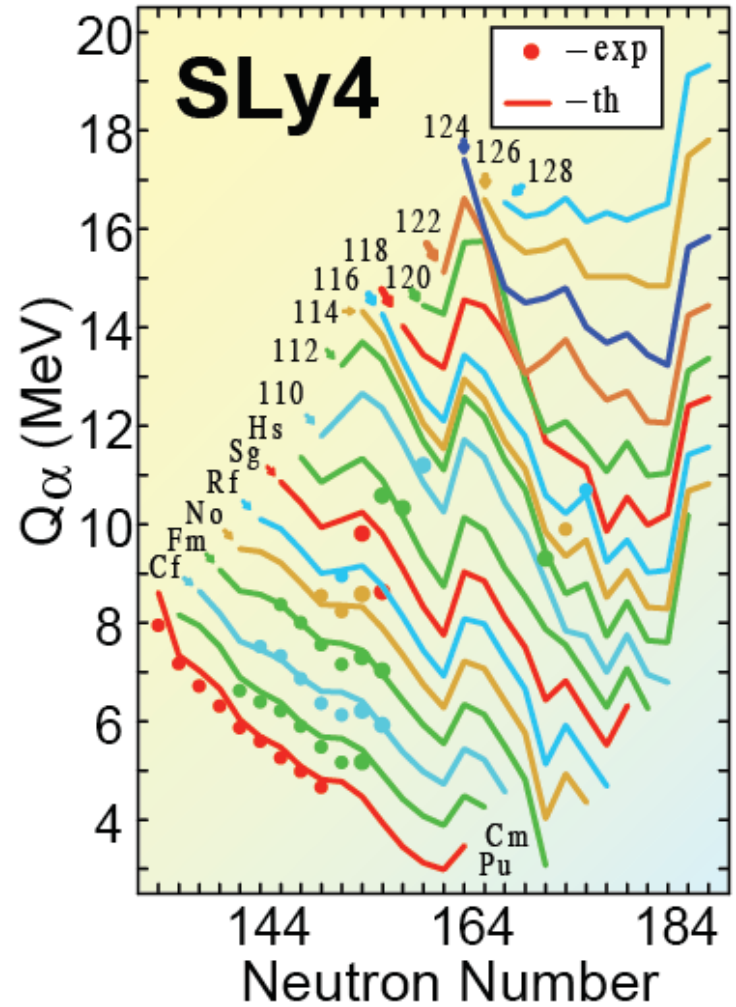
Examples: Nuclear Density Functional Theory

