Designer Nuclei: New Tools and New Applications

Argonne National Laboratory Physics Department Colloquium

26 March, 2010

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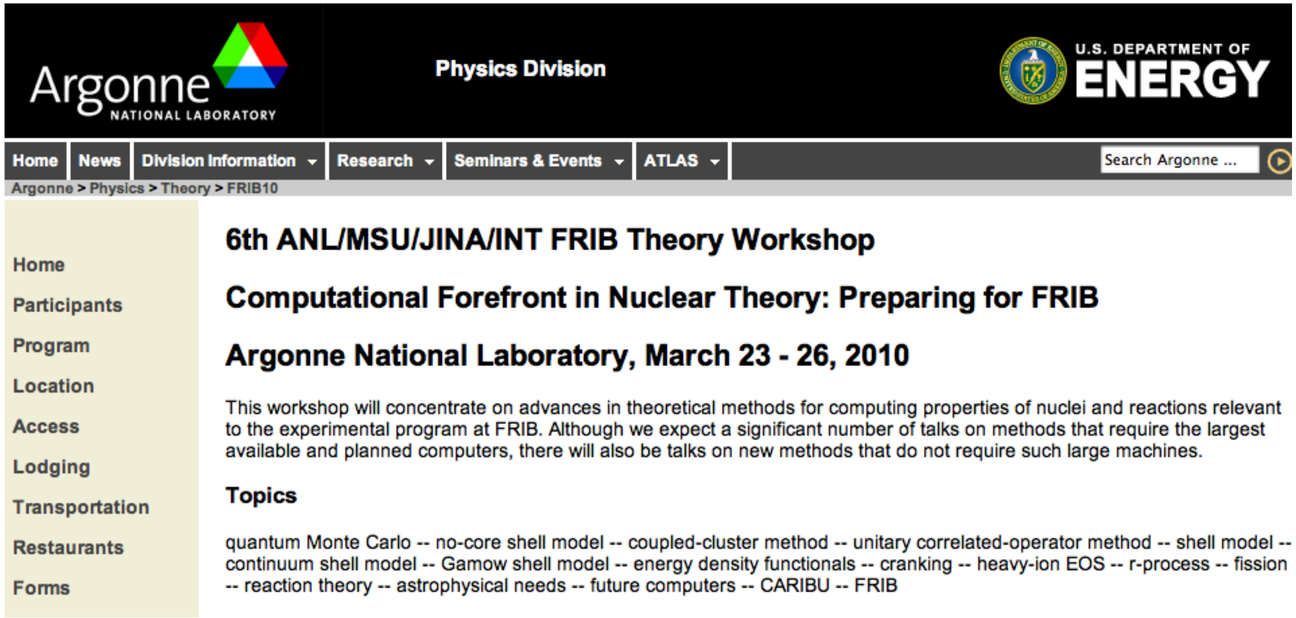
Michigan State University

U.S. DEPARTMENT OF ENERGY

Office of Science

Computational Forefront in Nuclear Theory
6th FRIB Theory Workshop

- This colloquium is the final talk of the Nuclear Theory workshop



6th ANL/MSU/JINA/INT FRIB Theory Workshop

Computational Forefront in Nuclear Theory: Preparing for FRIB

Argonne National Laboratory, March 23 - 26, 2010

This workshop will concentrate on advances in theoretical methods for computing properties of nuclei and reactions relevant to the experimental program at FRIB. Although we expect a significant number of talks on methods that require the largest available and planned computers, there will also be talks on new methods that do not require such large machines.

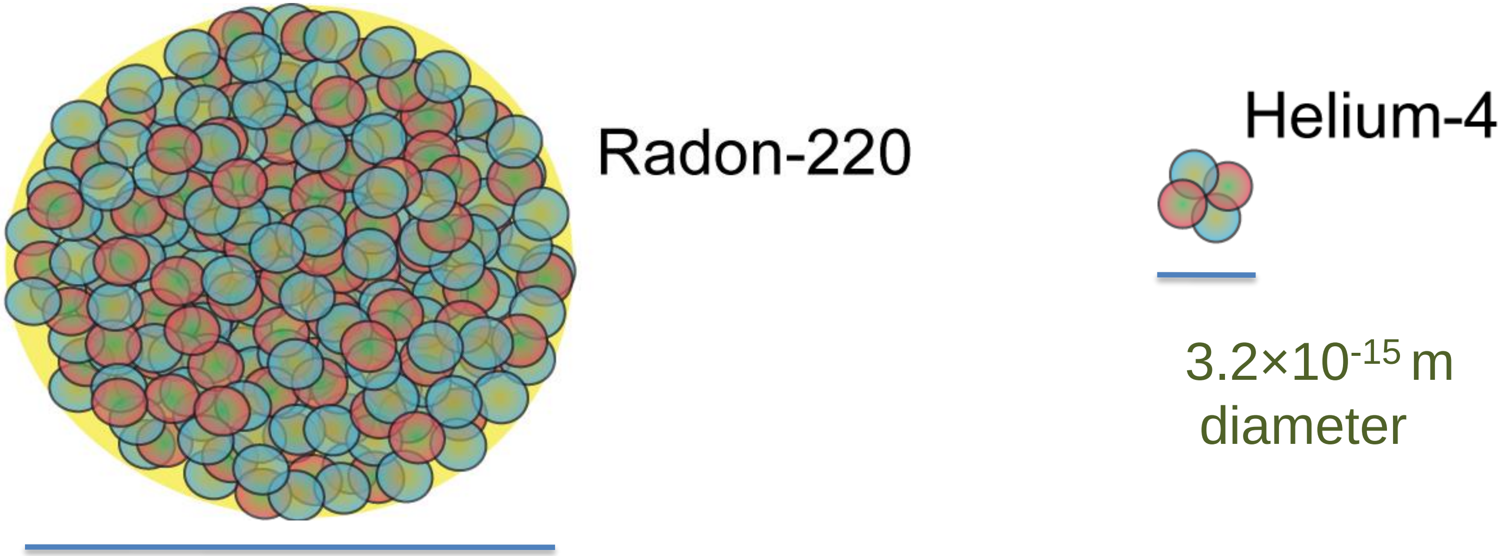
Topics

quantum Monte Carlo -- no-core shell model -- coupled-cluster method -- unitary correlated-operator method -- shell model -- continuum shell model -- Gamow shell model -- energy density functionals -- cranking -- heavy-ion EOS -- r-process -- fission -- reaction theory -- astrophysical needs -- future computers -- CARIBU -- FRIB

- Organizers
  - Filomena Nunes, Michigan State
  - Steven C. Pieper, Argonne
  - Craig Roberts, Argonne
  - Robert Wiringa, Argonne
  - David B. Kaplan, INT

The problem we want to solve

- Atomic nuclei and how they interact: Three of the four forces in nature are relevant, the dominant force, QCD, is nonperterbative.



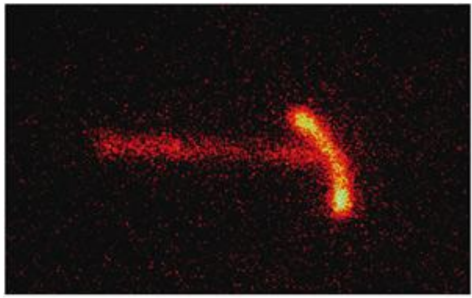
3.2×10^{-15} m diameter

1.5×10^{-14} m diameter

- Few body physics but also mesoscopic science
- Nuclear physics provides many examples of diverse mesoscopic phenomena, including phase transitions, superfluidity and superconductivity, and quantum chaos.

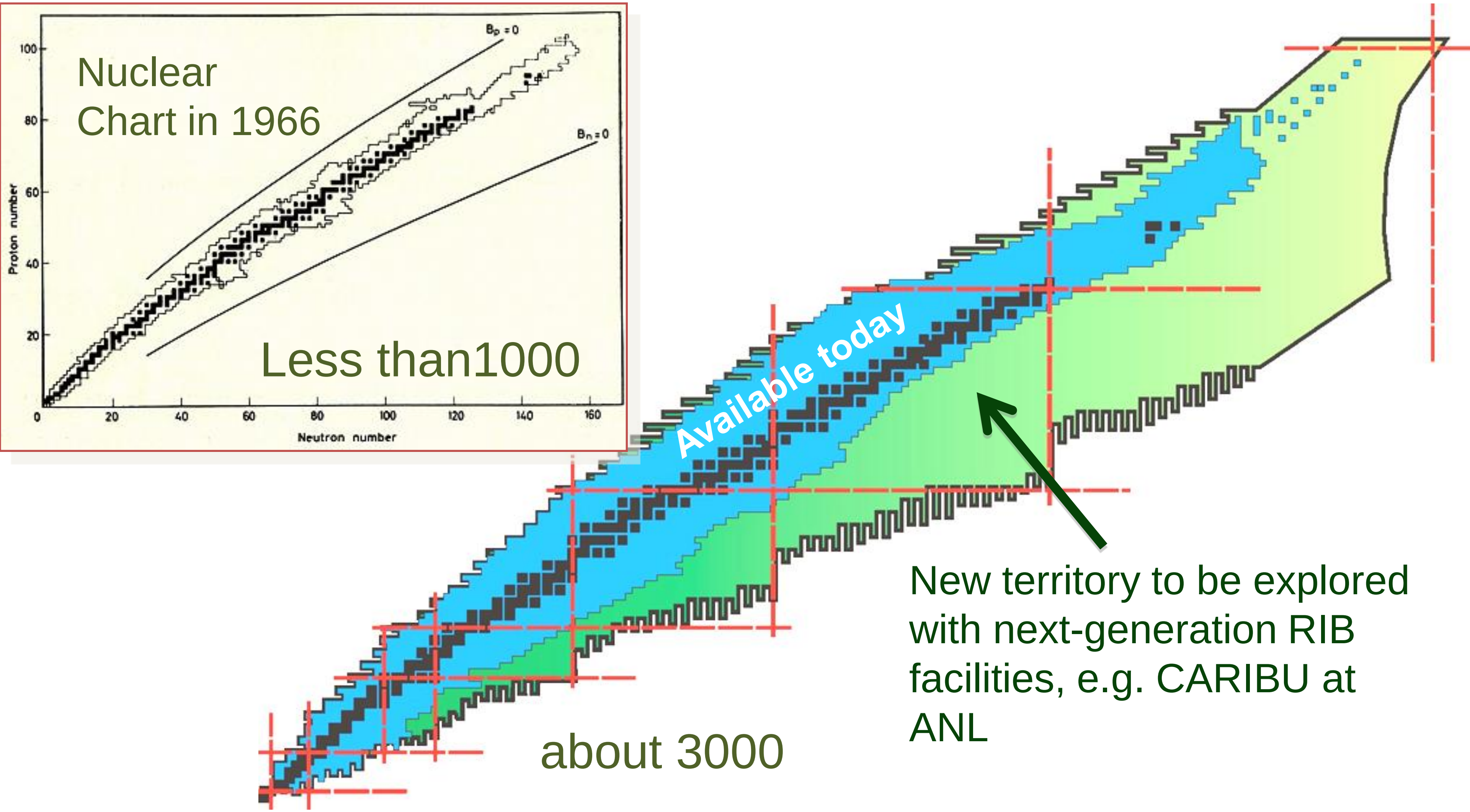
Designer atomic nuclei

- Designer Nuclei: The possibility for a researcher (theorist) to order a nucleus that has a specified number of neutrons and protons
- To make progress in nuclear physics, some astrophysics, and some high energy physics we need such a capability. In the talk I will give some examples from the workshop
- The term "designer nuclei" was introduced by Aurel Bulgac, Phys. Rev. Lett. 89, 050402 (2002) Dilute Quantum Droplets
- There are about 263 stable combinations found in nature, with about 1500 others studied in some detail. In 10 years we may have the capability to extend that to 5000 isotopes.
- Most combinations of neutrons and protons are radioactive; sometimes it is the novel radioactivity that is interesting
- Designer Nuclei ←→ Rare Isotopes



^{45}Fe two-proton decay: K Miernik *et al.* 2007 Phys. Rev. Lett. 99 192501

The availability of rare isotopes over time



Nuclear Chart in 1966

Less than1000

Available today

about 3000

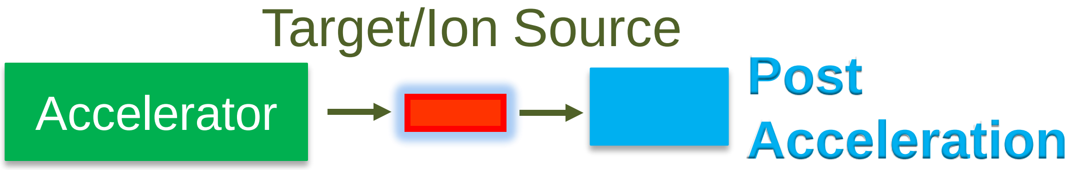
New territory to be explored with next-generation RIB facilities, e.g. CARIBU at ANL

Nuclei matter

- The atomic nucleus is a significant intellectual challenge. Can we construct a comprehensive and predictive model of its properties? How do we relate that model to QCD? Surprises are still likely.
- The properties of nuclei are relevant to other sciences
    - Fundamental symmetries studies, e.g., neutrinoless double-beta decay the rate is related to nuclear matrix elements
    - Modeling astrophysical environments; e.g., nucleosynthesis in supernovae, depends on properties of exotic isotopes, or, neutron star properties which are related to properties of very neutron-rich nuclei
- The properties of nuclei are important for a wide variety of applications
    - Nuclear power (nuclear data is needed to optimize reactor design)
    - Homeland security (forensics involves the same types of reactions, e.g. (n,2n), important for astrophysics; detection of nuclear material and other threats)
    - Stockpile stewardship (ditto)
    - Medical diagnostics (^{99}Mo ; ^{18}F; etc.)
    - Industrial and environmental tracers (^{7}Be, ^{210}Pb, ^{137}Cs, etc.)

Rare Isotope Production Techniques using Accelerators

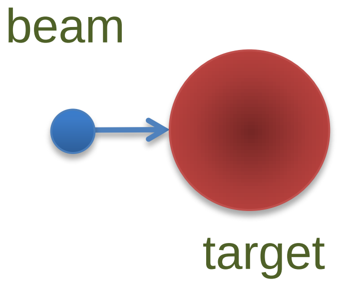
- Target spallation and fragmentation by light ions



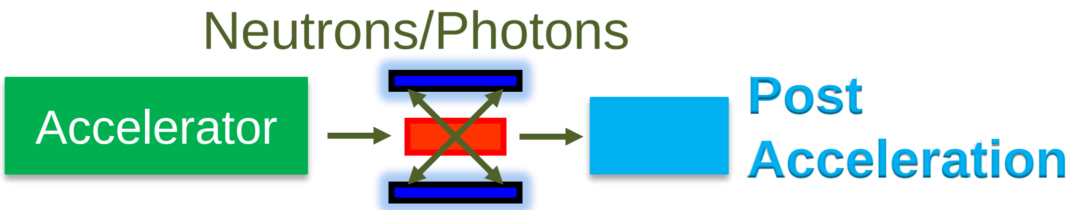
Target/Ion Source

Accelerator

Post Acceleration



- Neutron induced fission (2-step target)

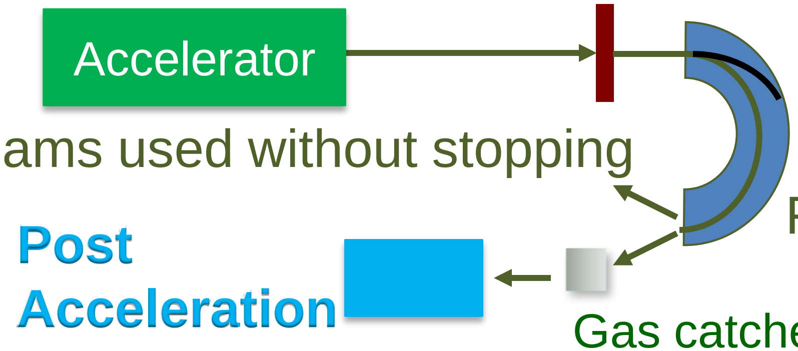


Neutrons/Photons

Accelerator

Post Acceleration

- In-flight Separation following projectile fragmentation/fission (Used by FRIB)