Traditional (limited) functionals provide quantitative description

Mass table

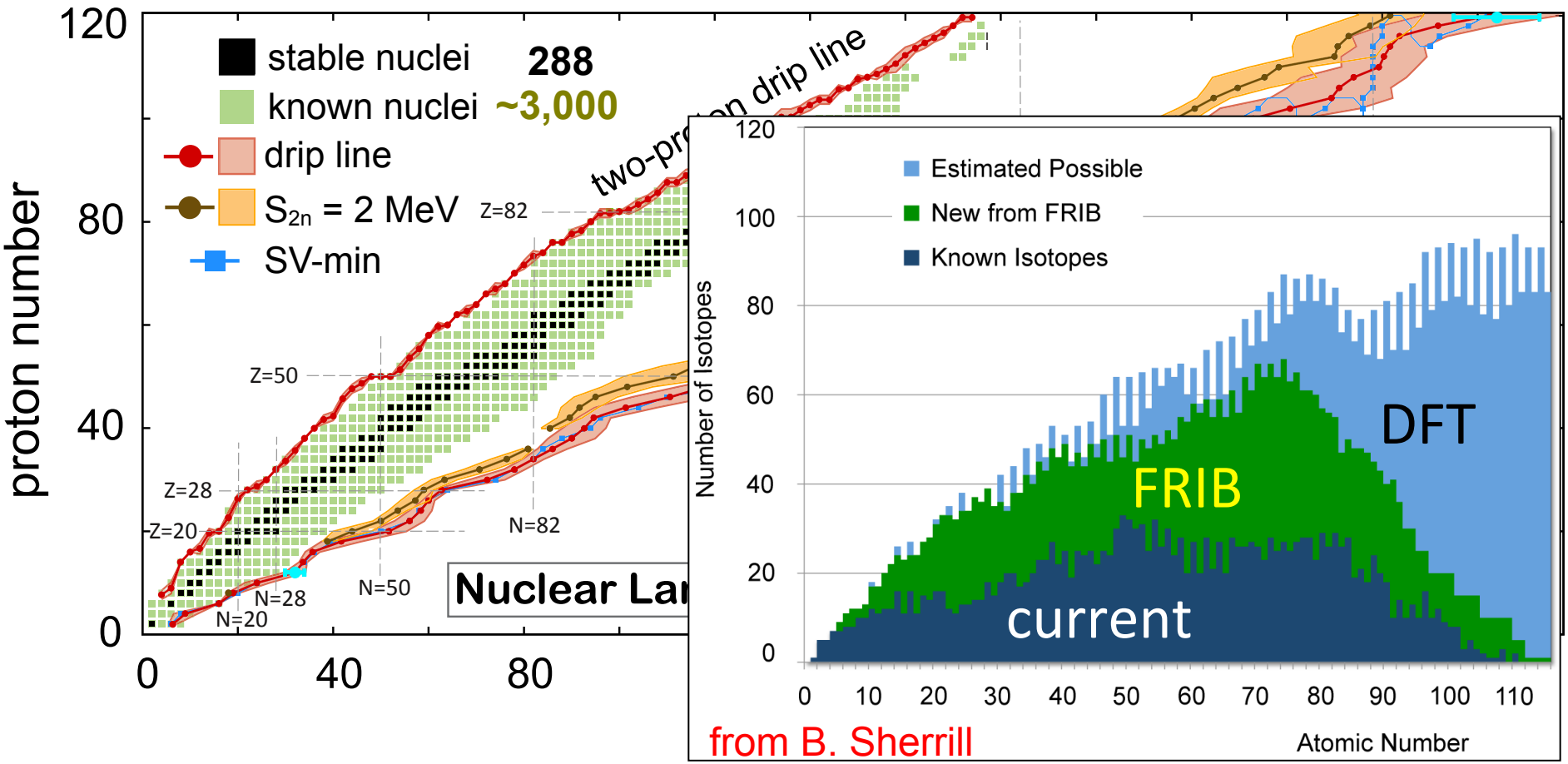


BE differences



Cwiok et al., Nature, 433, 705 (2005)

Quantified Nuclear Landscape



How many protons and neutrons can be bound in a nucleus?

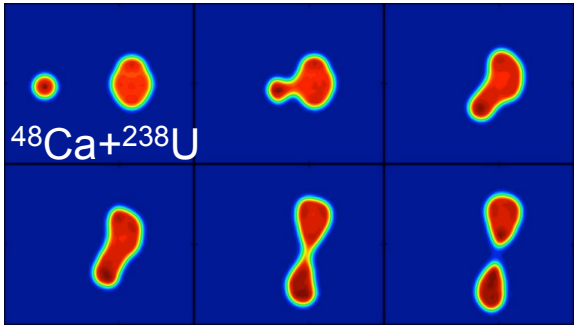
Erler et al.
Nature 486, 509 (2012)