Accelerator

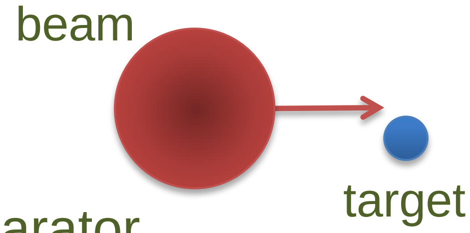
Beam

Beams used without stopping

Fragment Separator

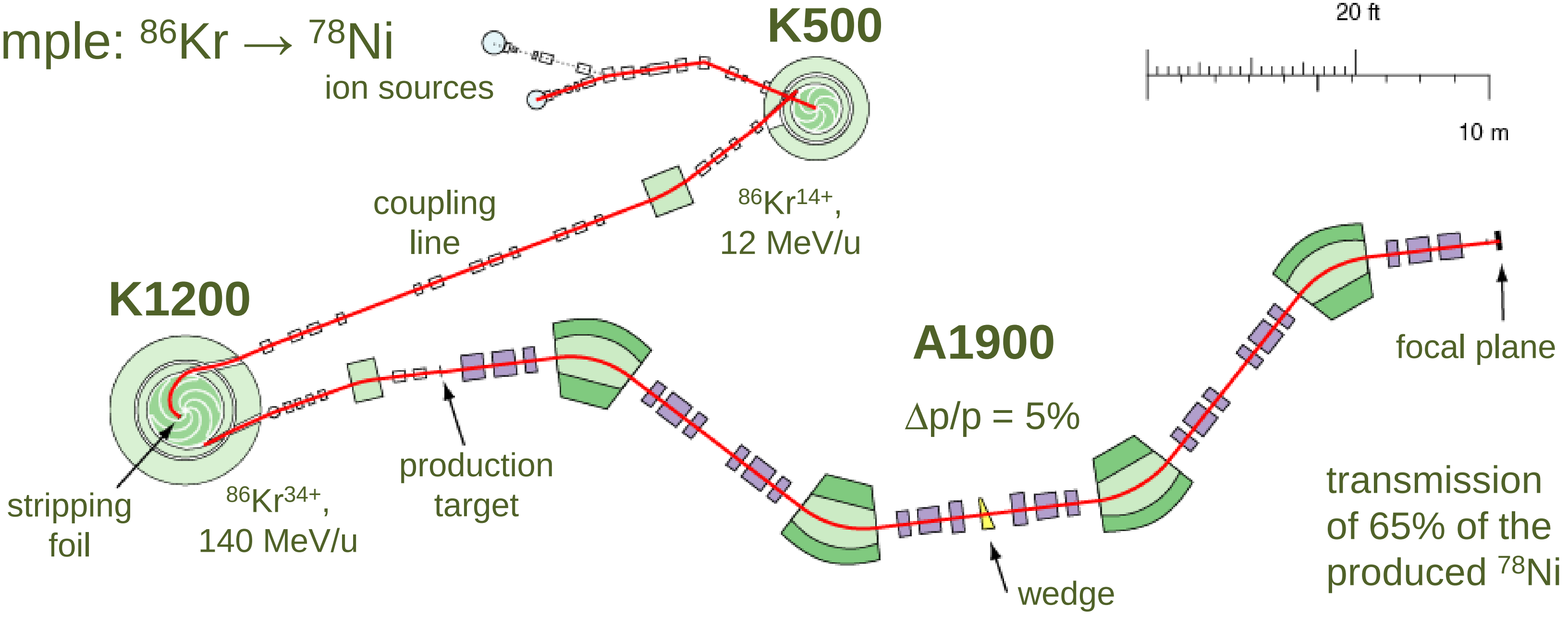
Post Acceleration

Gas catcher/ solid catcher + ion source



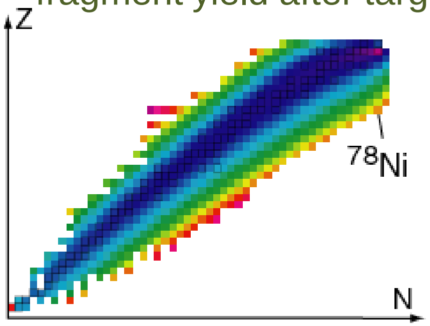
In-Flight Production of Rare Isotopes
Example: NSCL's CCF

Example: $^{86}Kr \rightarrow {}^{78}Ni$

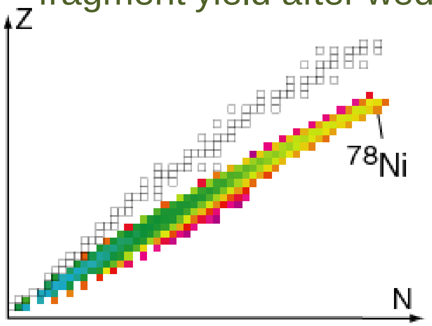


transmission of 65% of the produced ^{78}Ni

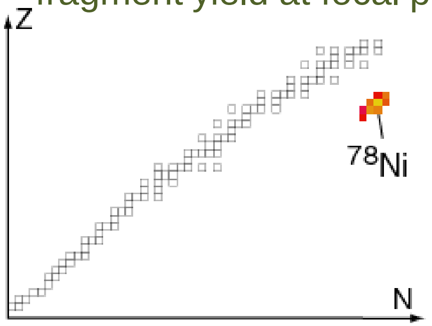
fragment yield after target



fragment yield after wedge

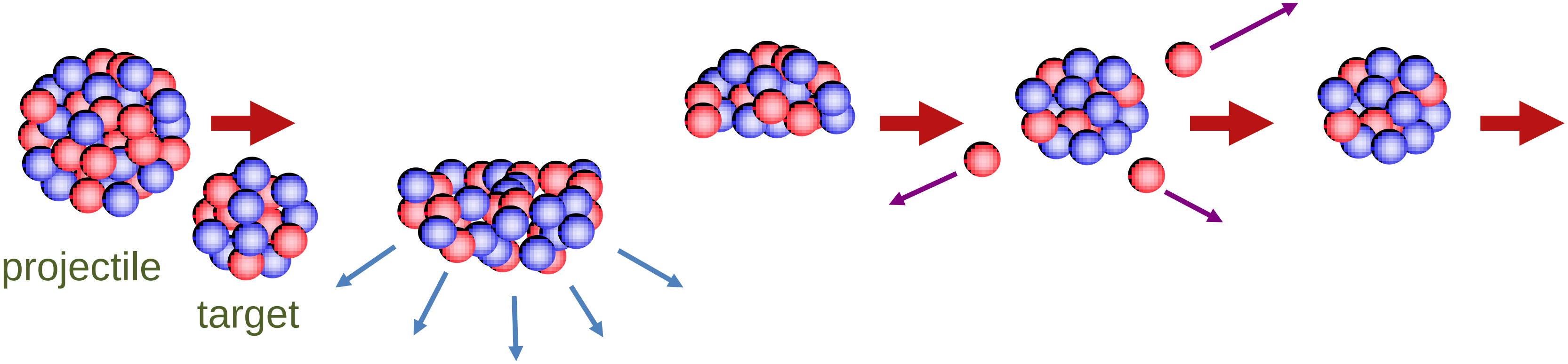


fragment yield at focal plane



Production of Rare Isotopes in Flight

1. Cartoon of the production process - fragmentation (fission is also used)

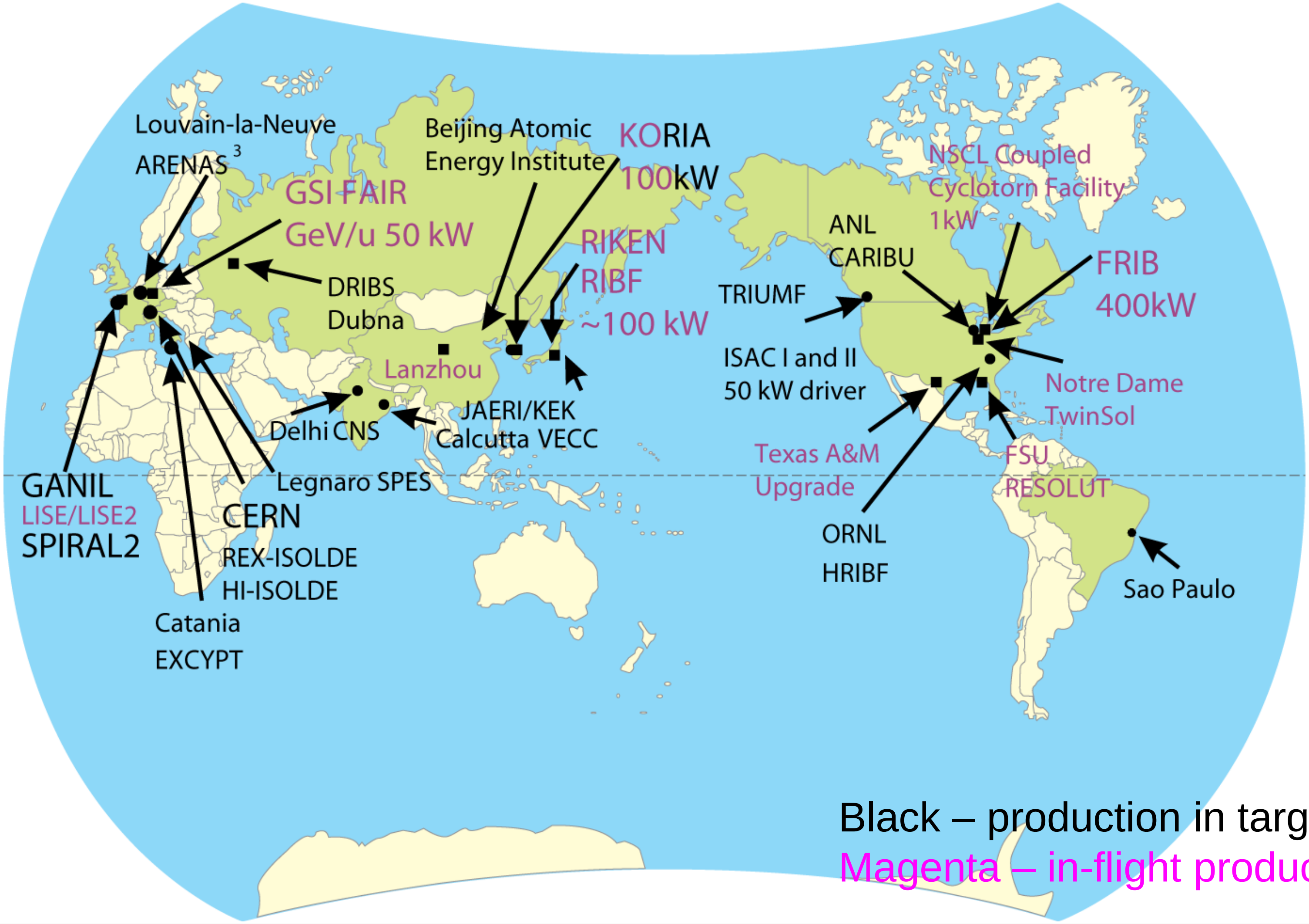


1. The production cross section for the most exotic nuclei is extremely small; but, facilities have tremendous sensitivity. The projectile intensity at the next generation facilities (^{48}Ca 400 kW, ≅ 2x10^{14} ion/s) is such that the cross section that corresponds to one atom/week is 3x10^{-20} b (30 zeptobarns, 3x10^{-48} m^2)

2. Neutrino elastic scattering cross sections are

$$\sigma_{\upsilon_e e^- \to \upsilon_e e^-} = 9.5\cdot 10^{-49}\ m^2 \left(\frac{E_\upsilon}{1\ MeV}\right)$$

World view of rare isotope facilities

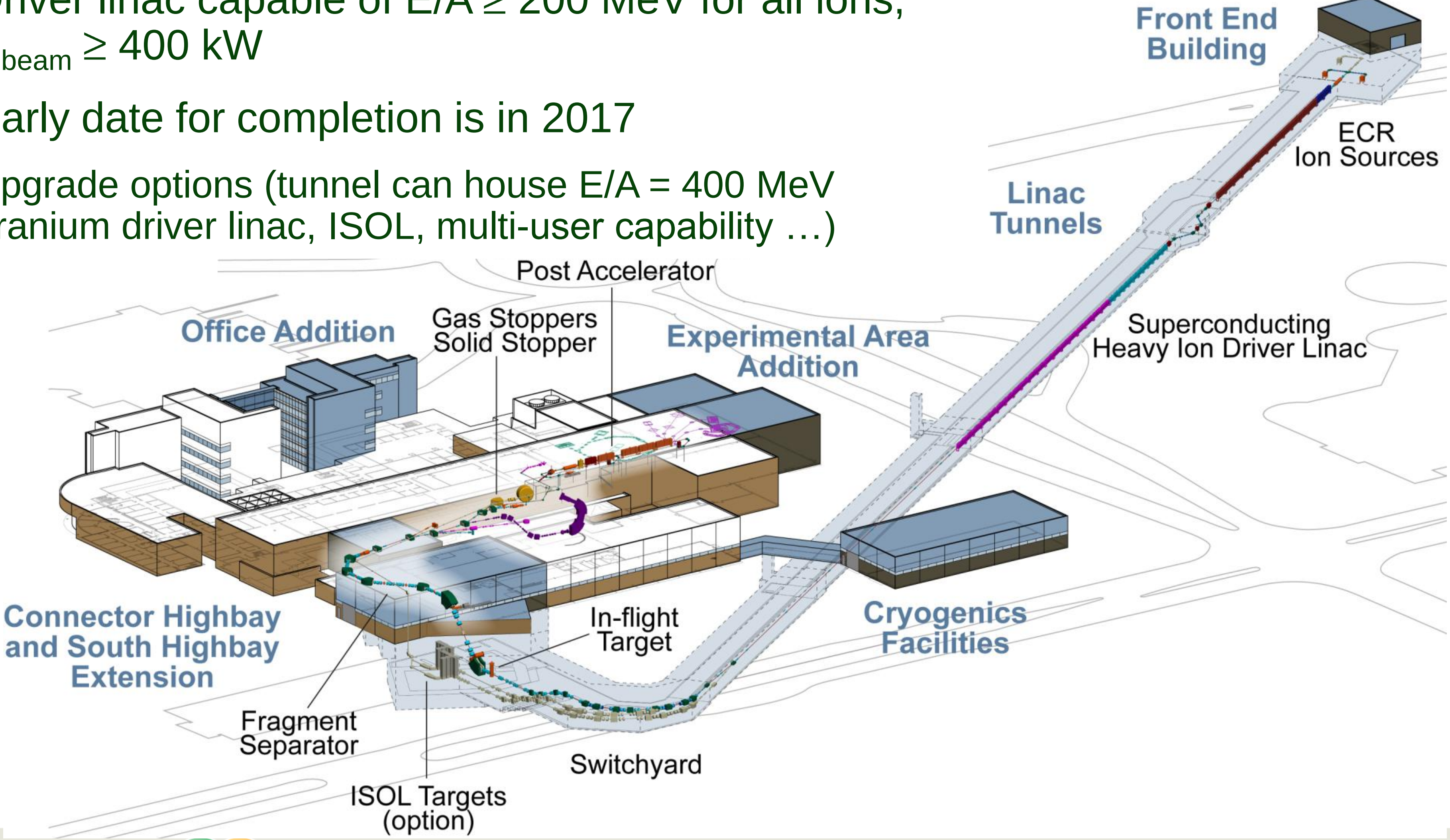


Black – production in target

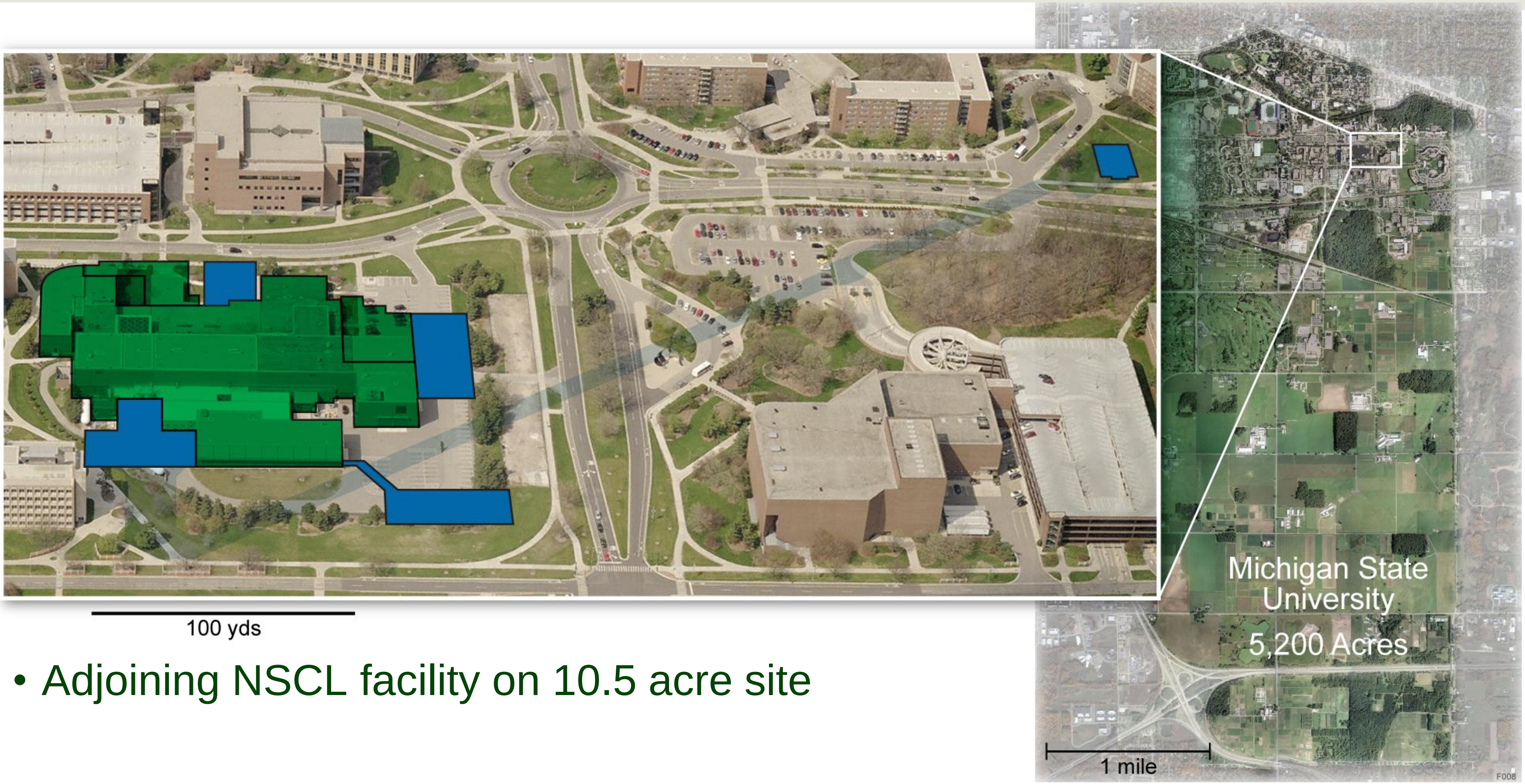
Magenta – in-flight production

Facility for Rare Isotope Beams, FRIB Broad Overview

- Driver linac capable of E/A ≥ 200 MeV for all ions, $P_{beam} \geq 400$ kW
- Early date for completion is in 2017
- Upgrade options (tunnel can house E/A = 400 MeV uranium driver linac, ISOL, multi-user capability …)

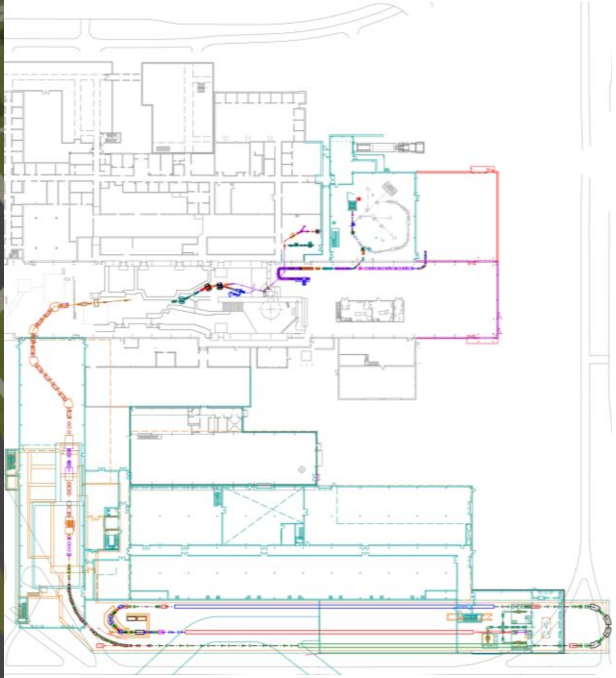


Facility placement on MSU campus



- Adjoining NSCL facility on 10.5 acre site

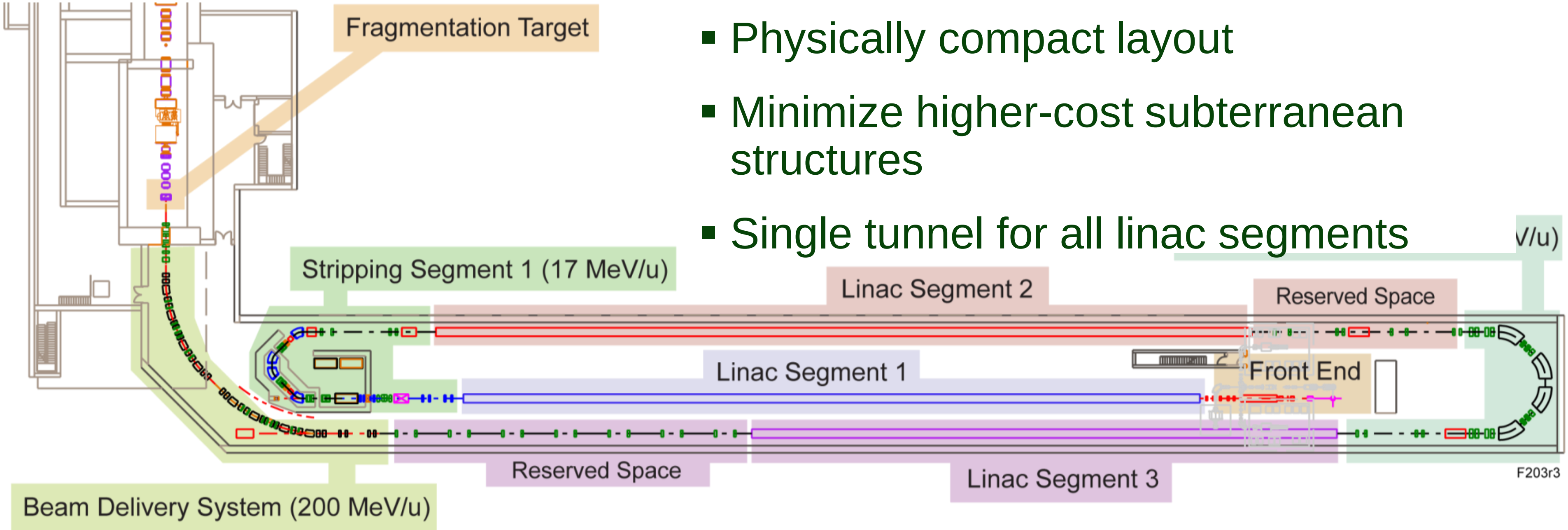
Compact, more cost-effective solution

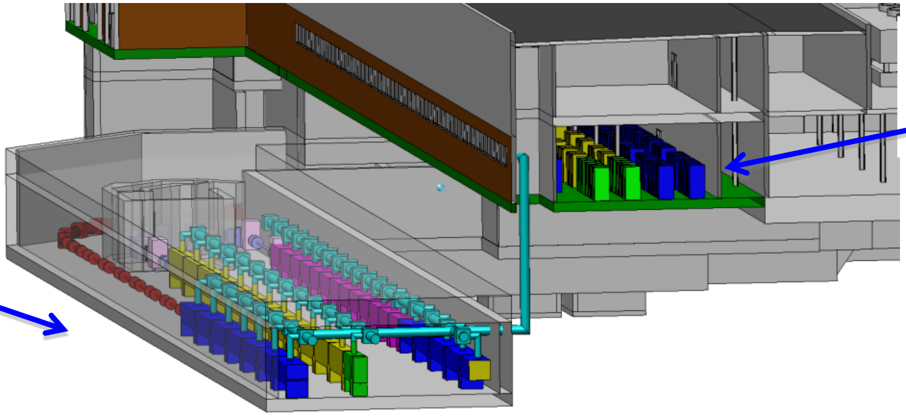


Rough (not baselined) TPC range $550M to $600M

Folded FRIB LINAC details

- Physically compact layout
- Minimize higher-cost subterranean structures
- Single tunnel for all linac segments

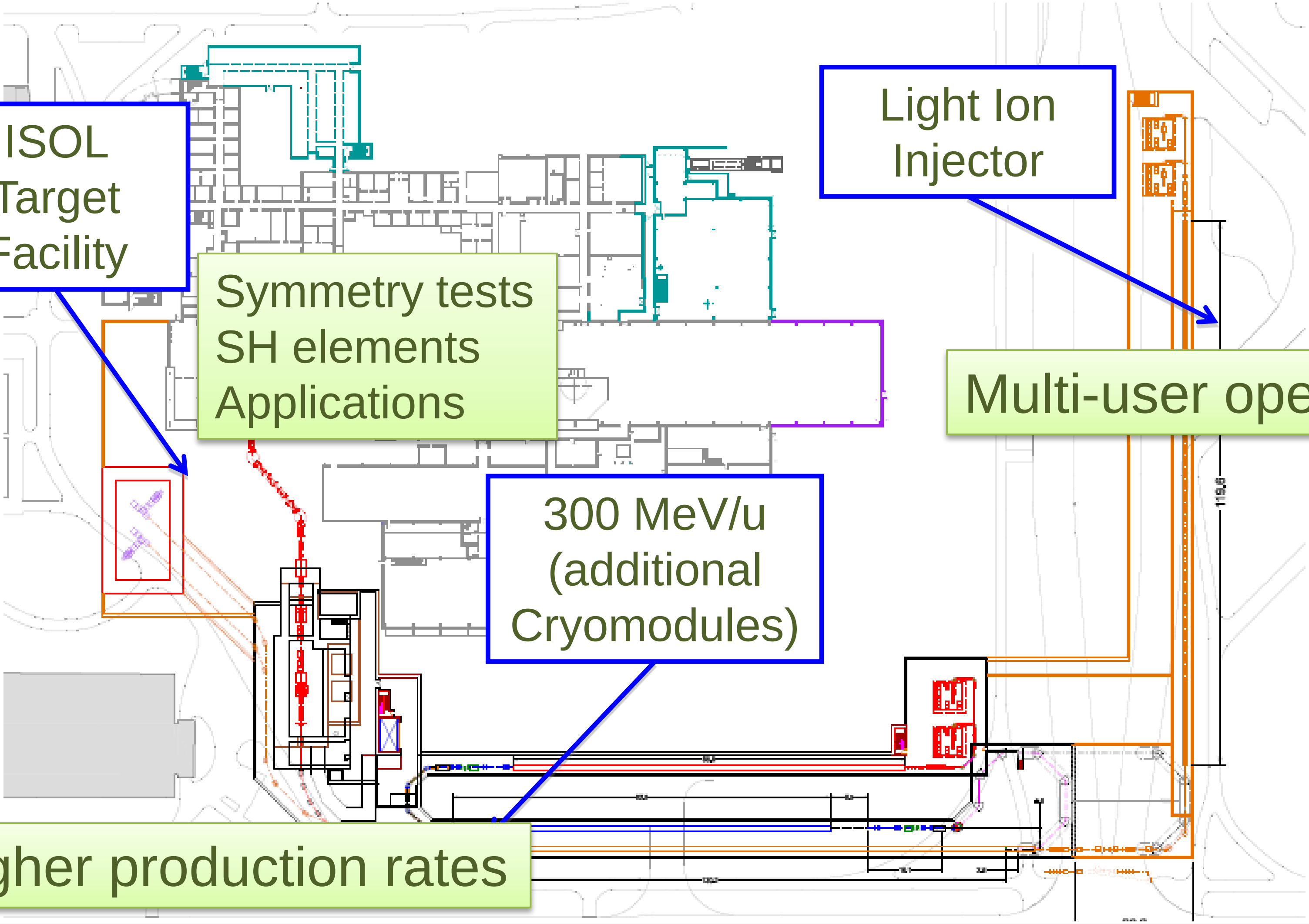




Grade (ground) level

Tunnel Floor ~40 ft below grade

FRIB Facility Upgrade Options



ISOL Target Facility

Symmetry tests
SH elements
Applications

Light Ion Injector

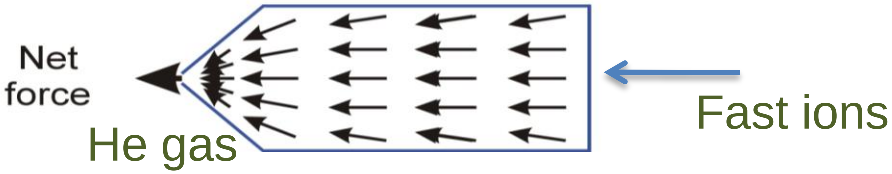
Multi-user operation

300 MeV/u (additional Cryomodules)

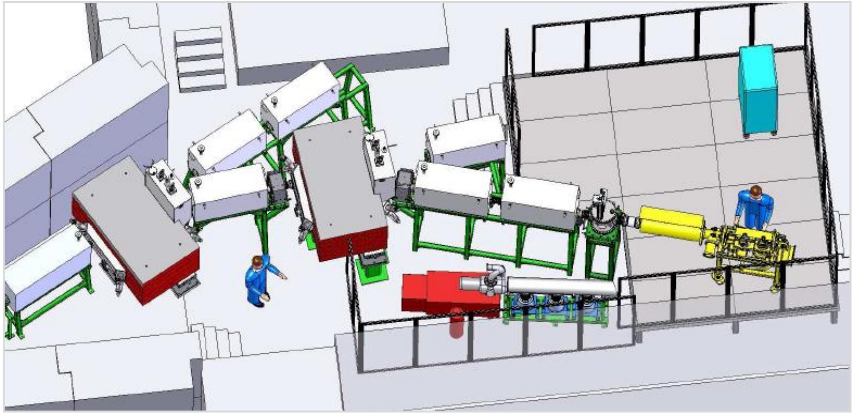
Higher production rates

Key FRIB component: Beam Stopping

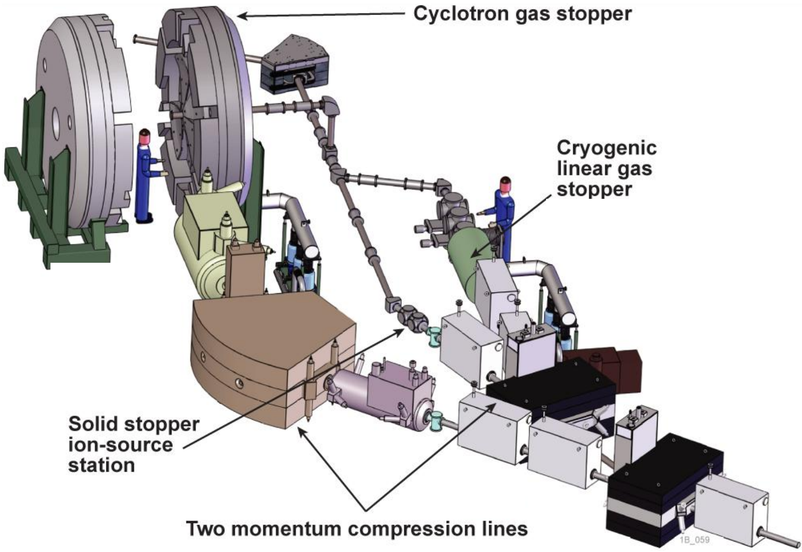
Concepts develop at ANL by G. Savard *et al.*



Beams for precision experiments at very low-energies or at rest and for reacceleration
- Cyclotron gas stopper
- Linear gas stopper
- Solid stopper (FRIB)

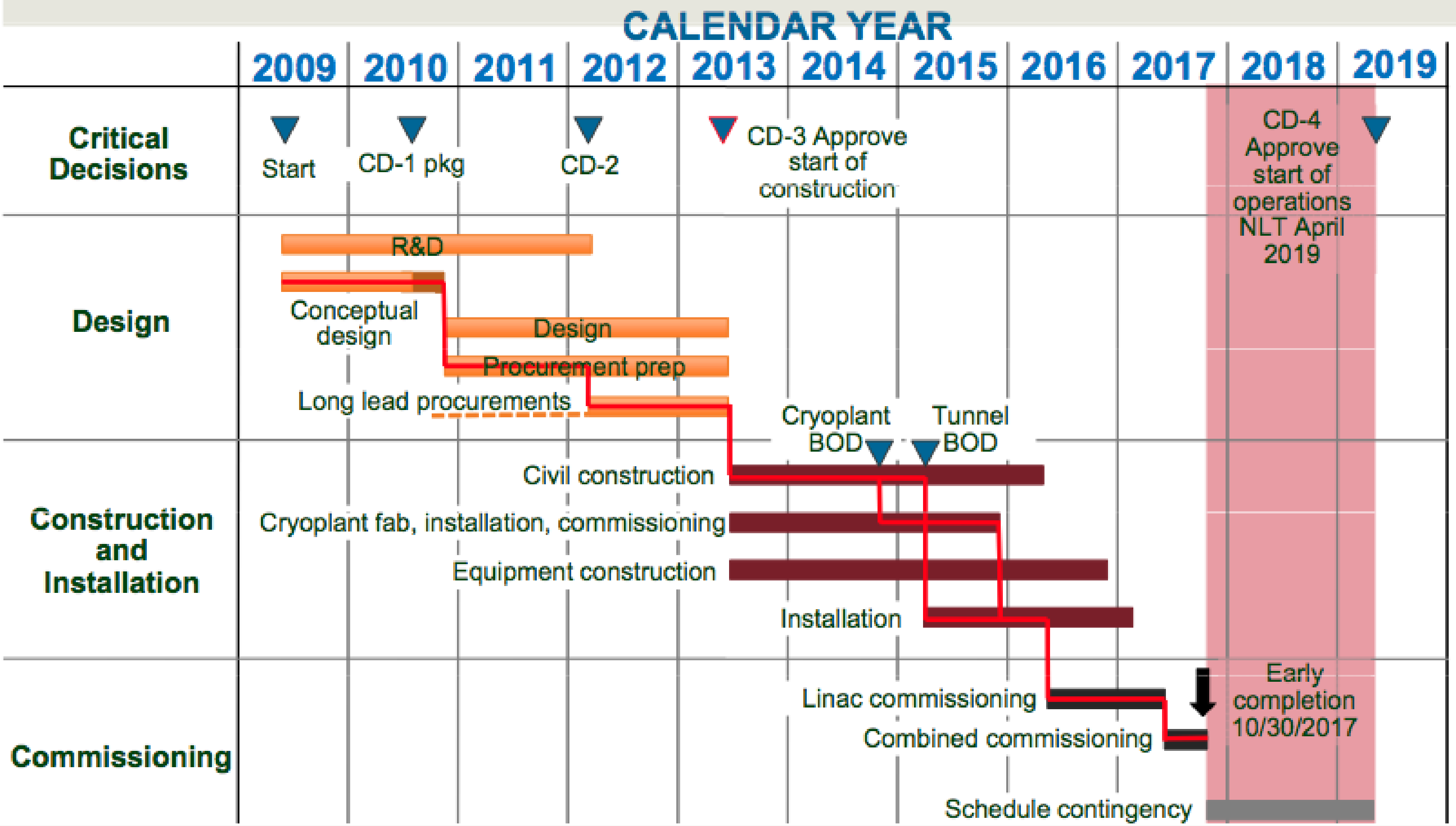


- Phase 1 (by 2011), two momentum compression lines
  - MSU linear cryogenic gas cell and
  - ANL gas catcher (FRIB R&D)
- Phase 2 (after 2012):
  - One linear gas stopper
  - Gas-filled cyclotron stopper (funded as NSF-MRI)
  - Solid-stopper/reionizer (FRIB)