Literature: 5,000-12,000

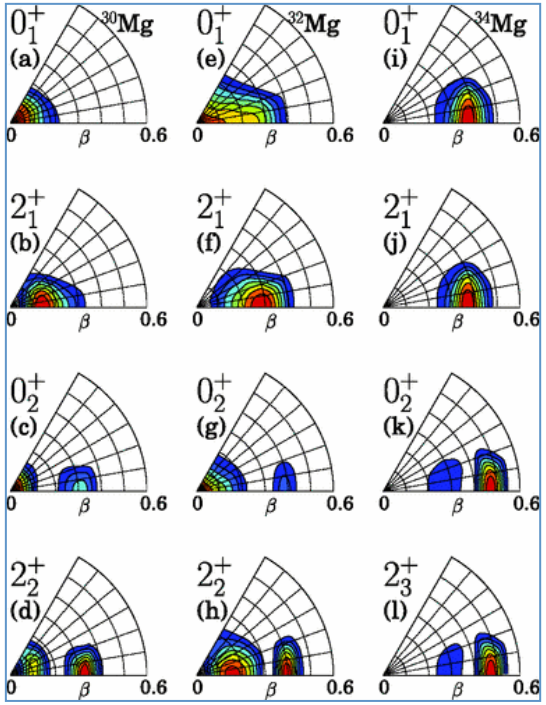
Skyrme-DFT: 6,900±500$_{syst}$

Small and Large-Amplitude Collective Motion

- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena



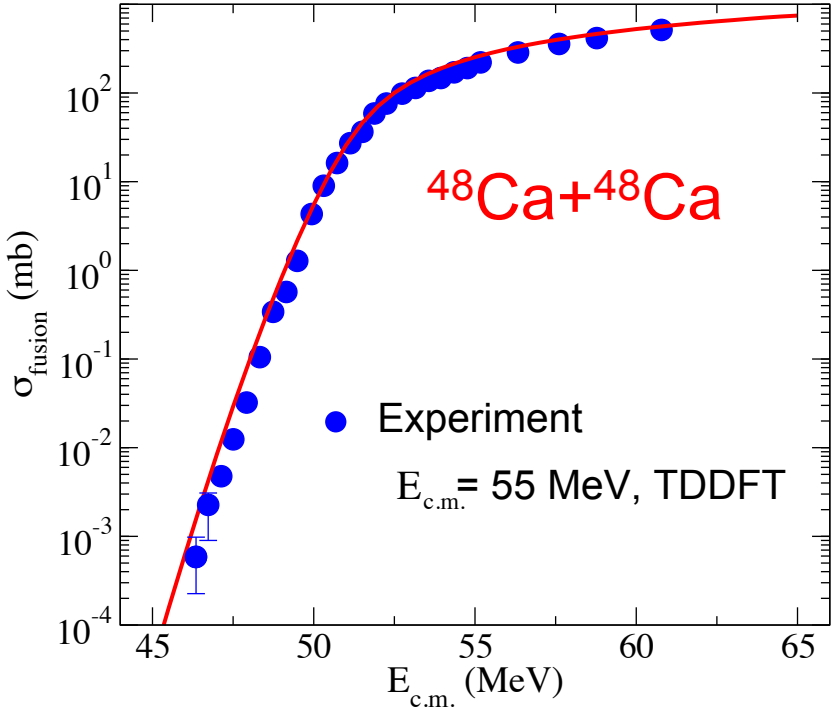
Shape coexistence



Hinohara et al. PRC 84, 061302(R) (2011)

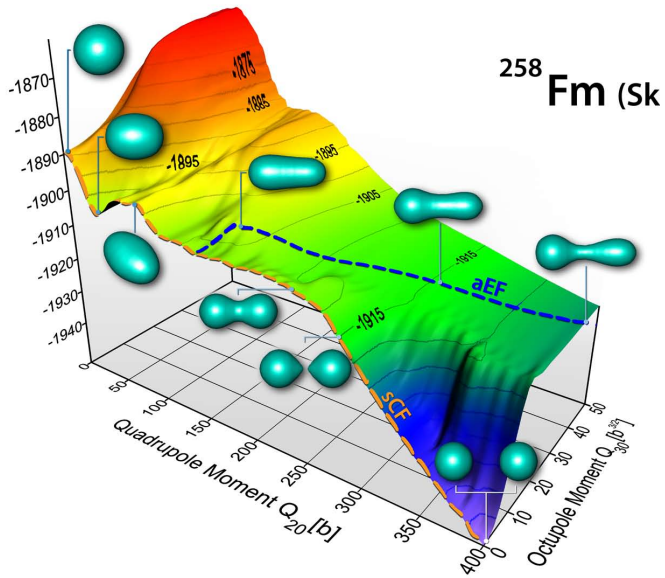
also: Tsunoda et al. Phys. Rev. C 89, 031301(R) (2014); HPCI