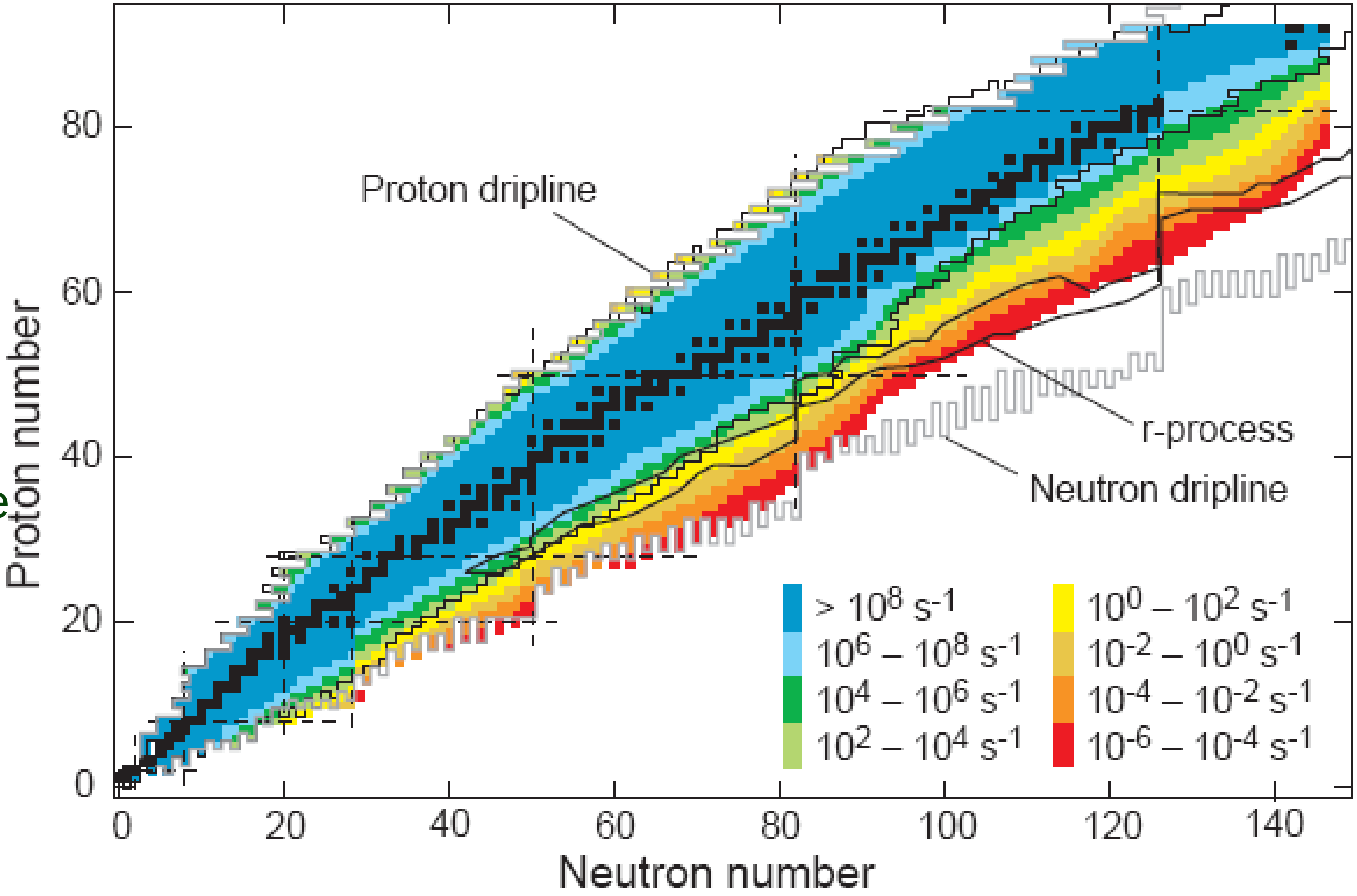
Timeline for establishment of FRIB

- The timeline for FRIB is dependent on funding by congress and approval by DOE



What New Nuclides Will FRIB Produce?

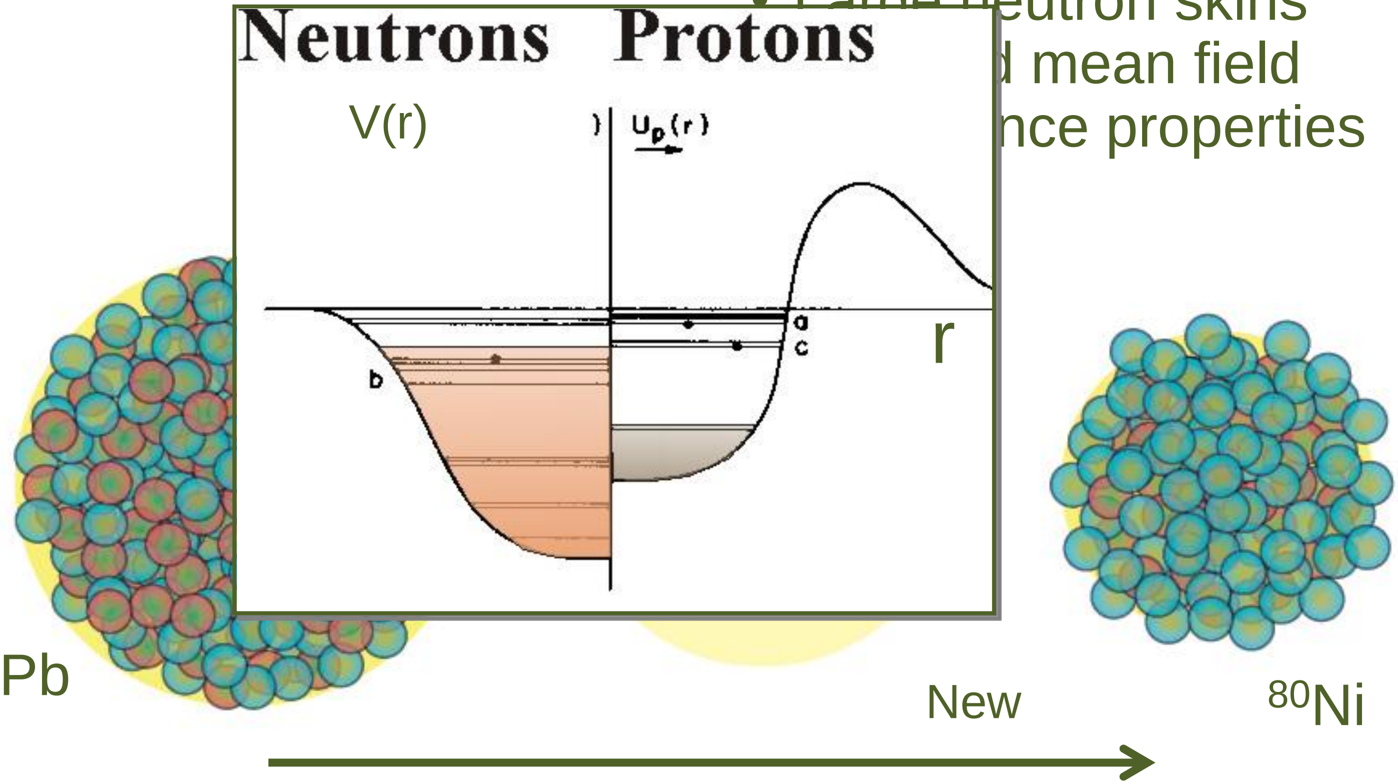
- FRIB will produce more than 1000 NEW isotopes at useful rates (4500 available for study)
- Theory is key to making the right measurements
- Exciting prospects for study of nuclei along the drip line to mass 120 (compared to 24)
- Production of most of the key nuclei for astrophysical modeling
- Harvesting of unusual isotopes for a wide range of applications



Rates are available at http://groups.nscl.msu.edu/frib/rates/

FRIB specialty – Produce new exotic isotopes

- Large neutron skins
- d mean field
- nce properties

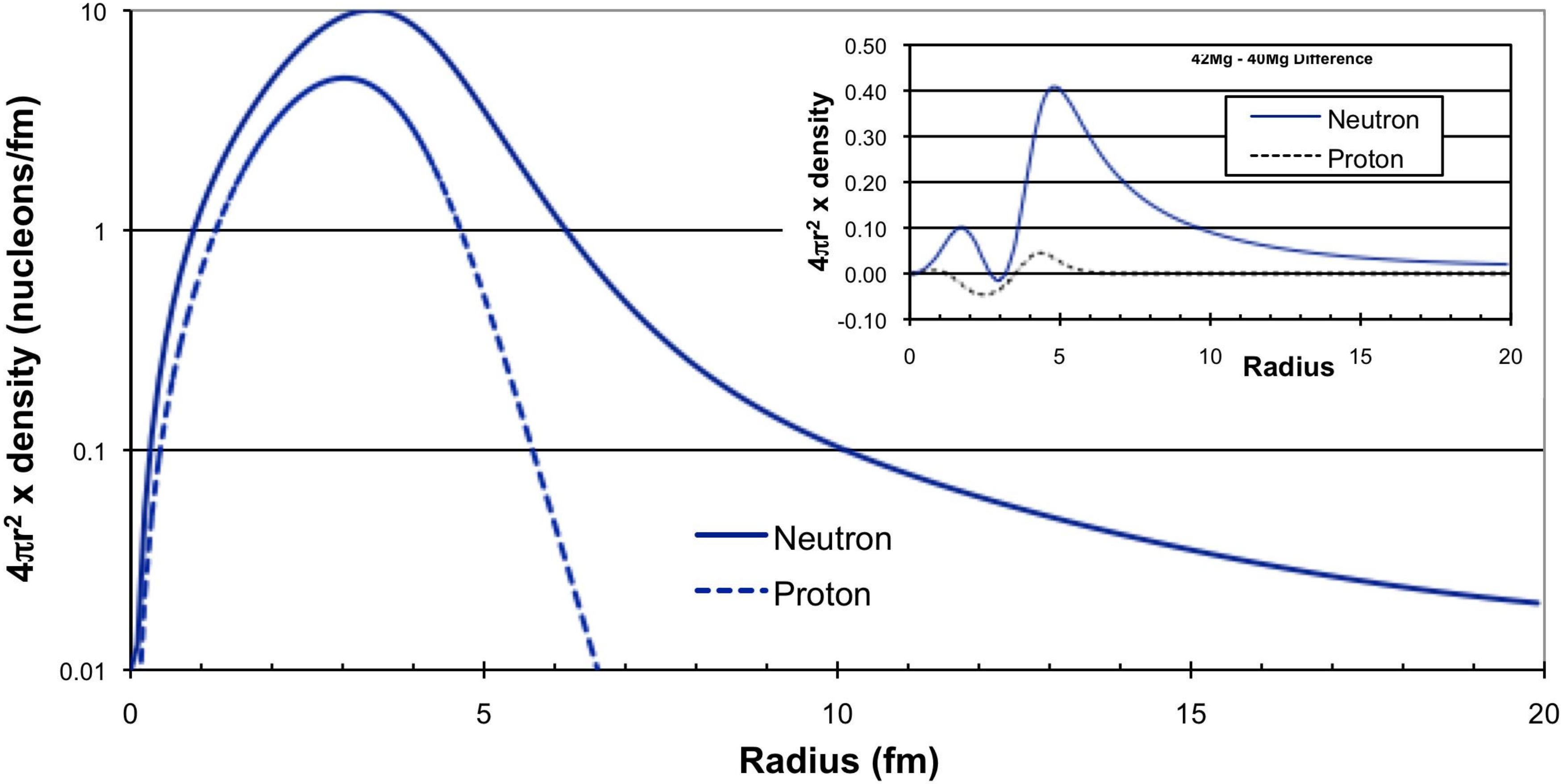


Science: Pairing in low-density material, new tests of nuclear models, open quantum system, interaction with continuum states - Efimov States - Reactions

New insight and physics from extreme halos and skins

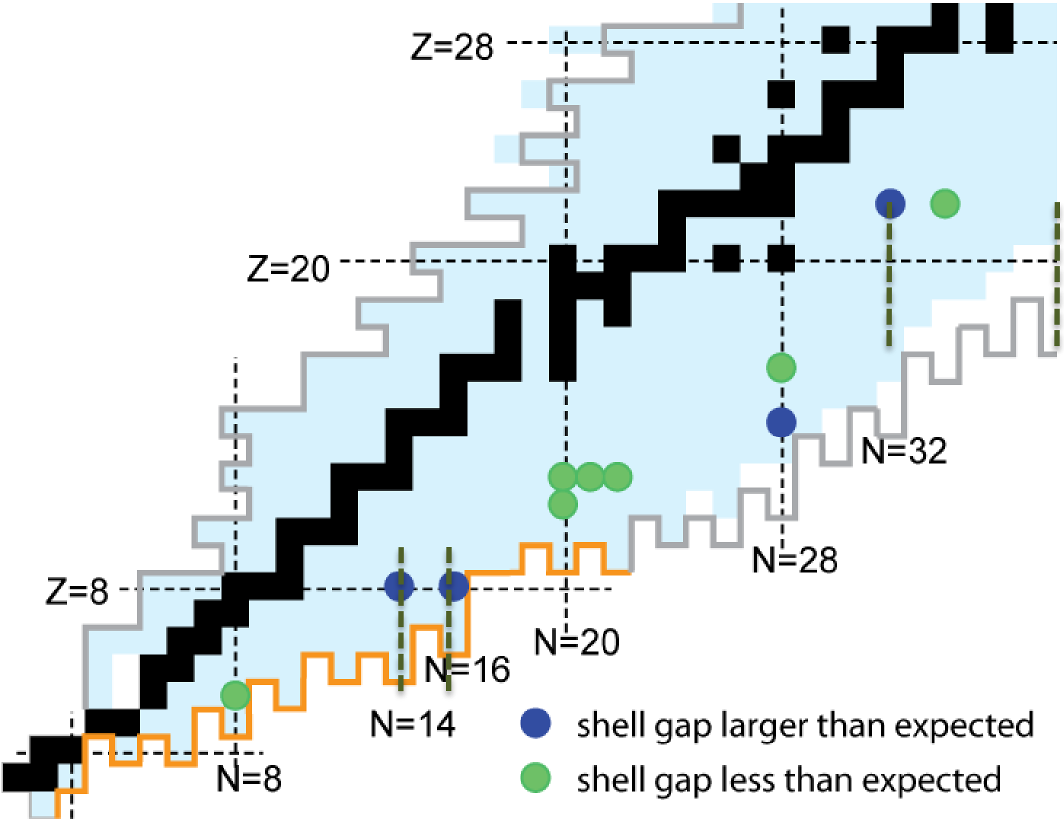
Example: ^{42}Mg (Predicted to be produced at 10 atoms/day)

Theory - 100 keV S_n BA Brown



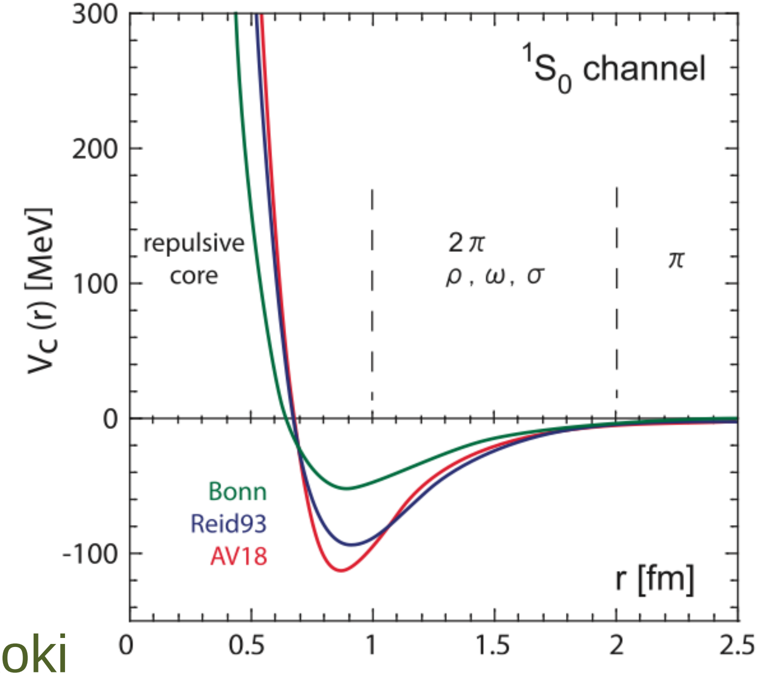
Nuclear Magic Numbers – New Picture

- The standard magic numbers are generally only correct for stable and near stable isotopes
- Study of new isotopes has given insight into the role of tensor and 3-body forces in nuclei (e.g. Otsuka et al.)
- The continuum will also play a role in more weakly bound nuclei (Nazarewicz, Papenbrook, Volya, et al.)
- May have implications for astrophysics…



How do we model nuclei?

- The origin of the strong force that binds nuclei is QCD (How would we prove that? Surprises are likely.)
- We construct potentials based on neutron and proton scattering data and properties of light nuclei (Bonn, Reid, Illinois AV18, Nijmegen, etc.)
- QCD Inspired EFT (String Theory Inspired – Hashimoto et al.)



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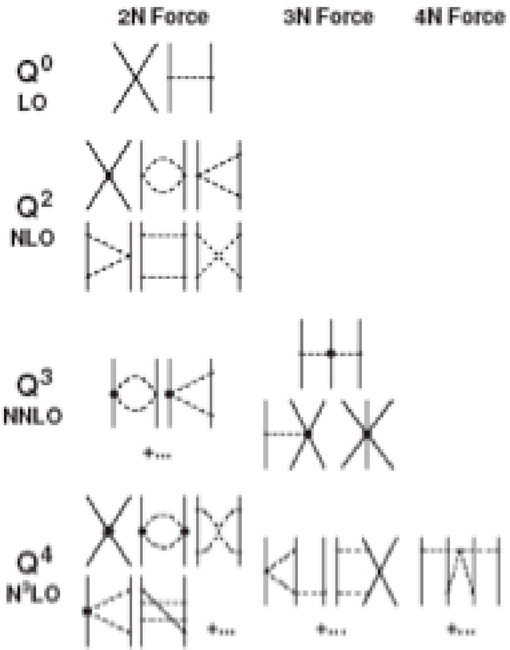
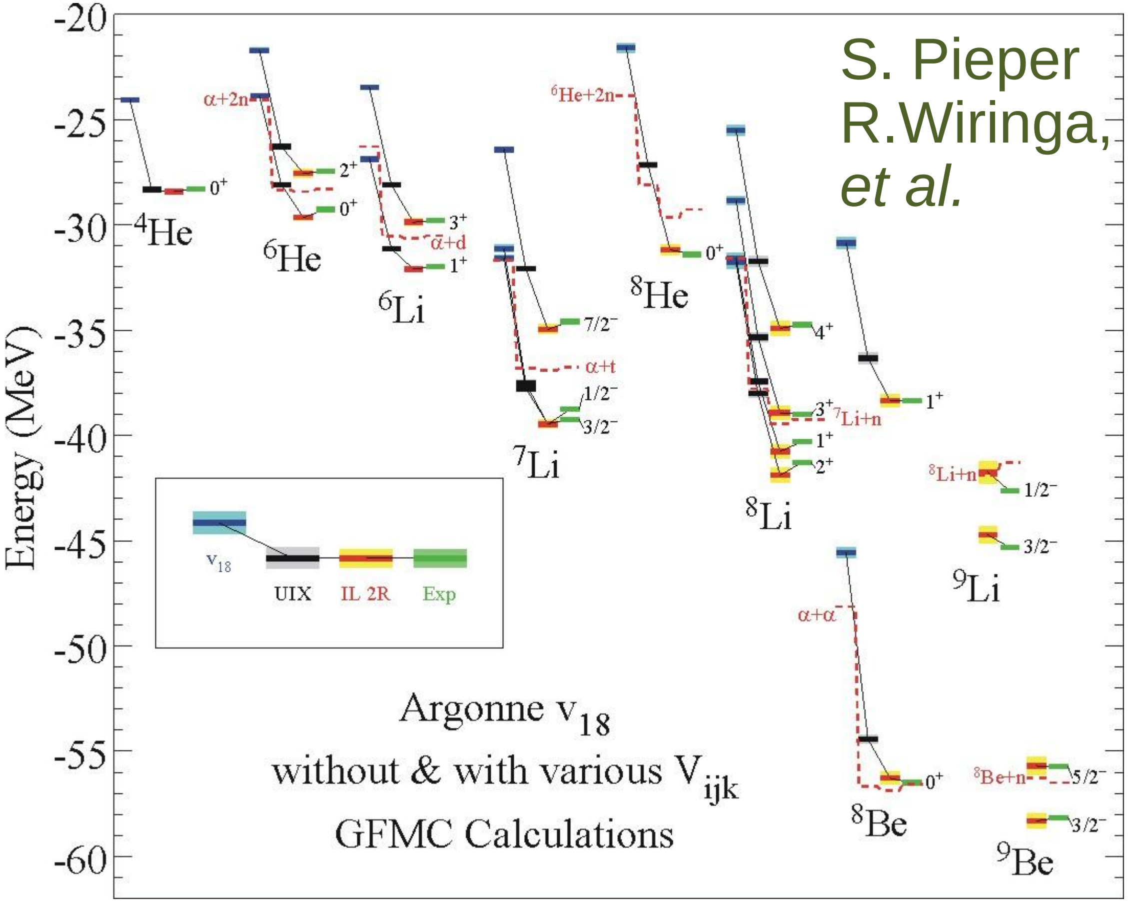


Goal: Develop an Effective Field Theory based on QCD Symmetries (Furnstahl, van Kolck, Navrátil, Vary, Machliedt…)

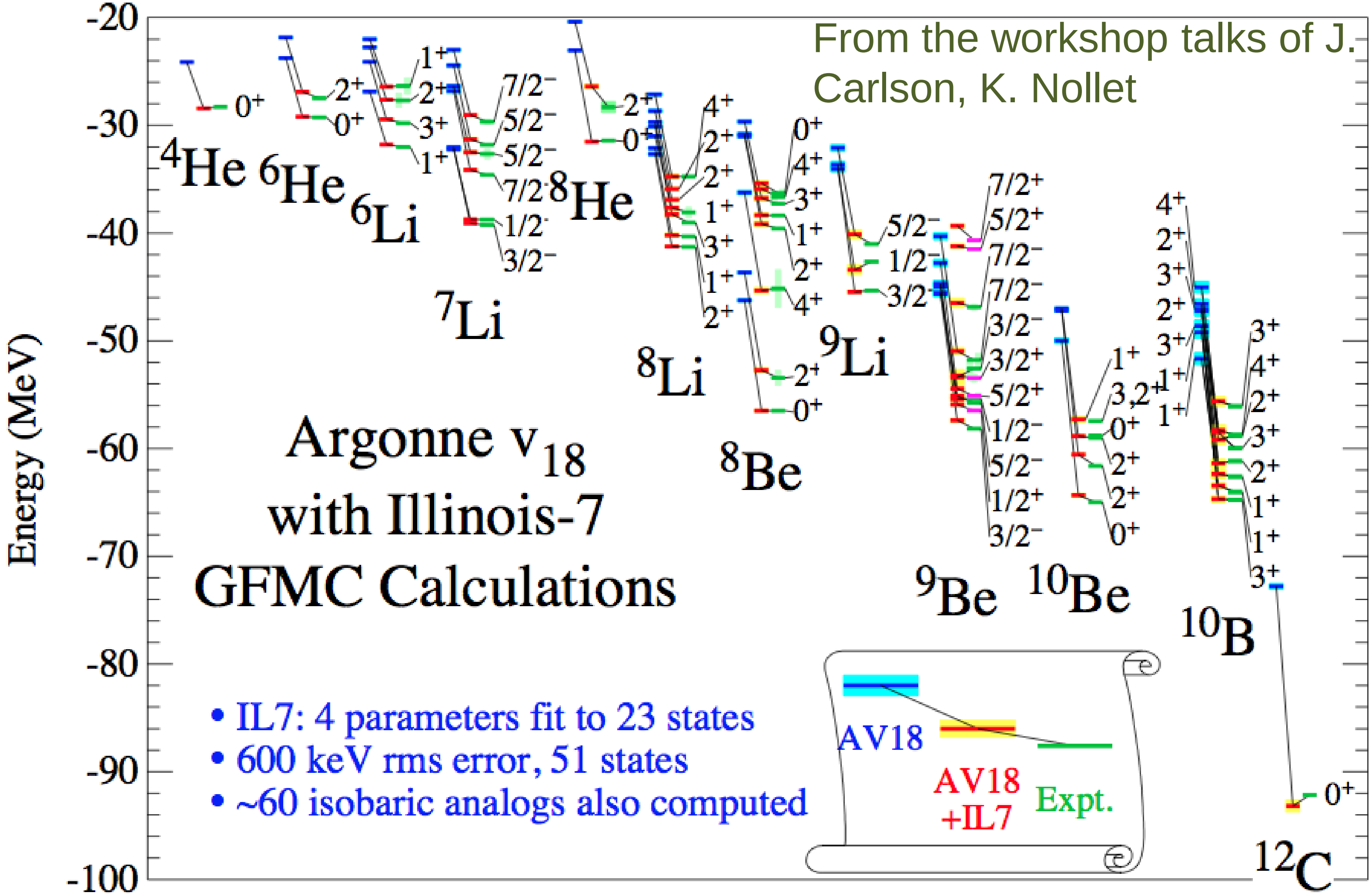
Properties of exotic isotopes are essential in determining NN and NNN potentials

- Neutron rich nuclei were key in determining the isospin dependence of 3-body forces and the development of IL-2R from UIX
- New data on exotic nuclei continues to lead to refinements in the interactions
- EFT developments, LQCD and even computational power are providing insight for *ab initio* theories, but they need grounding in data



S. Pieper
R.Wiringa,
et al.

Current status of the GFMC calculations



From the workshop talks of J. Carlson, K. Nollet

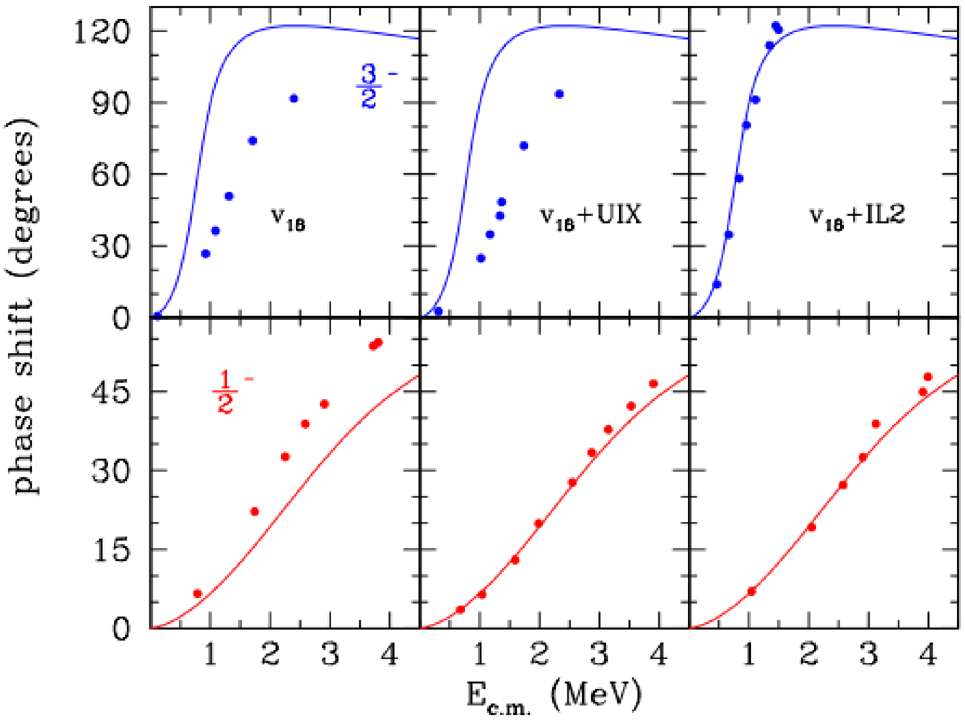
Argonne v_{18} with Illinois-7 GFMC Calculations

- IL7: 4 parameters fit to 23 states
- 600 keV rms error, 51 states
- ~60 isobaric analogs also computed

Application of GFMC technique to reactions of nuclei

- Resonance states in ^{5}He (n+^{4}He) From the workshop talk of K. Nollett

Results illuminate origins of spin-orbit splitting between $3/2^-$ and $1/2^-$ resonances



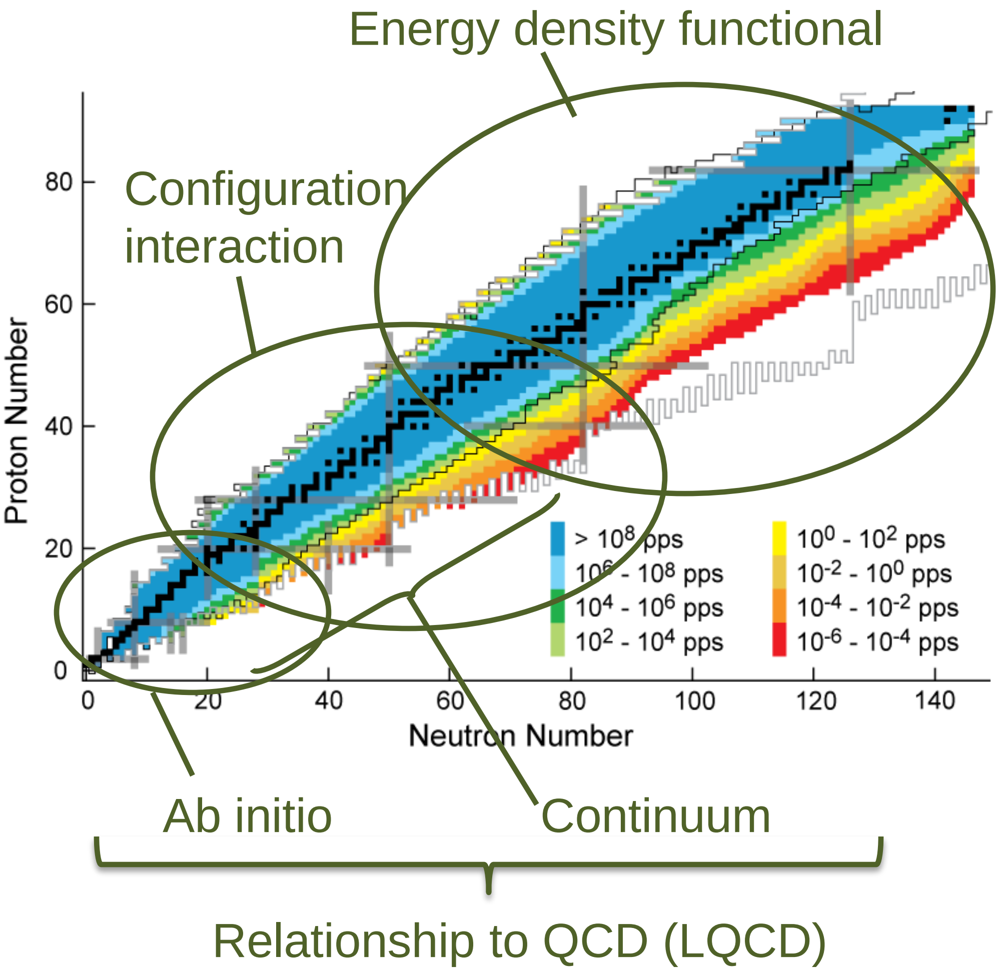
These are also the first-ever calculations of resonance widths in GFMC

Nollett, et al, PRL 2007; motivated by BBN modeling

Extraction of S-matrix poles shows agreement with pseudo-bound for $\frac{3}{2}^-$, a few hundred keV difference for $\frac{1}{2}^-$

Theory Road Map: Comprehensive Model of Nuclear Structure and Reactions

- Theory Road Map – comprehensive description of the atomic nucleus
  - Ab initio models – study of neutron-rich, light nuclei helps determine the force to use in models (measurement of sensitive properties for N=14, 16 nuclei)
  - Configuration-interaction theory; study of shell and effective interactions (study of key nuclei such as ^{54}Ca, ^{60}Ca, ^{122}Zr)
  - The universal energy density functional (DFT) – determine parameters (broad view of mass surface, BE(2)s, BE(4)s, fission barrier surface, etc.)
  - The role of the continuum and reactions and decays of nuclei (halo studies up to A ~100)
- IMPORTANT: Understand and select the most sensitive measurements



Energy density functional

Configuration interaction

Ab initio

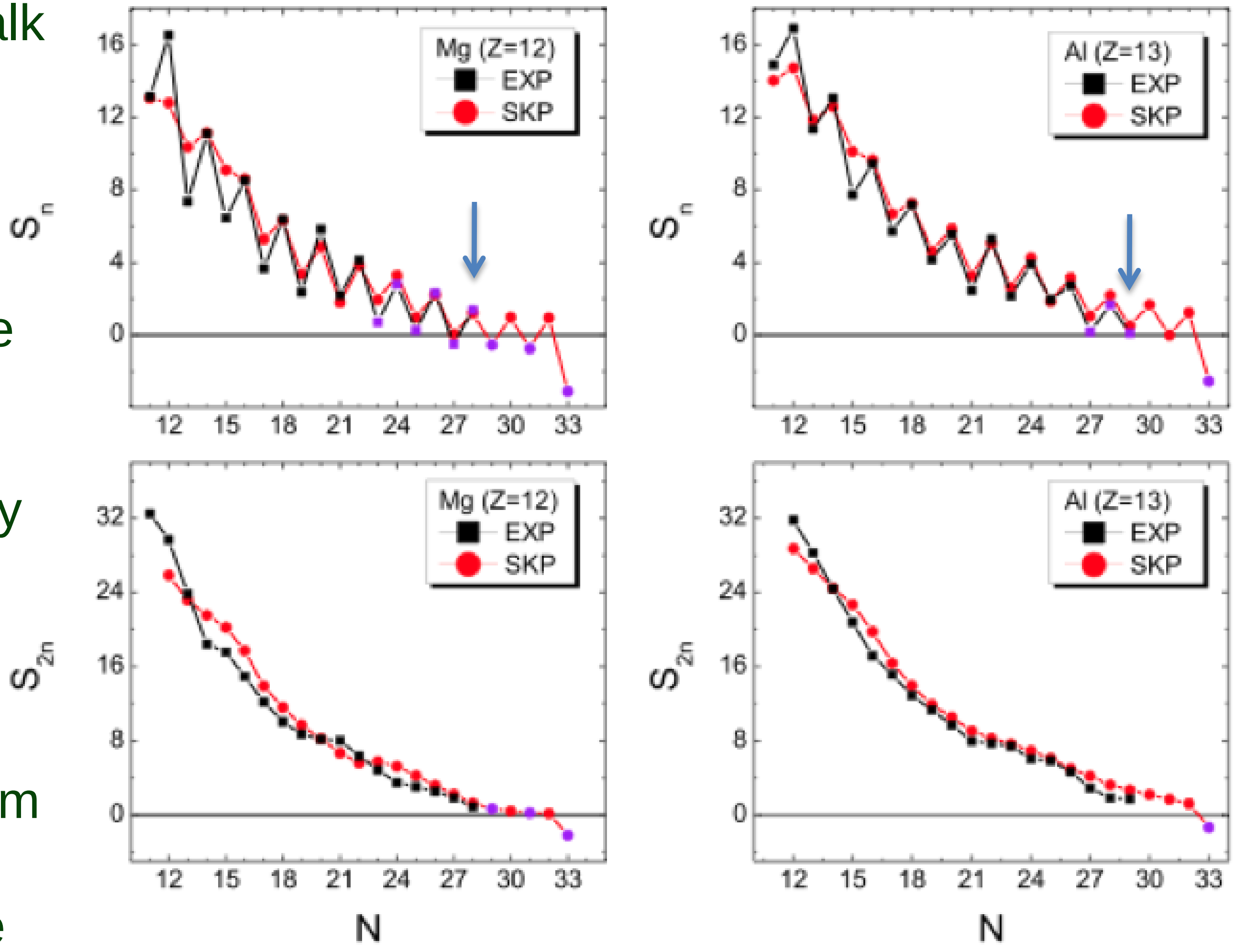
Continuum

Relationship to QCD (LQCD)