Fusion cross section



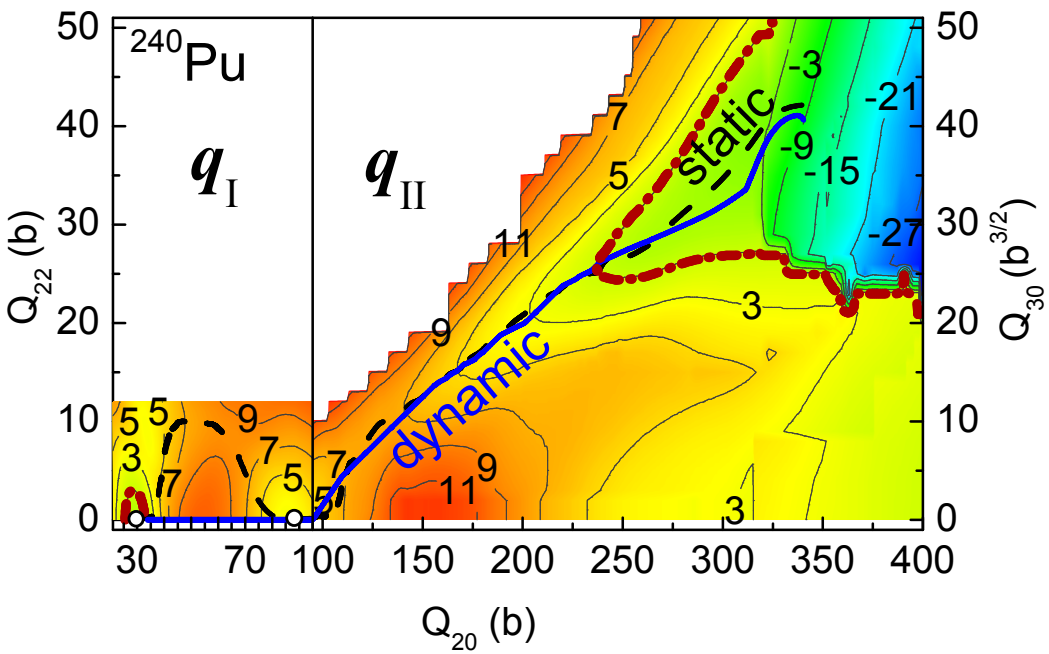
R. Keser et al., PRC 85, 044606 (2012)

Nuclear Fission

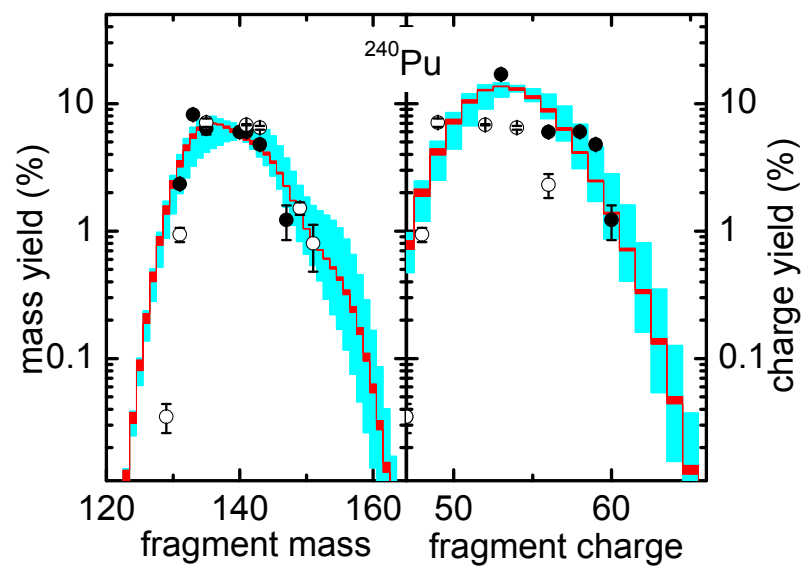


$$T_{1/2} = \ln 2/(nP) \quad P = 1/(1+e^{2S})$$

$$S(L) = \int_{s_{\rm in}}^{s_{\rm out}} \frac{1}{\hbar}\sqrt{2\mathcal{M}_{\rm eff}(s)\,(V(s)-E_0)}\,ds$$