FRIB Facility for Rare Isotope Beams
U.S. Department of Energy Office of Science
Michigan State University

Density Functional Theory

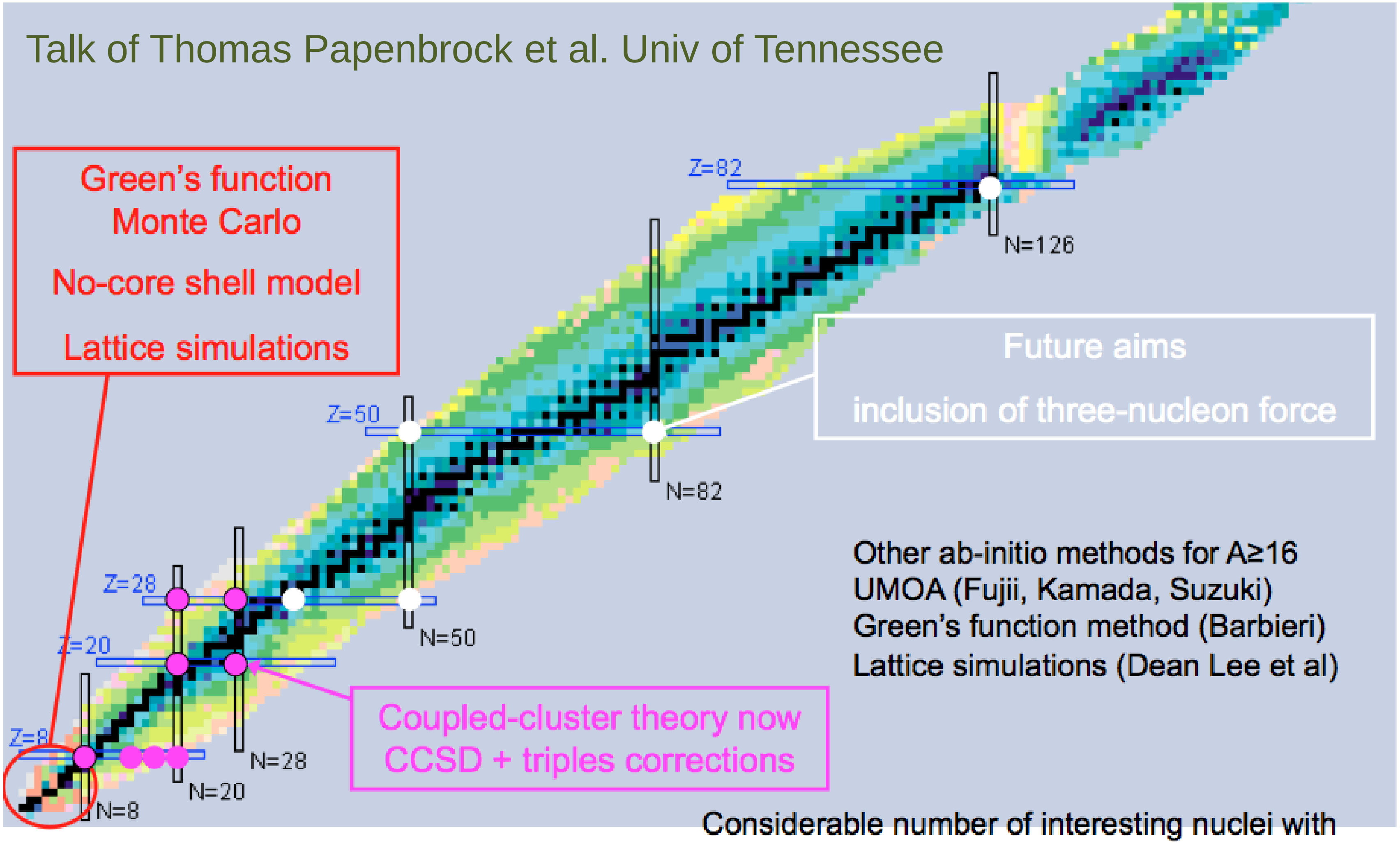
- From the workshop talk of D. Furnstahl
- Talk of S. Bogner on QCD inspired functional forms
- EDF calculation of the binding energies of 9000 isotopes
- Key tests of the theory come at the limits of binding (see figure)
- Remarkable success so far; Global DFT mass calculations from HFB Δm~700keV
- Goal is to achieve the results



M. Stoitsov et al.

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

Configuration space models – Example Coupled Cluster



Talk of Thomas Papenbrock et al. Univ of Tennessee

Green's function Monte Carlo

No-core shell model

Lattice simulations

Future aims

inclusion of three-nucleon force

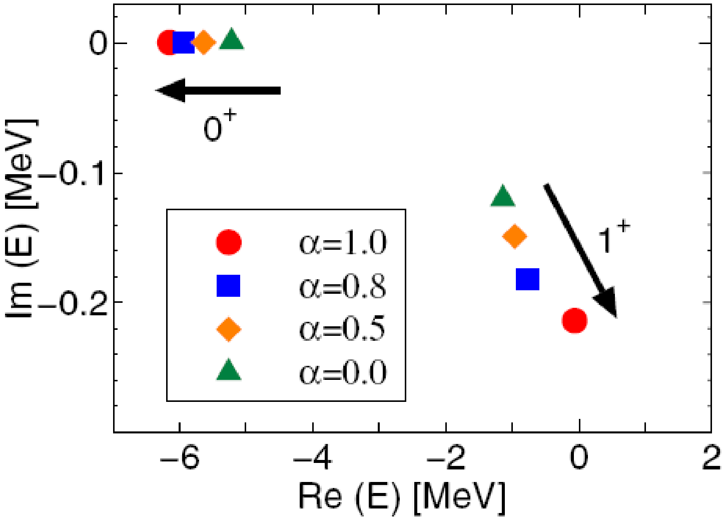
Coupled-cluster theory now
CCSD + triples corrections

Other ab-initio methods for A≥16
UMOA (Fujii, Kamada, Suzuki)
Green's function method (Barbieri)
Lattice simulations (Dean Lee et al)

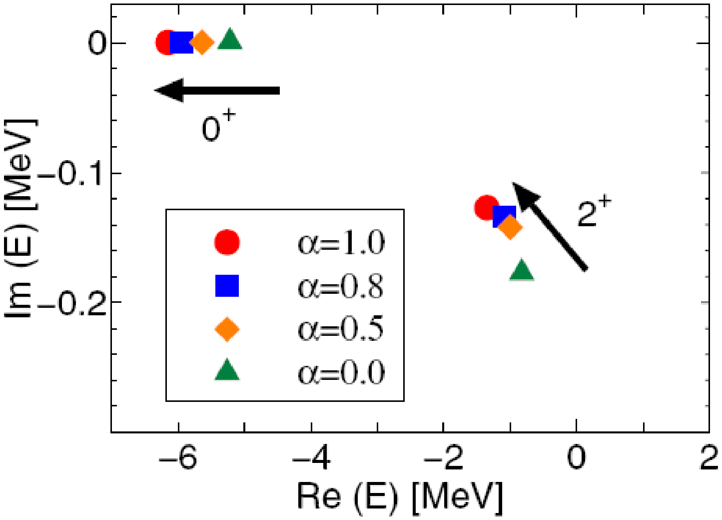
Considerable number of interesting nuclei with closed subshells…

Sensitivity of Nuclear Properties to Model Parameters

- Example: Level structure of ^{24}O and the $^1S_0$ NN interaction
- Structure of these loosely bound or unbound isotopes is strongly influenced by the $^1S_0$ component of the NN interaction
- Calculation of ^{24}O in a shell model that correctly treats weakly-bound and continuum states (specifically Gamow Shell Model)



(a)The ground state and the 1^+ in ^{24}O

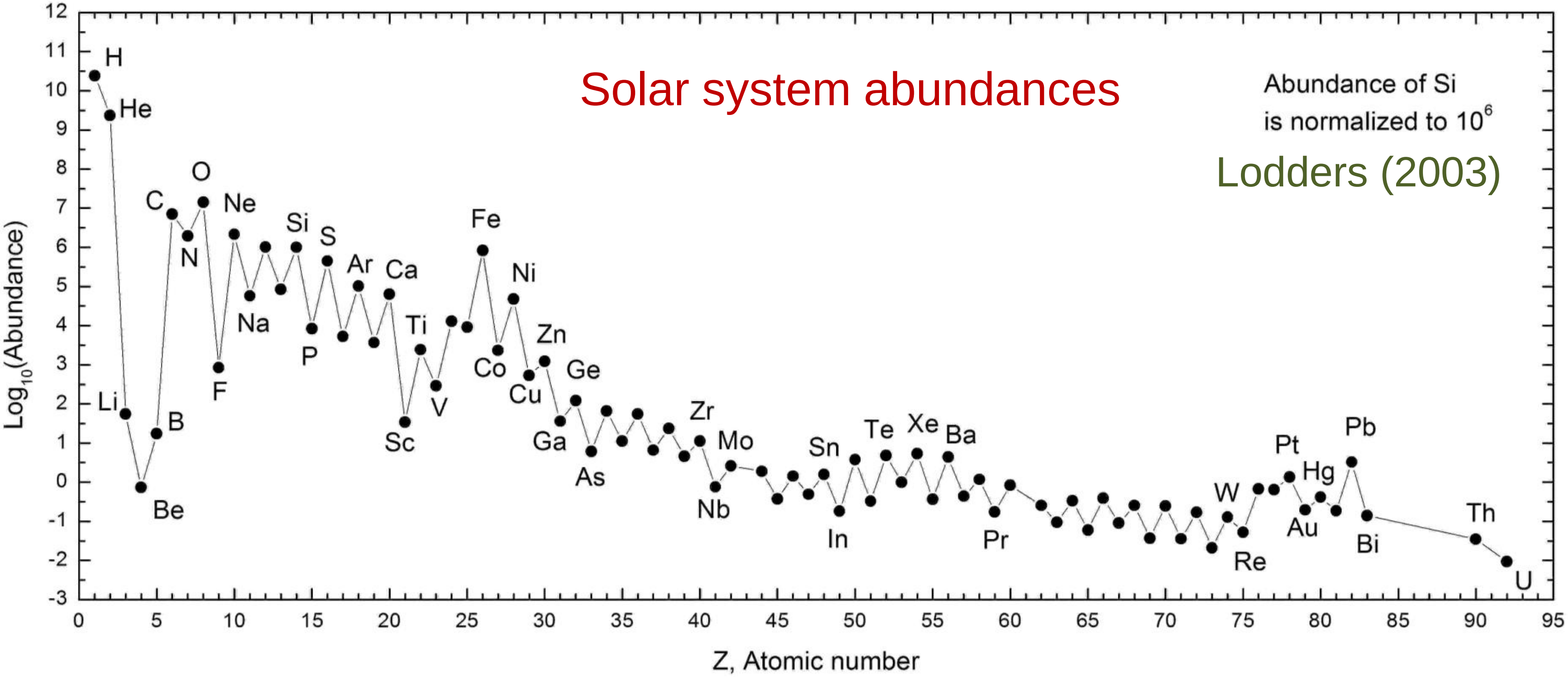


(b)The ground state and the 2^+ in ^{24}O

Tsukiyama, Horth-Jensen, Hagen PRC 80 051301(2009)

Solar System Elemental Abundances

- Understanding the chemical history of the universe – J. Truran, B. Meyers
- The abundance of elements tell us about the history of events prior to stellar formation

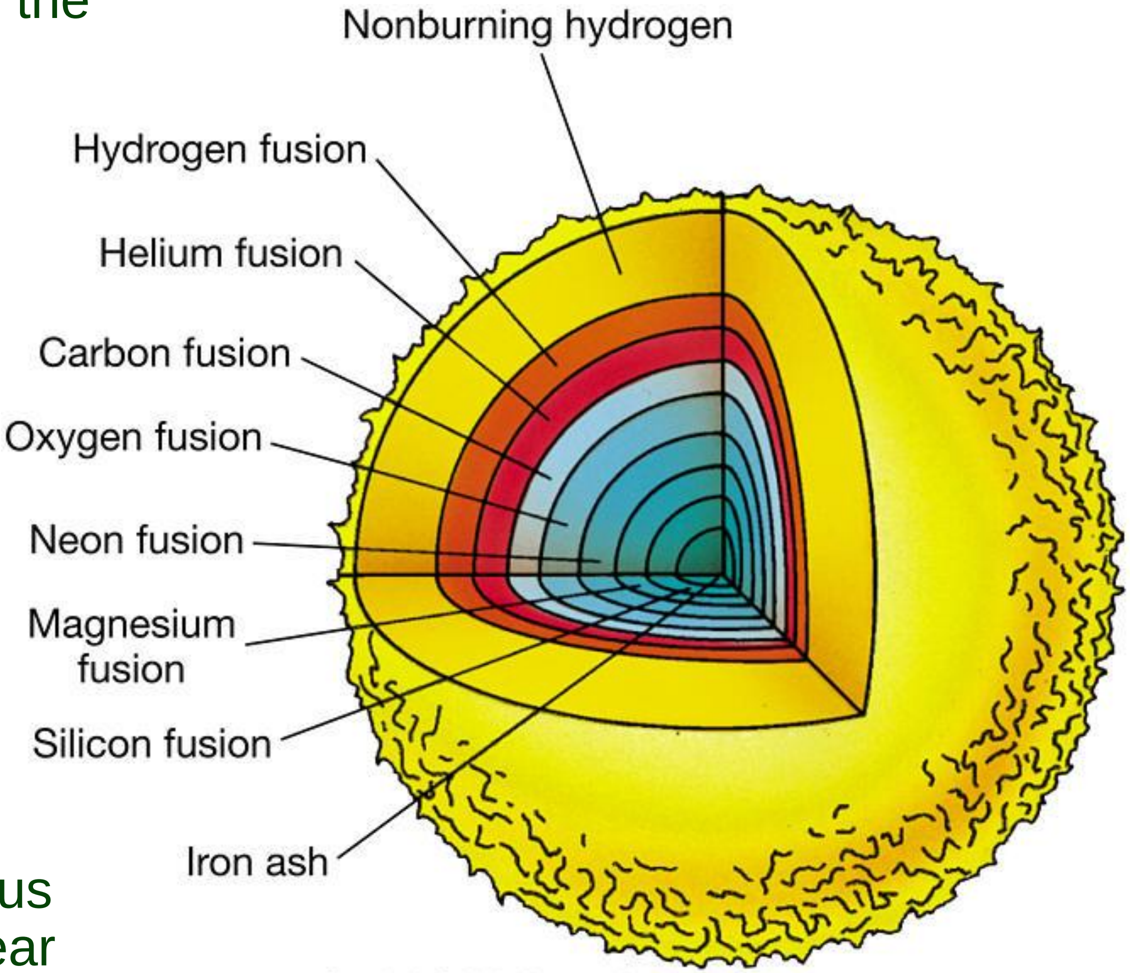

Solar system abundances

Abundance of Si is normalized to 10^6

Lodders (2003)

Stellar evolution of massive stars

- Stars with more than 8 times the mass of our Sun develop multiple burning layers
- Hydrogen to helium
- Helium to carbon
- Carbon to oxygen, neon, magnesium
- Oxygen to neon
- Neon to magnesium
- Magnesium to Silicon
- Silicon to Iron
- Iron is the most bound nucleus and has no exothermic nuclear reactions



Simulation of Solar System Abundances

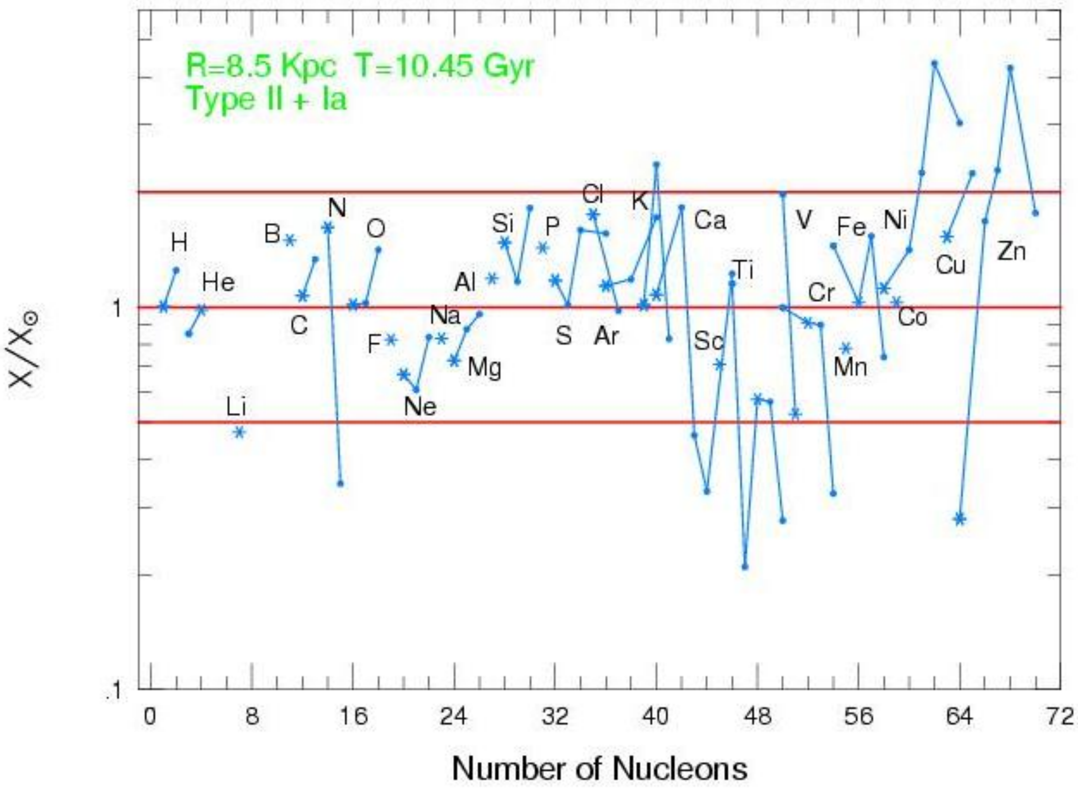
Parameters:

- Supernovae type Ia and II
- Number (77 supernovae with M_s 11-40 M_{sun})
- Progenitor mass distributions
- Age of the galaxy
- …

Results:

- SN rate1/3 comes from type Ia
- Reproduction of measured ^{7}Li abundance metalicity vs. time etc.

Timmes, Woosley, Weaver
Astrophysical Journal 1995

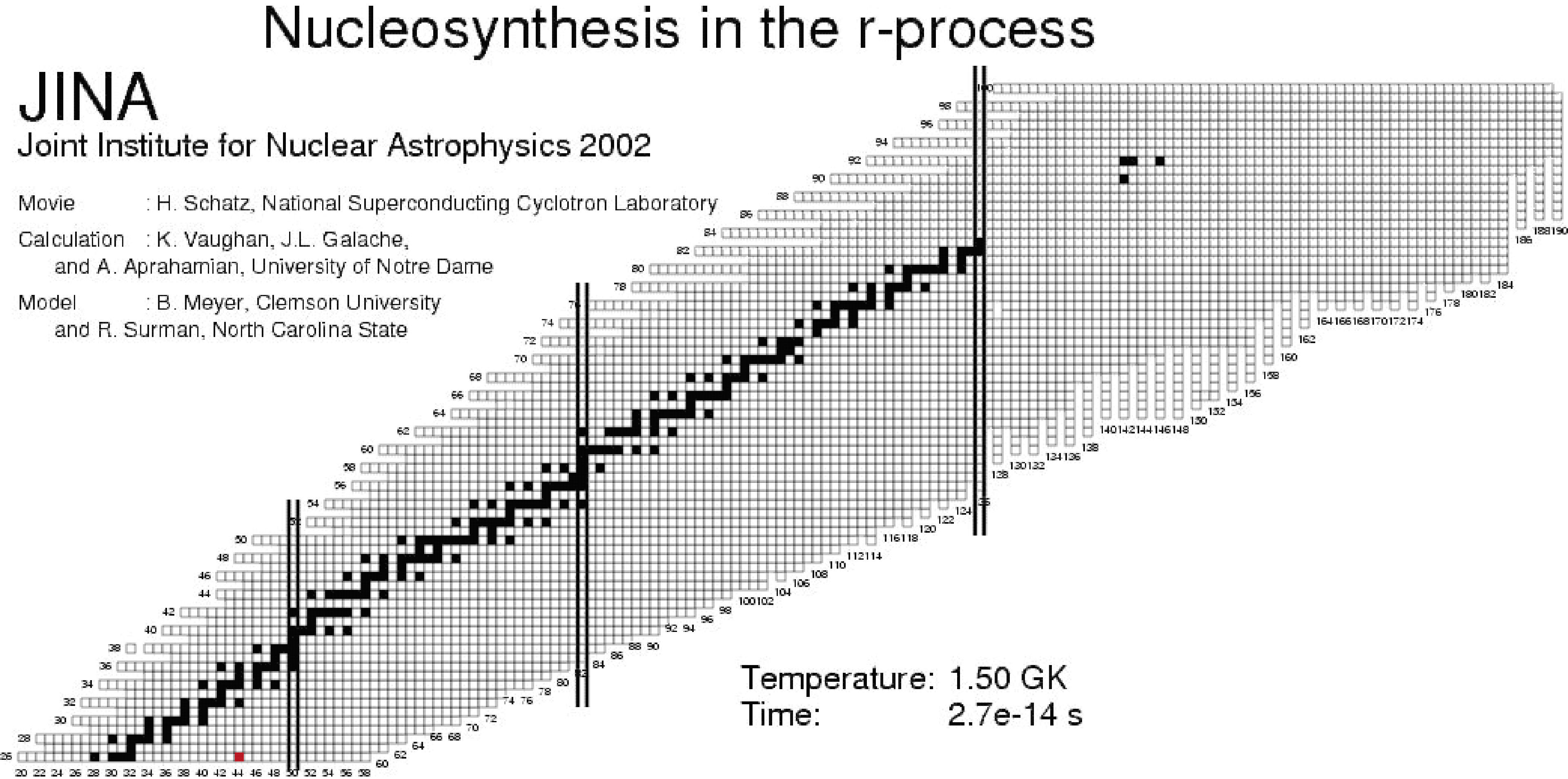


Success ! ? Above 72 we can’t model well

Where do gold atoms come from?
An r-process

- E. M. Burbidge, G. R. Burbidge, W. A. Fowler, and F. Hoyle. (1957). "Synthesis of the Elements in Stars". Rev Mod Phy 29: 547, must be an r-procees, but …
- We know they must be made in a neutron-rich environment $T > 10^9$ K, $\rho_{neutron} \approx 10^{20\text{-}28}$ cm^{-3} , that lasts for about 1 second; called the rapid-neutron capture process, r-process
- Type II supernovae are a possible site (variants)
  - Neutrino driven shock wave
  - Models do not produce the entropy and neutron flux needed to match abundance data (although we can't say that for sure)
  - Shock waves in C-O layers
  - Magnetic outflows
- Colliding neutron stars would also work, but there does not seem to be enough of these in the early universe to explain how much heavier elements we see
- Once the underlying physics is known, we can infer information of the site

About Half of Heavier Elements must be made in an r-Process



Nucleosynthesis in the r-process

JINA
Joint Institute for Nuclear Astrophysics 2002

Movie : H. Schatz, National Superconducting Cyclotron Laboratory

Calculation : K. Vaughan, J.L. Galache, and A. Aprahamian, University of Notre Dame

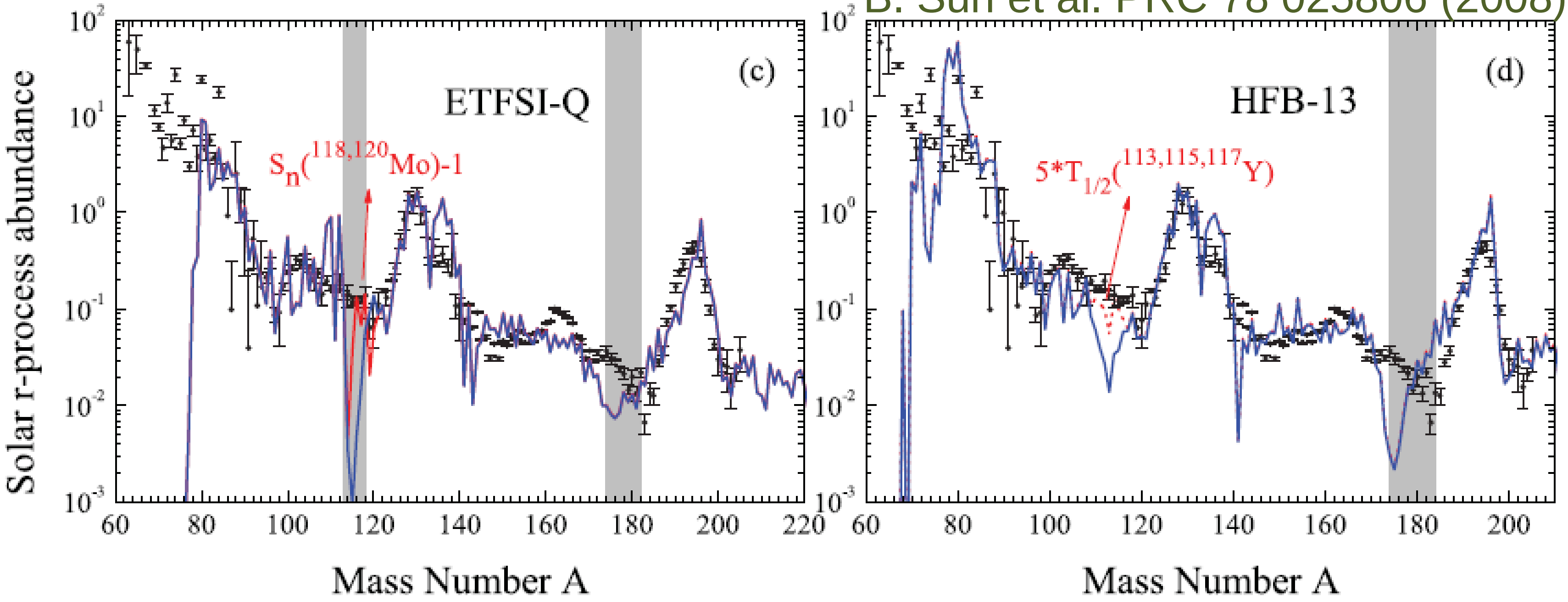
Model : B. Meyer, Clemson University and R. Surman, North Carolina State

Nuclear physics shapes the characteristic final abundance pattern for a given r-process model

Mass Uncertainties and r-process

- Are the fine details a reflection of the site or of nuclear physics?

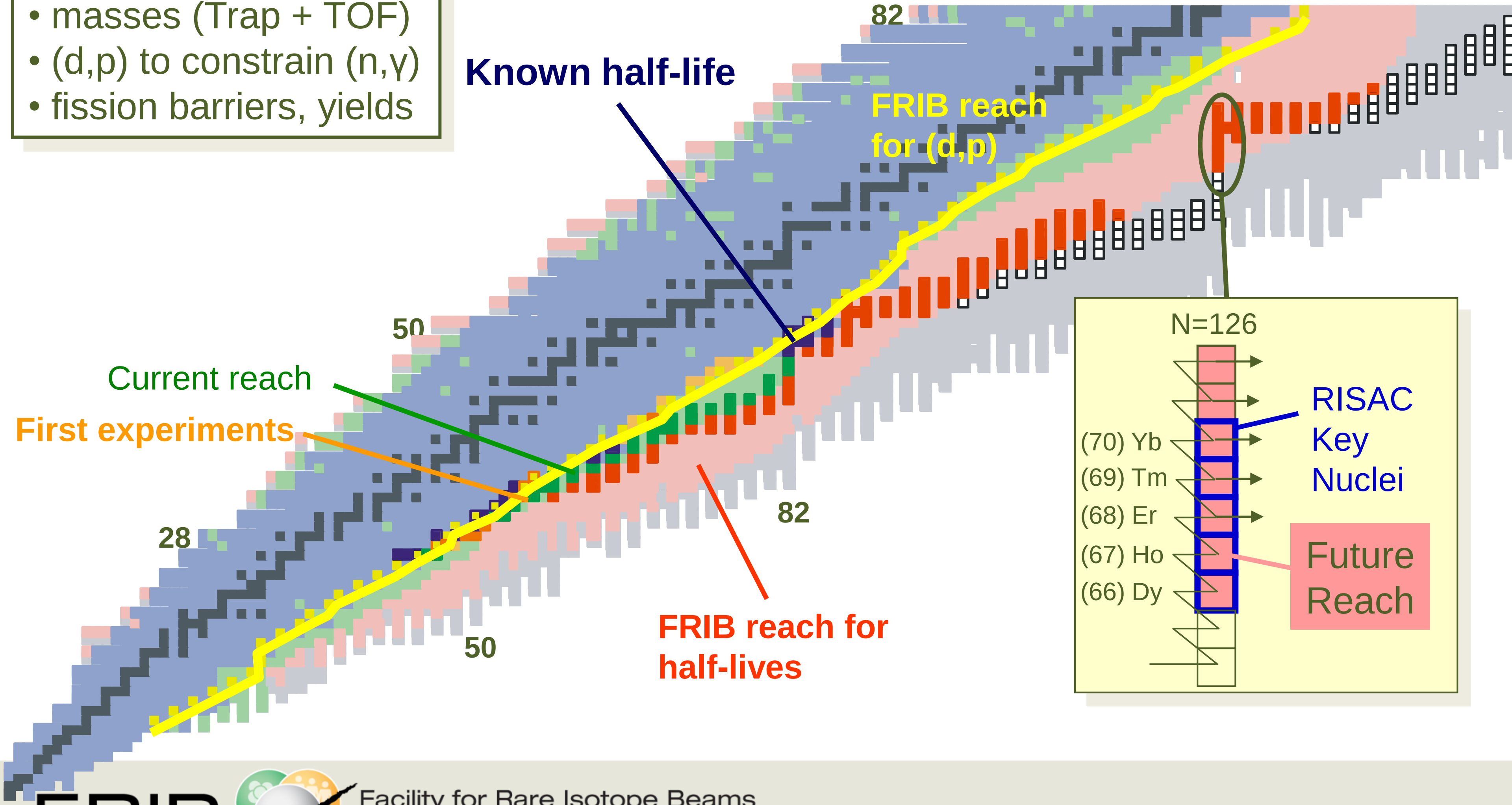
B. Sun et al. PRC 78 025806 (2008)



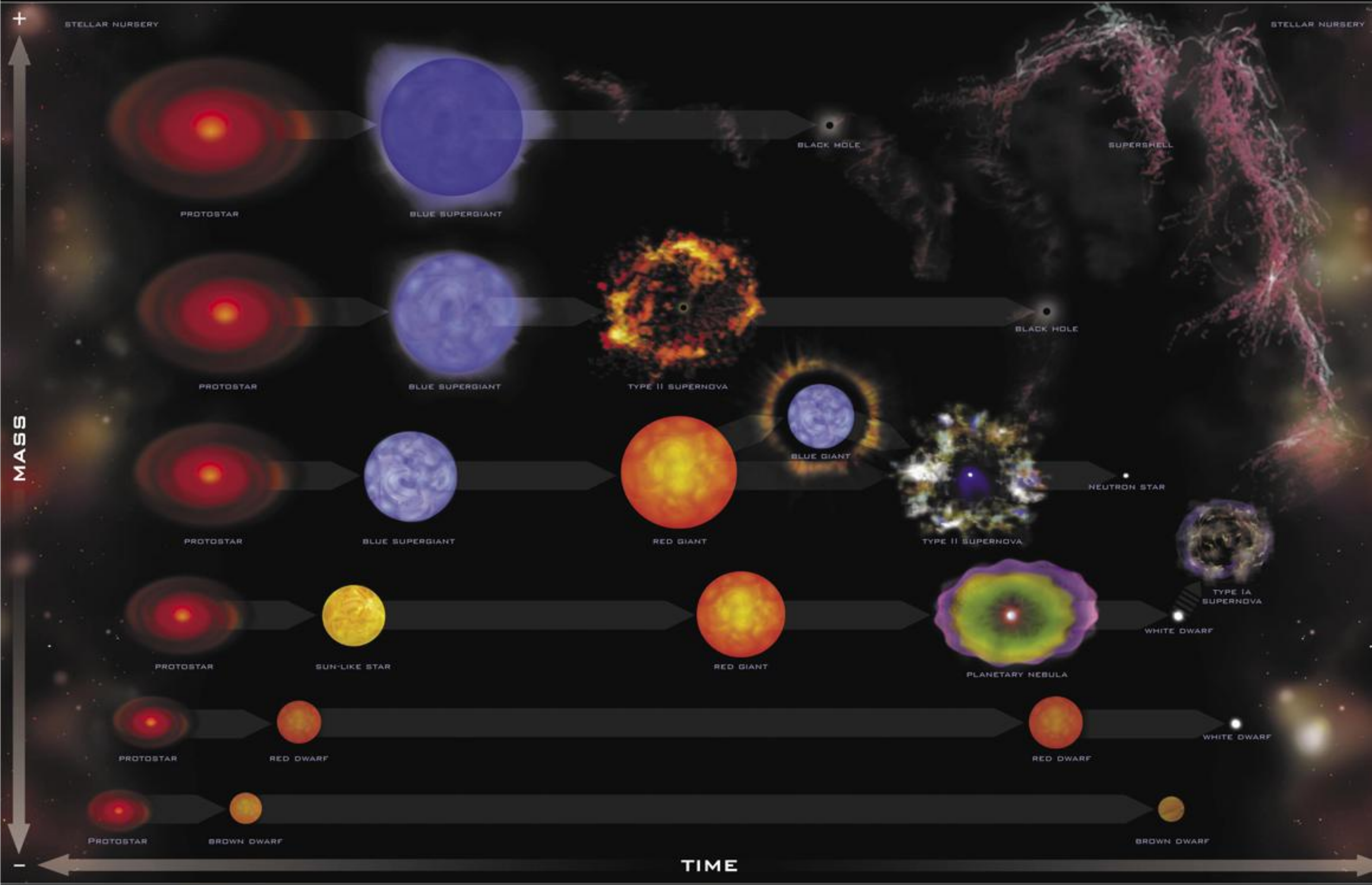
- "Site independent model" – Fe seed nuclei are irradiated with ≈ 20 flashes of 10^{20} to 10^{28} n/cm^3 over a time scale of seconds (T ≈ 1 GK)