Spontaneous fission yields

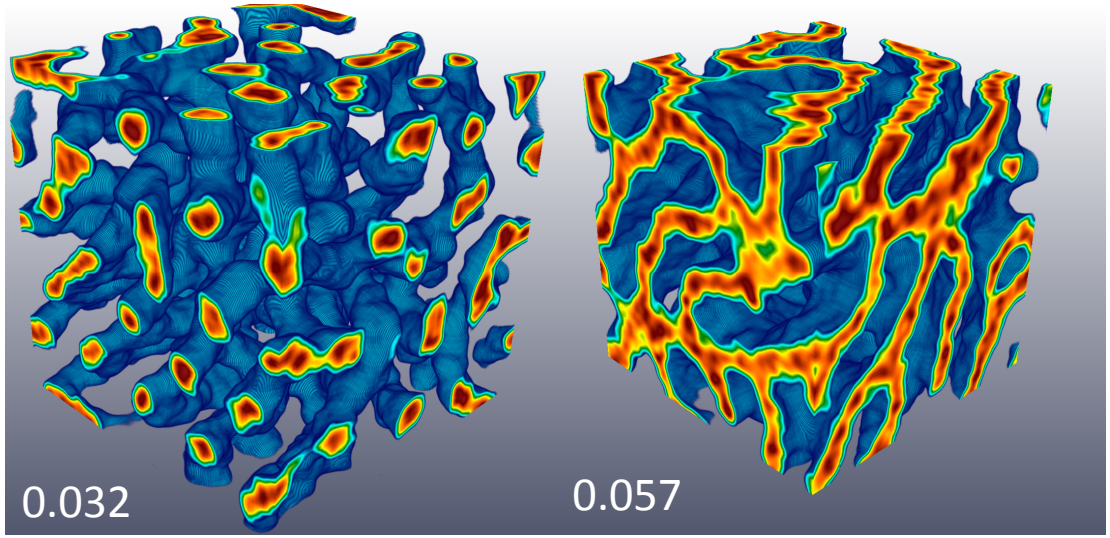


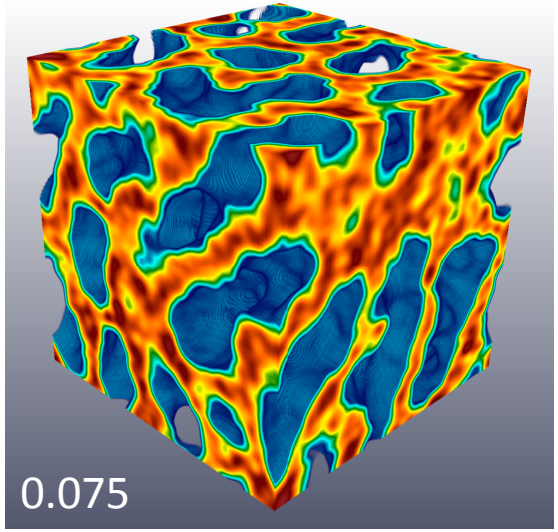
Sadhukhan et al. Phys. Rev. C 90 061304(R) (2014) and arXiv:1510.08003

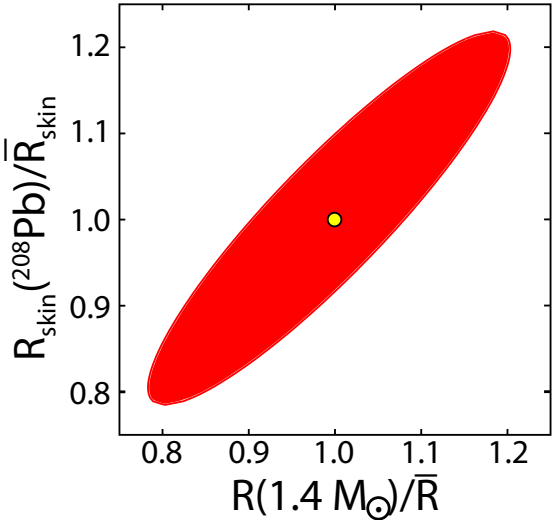
http://science.energy.gov/ascr/highlights/2015/ascr-2015-08-a/

Quest for understanding the neutron-rich matter on Earth and in the Cosmos

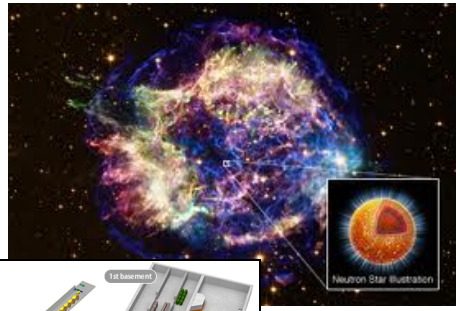
Crustal structures in neutron stars

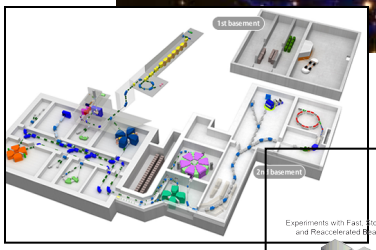


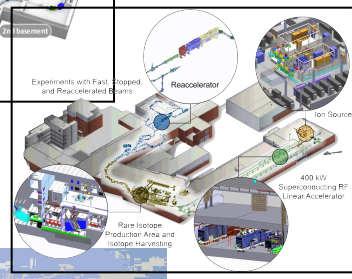




Data







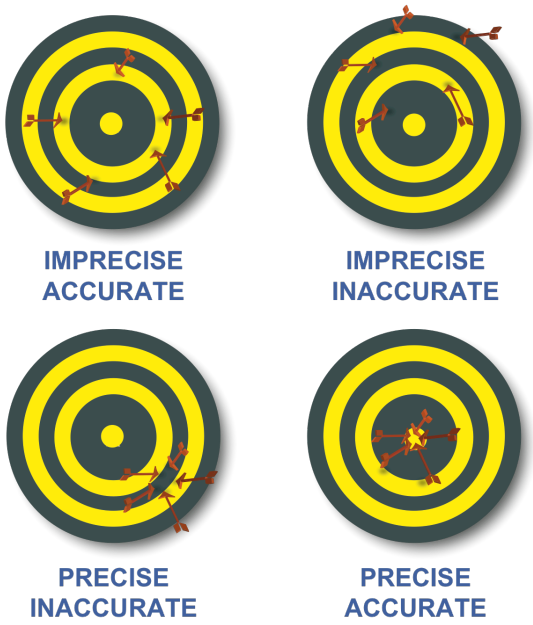
The covariance ellipsoid for the neutron skin R_{skin} in ^{208}Pb and the radius of a $1.4M_\odot$ neutron star. The mean values are: $R(1.4M_\odot)=10$ km and $R_{skin}= 0.17$ fm.

ISNET: Enhancing the interaction between nuclear experiment and theory through information and statistics

JPG Focus Issue: http://iopscience.iop.org/0954-3899/page/ISNET

Around 35 papers (including nuclear structure, reactions, nuclear astrophysics, medium energy physics, statistical methods… and fission…)

"Remember that all models are wrong; the practical question is *how wrong do they have to be to not be useful*" (E.P. Box)