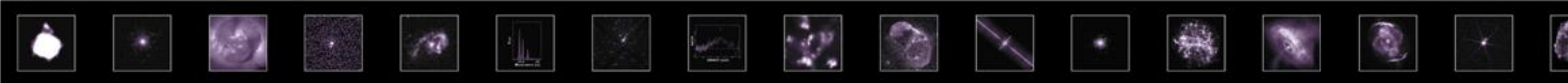
Reach of FRIB – Will Allow Modeling of the r-Process

- β-decay properties
- masses (Trap + TOF)
- (d,p) to constrain (n,γ)
- fission barriers, yields

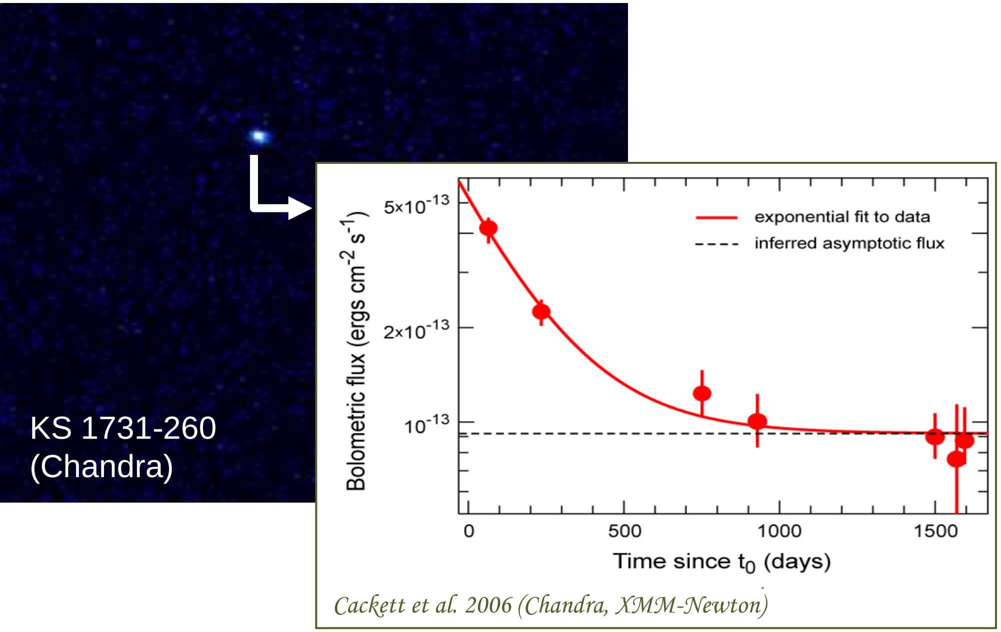


STELLAR EVOLUTION: A JOURNEY WITH CHANDRA



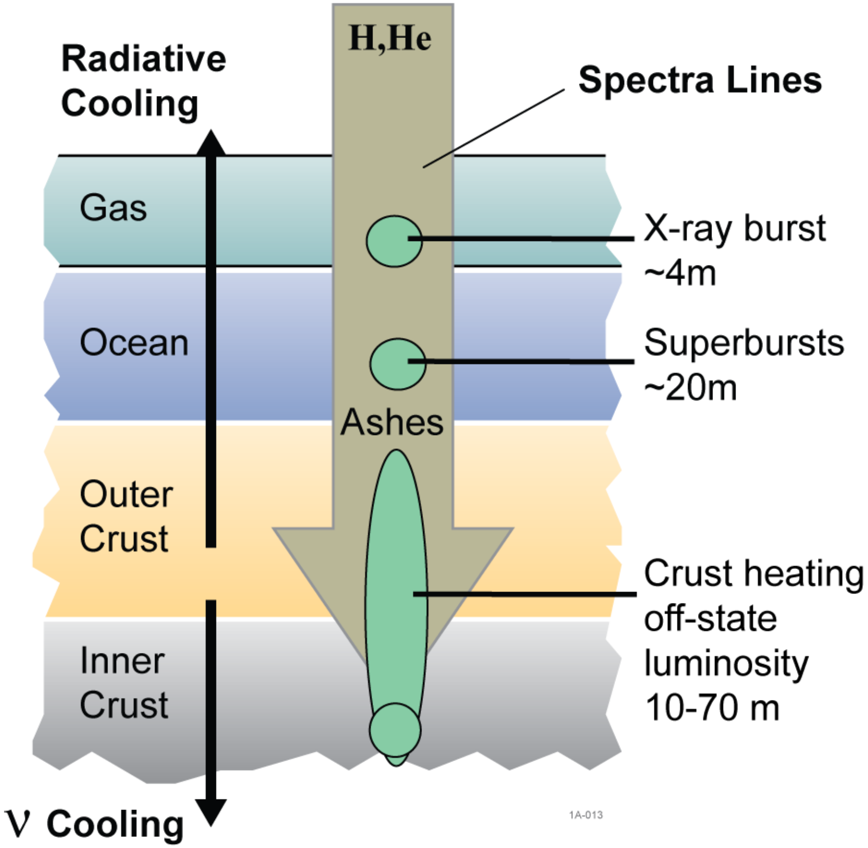


Rare Isotope Crusts of Accreting Neutron Stars



Cackett et al. 2006 (Chandra, XMM-Newton)

Neutron Star Surface

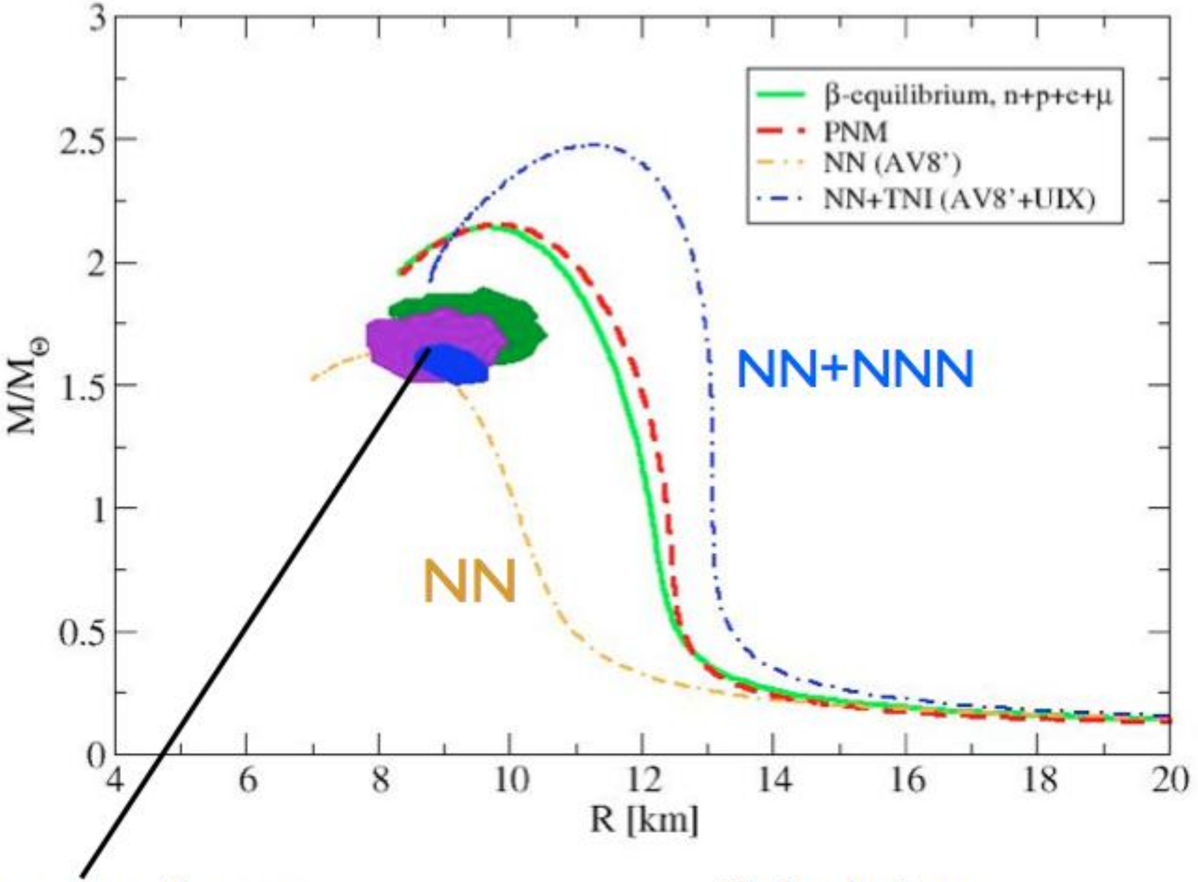


- Nuclear reactions in the crust set thermal properties
- Can be directly observed in transients
- Directly affects superburst ignition

Understanding of crust reactions offers possibility to constrain neutron star properties (core composition, neutrino emission…)

Relevance to neutron star radii and NNN force

From the talk of J. Carlson, LANL



Observations:

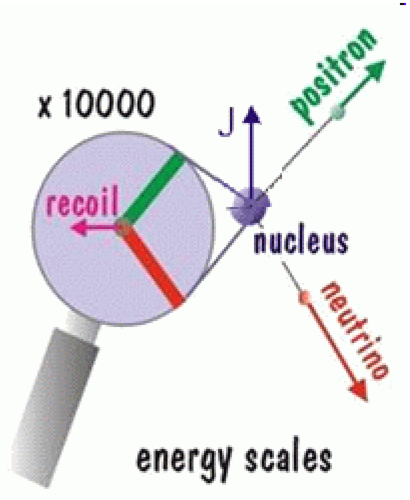
Ozel, Baym, Guyver arXiv:1002.3153

Calculations

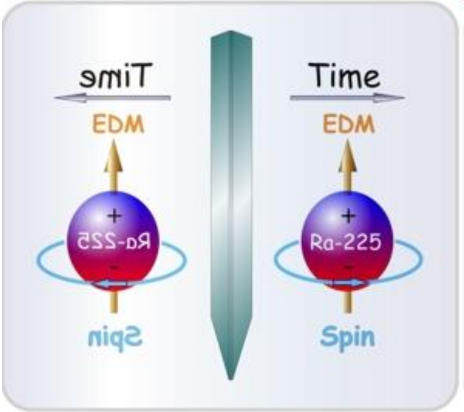
Gandolfi, Illarionov, Fantoni,
Miller, Pederivak, Schmidt : arxiv 0909.3487

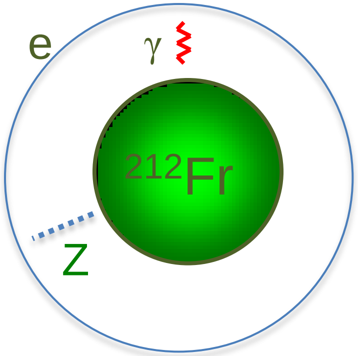
Tests of Nature's Fundamental Symmetries

- Angular correlations in β-decay and search for scalar currents
  - Mass scale for new particle comparable with LHC
  - ^{6}He and ^{18}Ne at 10^{12}/s
- Electric Dipole Moments
  - ^{225}Ac, ^{223}Rn, ^{229}Pa (30,000 more sensitive than ^{199}Hg; I > 10^{10}/s)
- Parity Non-Conservation in atoms
  - weak charge in the nucleus (francium isotopes; 10^{9}/s)
- Unitarity of CKM matrix
  - V_{ud} by super allowed Fermi decay
  - Probe the validity of nuclear corrections



Chupp, Lu, Mueller, Savard et al.



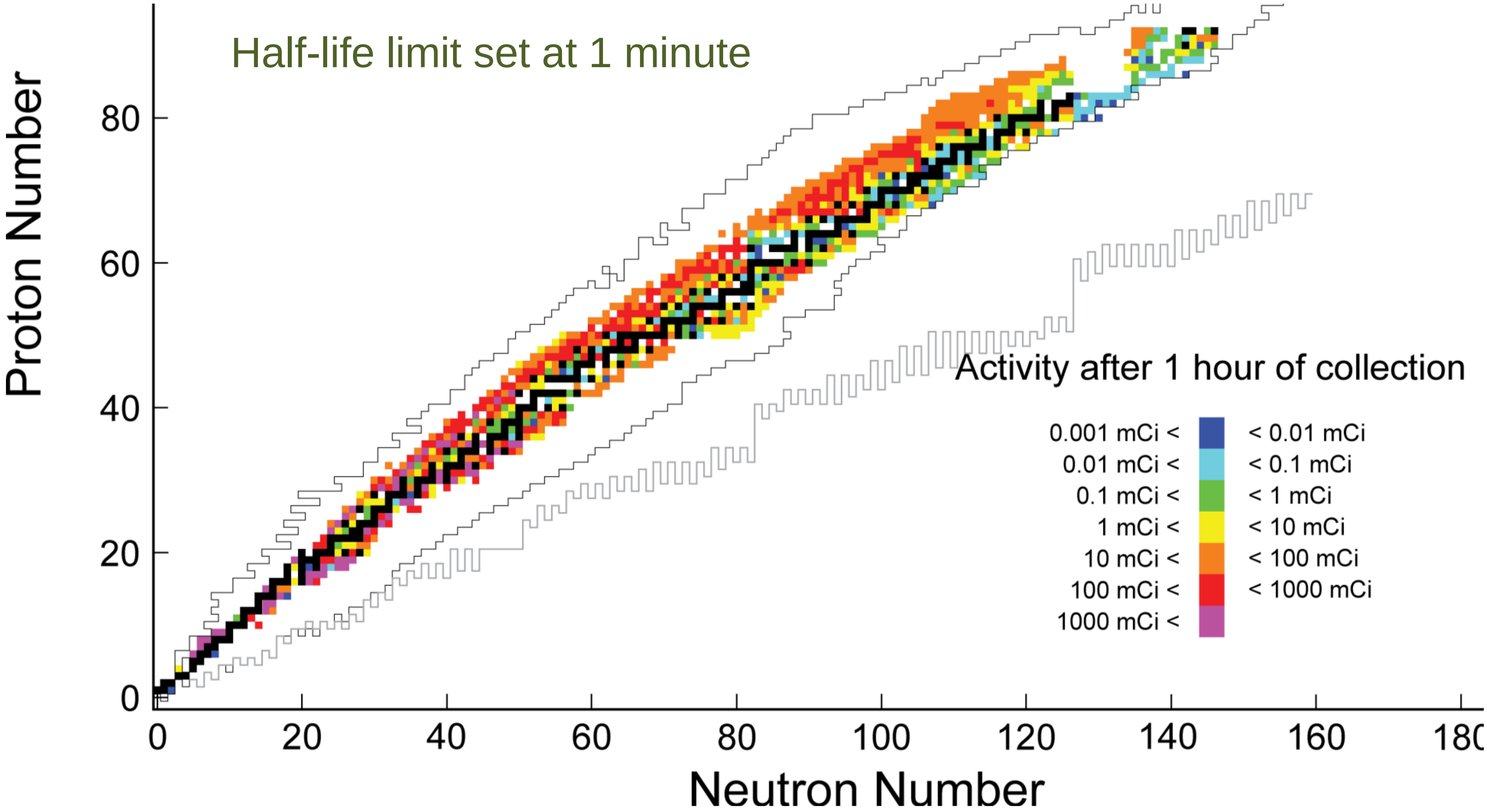


$$\begin{vmatrix} \mathbf{V_{ud}} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{vmatrix}$$

Rare Isotopes For Society

- Isotopes for medical research
  - Examples: ^{47}Sc, ^{62}Zn, ^{64}Cu, ^{67}Cu, ^{68}Ge, ^{149}Tb, ^{153}Gd, ^{168}Ho, ^{177}Lu, ^{188}Re, ^{211}At, ^{212}Bi, ^{213}Bi, ^{223}Ra (DOE Isotope Workshop)
  - α-emitters ^{149}Tb, ^{211}At: potential treatment of metastatic cancer
  - Cancer therapy of hypoxic tumors based on ^{67}Cu possible is a source would be available
- Reaction rates important for stockpile stewardship and nuclear power – related to astrophysics network calculations
  - Determination of extremely high neutron fluxes by activation analysis
  - Rare isotope samples for (n,γ), (n,n'), (n,2n), (n,f) e.g. ^{88,89}Zr
    - » Same technique important for astrophysics
  - More difficult cases studied via surrogate reactions (d,p), (^{3}He,α xn) …
- Tracers for Geology (^{32}Si), Condensed Matter (^{8}Li), material studies, …
- Special isotopes for homeland security applications (β-delayed neutron emitters to calibrate detectors, etc.)

Separated Isotopes from FRIB



Summary

- We have entered the age of designer atoms – new tool for science
- FRIB (and other facilities like CARIBU) will allow production of a wide range of new designer isotopes
  - Necessary for the next steps in accurate modeling of atomic nuclei
  - Necessary for progress in astronomy (chemical history, mechanisms of stellar explosions)
  - Opportunities for the tests of fundamental symmetries
  - Important component of a future U.S. isotopes program
- New applications range from nuclear modeling, astrophysics, fundamental interactions, and use of isotope