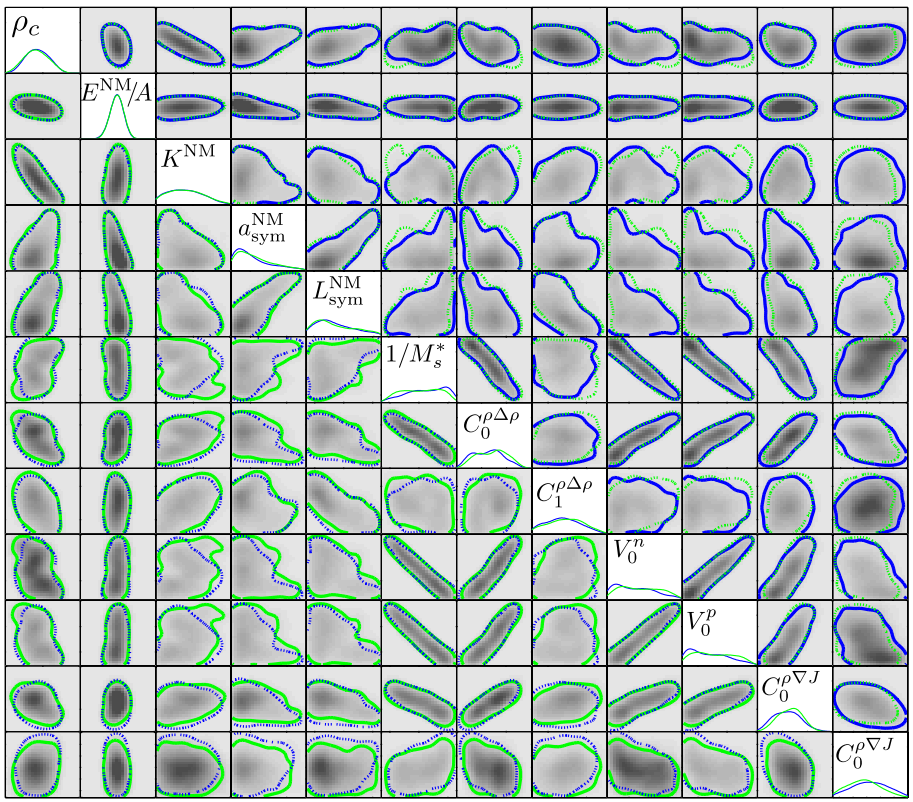


Error estimates of theoretical models: a guide

J. Phys. G **41** 074001 (2014)

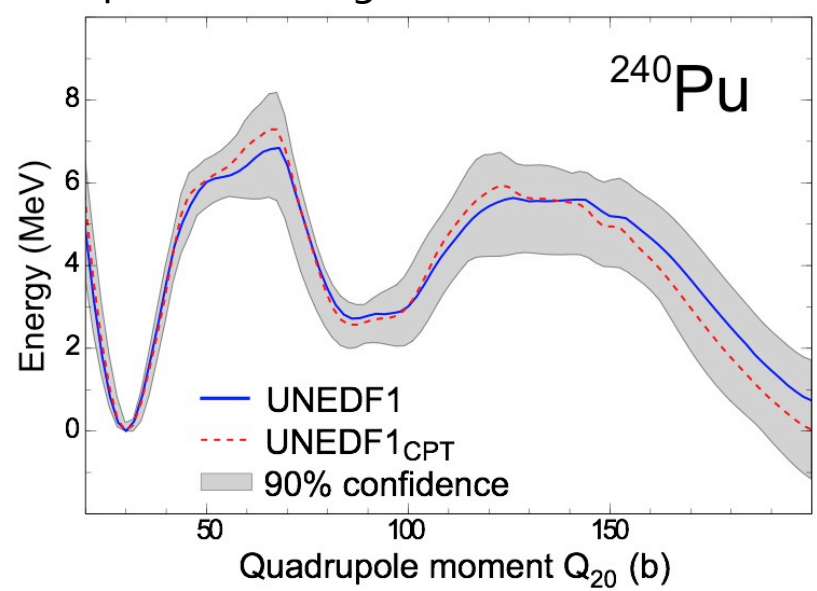
Information Content of New Measurements

J. McDonnell et al. Phys. Rev. Lett. 114, 122501 (2015)



Bivariate marginal estimates of the posterior distribution for the 12-dimensional DFT UNEDF$_1$ parameterization.

- Developed a Bayesian framework to quantify and propagate statistical uncertainties of EDFs.
- Showed that new precise mass measurements do not impose sufficient constraints to lead to significant changes in the current DFT models (models are not precise enough)



Theoretical Tools and Connections to Computational Science

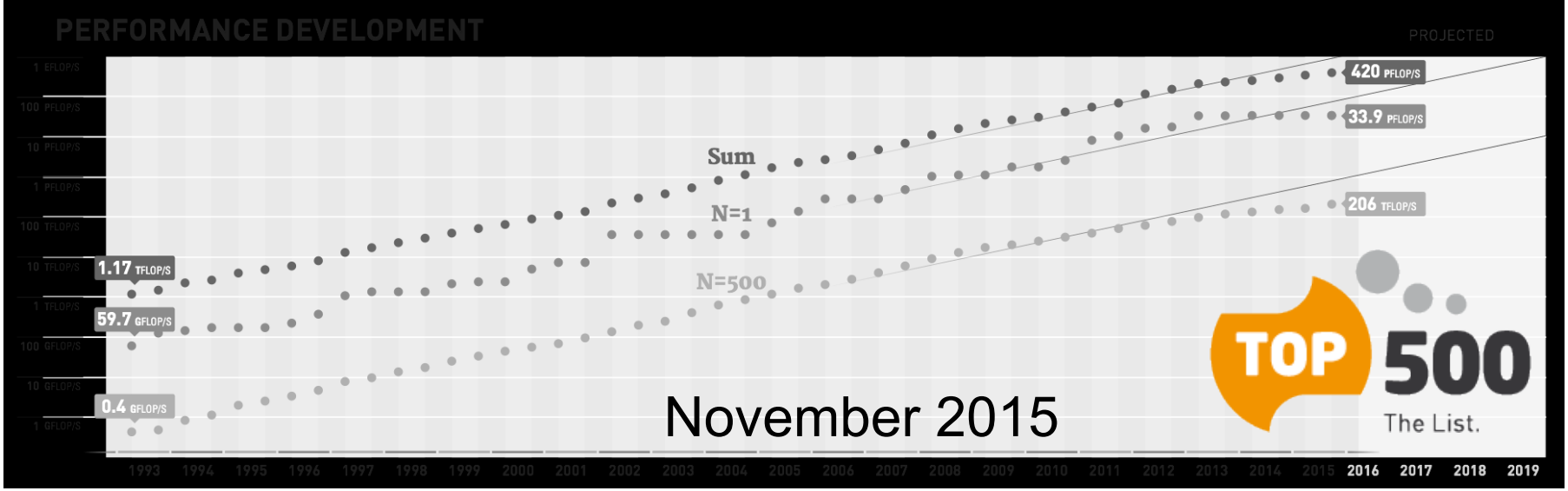
1teraflop=10^{12} flops
1peta=10^{15} flops (today)
1exa=10^{18} flops (next 10 years)

Tremendous opportunities for nuclear theory!

3,120,000 cores

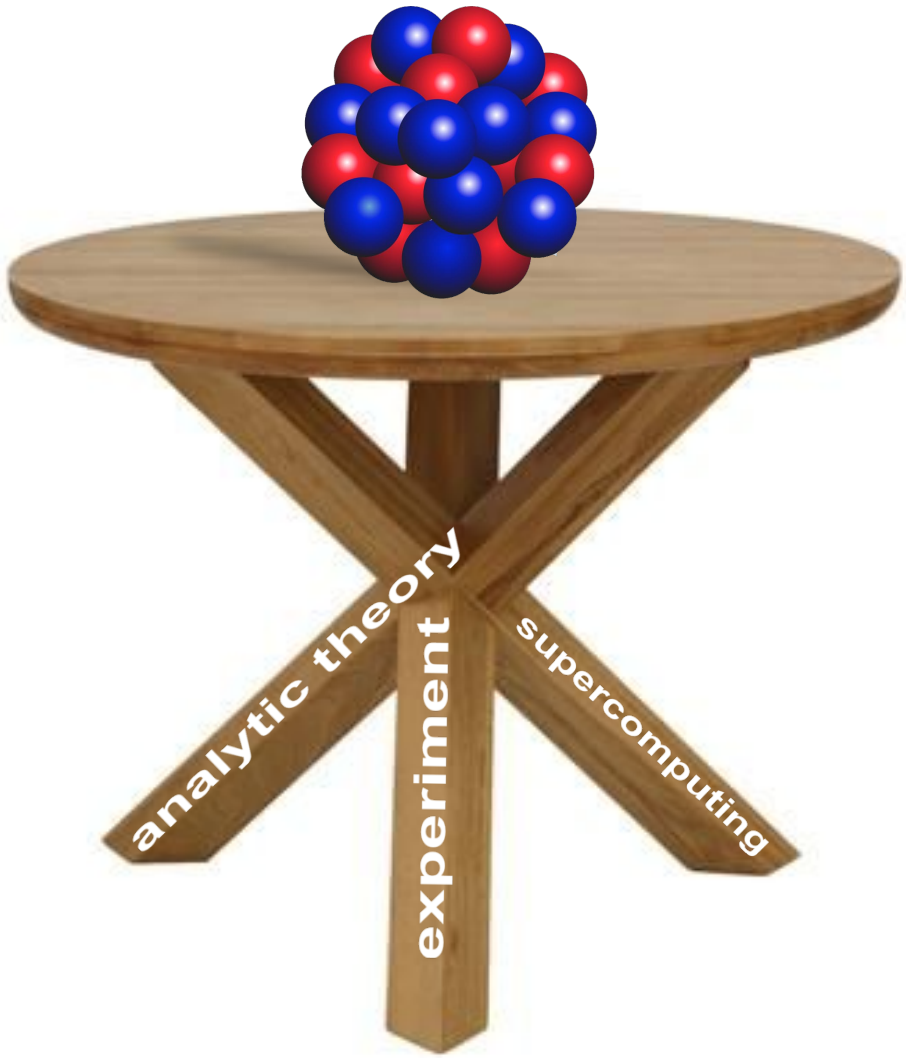
33.9 pflops

	NAME	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Tianhe-2 (Milkyway-2)	Intel Ivy Bridge (12C 2.2 GHz) & Xeon Phi (57C 1.1 GHz), Custom interconnect	NUDT	China	3,120,000	33.9	17.8
2	Titan	Cray XK7, Opteron 6274 (16C 2.2 GHz) + Nvidia Kepler GPU, Custom interconnect	DOE/SC/ORNL	USA	560,640	17.6	8.2
3	Sequoia	IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	17.2	7.9
4	K computer	Fujitsu SPARC64 VIIIfx (8C 2.0 GHz), Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
5	Mira	IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect	DOE/SC/ANL	USA	786,432	8.59	3.95



http://top500.org

High Performance Computing and Nuclear Theory



"High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, *it becomes a third leg supporting the field of nuclear physics*." (NAC Decadal Study Report)

Future: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math