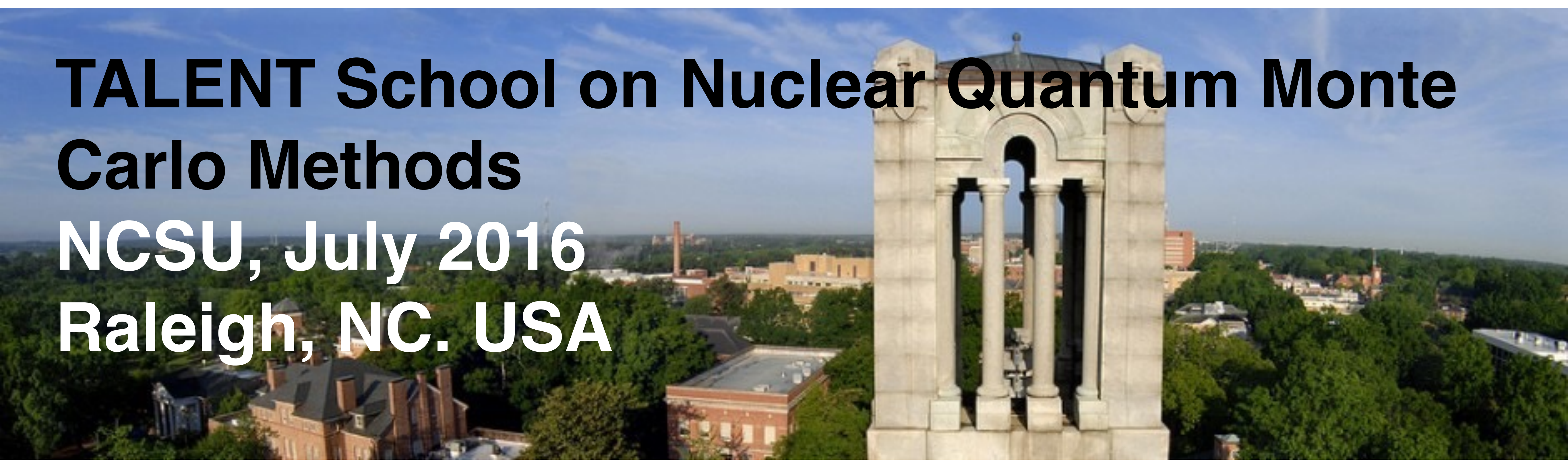
Finite-temperature lattice methods
Lecture 1.

Joaquín E. Drut

University of North Carolina at Chapel Hill

THE UNIVERSITY *of* NORTH CAROLINA *at* CHAPEL HILL



TALENT School on Nuclear Quantum Monte Carlo Methods

NCSU, July 2016

Raleigh, NC. USA

Goals

- **Lecture 1**:
  General motivation. Review of thermodynamics and statistical mechanics. Non-interacting quantum gases at finite temperature.

- **Lecture 2**:
  QRL1. Formalism at finite temperature: Trotter-Suzuki decompositions; Hubbard-Stratonovich transformations. From traces to determinants. Bosons and fermions. The sign problem.

- **Lecture 3**:
  QRL2. Computing expectation values (finally!). Particle number. Energy. Correlation functions: static and dynamic. Sampling techniques. Signal-to-noise issues and how to overcome them.

Goals

- **Lecture 4**:
  Quantum phase transitions and quantum information. Entanglement entropy. Reduced density matrix. Replica trick. Signal-to-noise issues.

- **Lecture 5**:
  QRL3. Finite systems. Particle-number projection. The virial expansion. Signal-to-noise issues. Trapped systems.

- **Lecture 6**:
  QRL5. Spacetime formulation. Finite-temperature perturbation theory on the lattice.

- **Lecture 7**:
  Applications to ultracold atoms in a variety of situations. Beyond equilibrium thermodynamics.

Motivation

Questions that drive low-energy nuclear physics

- How do protons and neutrons make stable nuclei and rare isotopes? Where are the limits?
- What are the heaviest nuclei that can exist?
- What is the equation of state of nucleonic matter?
- What is the origin of simple patterns in complex nuclei?
- How do we describe fission, fusion, reactions, . . . ?

Physics of Nuclei

- How did the elements from iron to uranium originate?
- How do stars explode?
- What is the nature of neutron star matter?

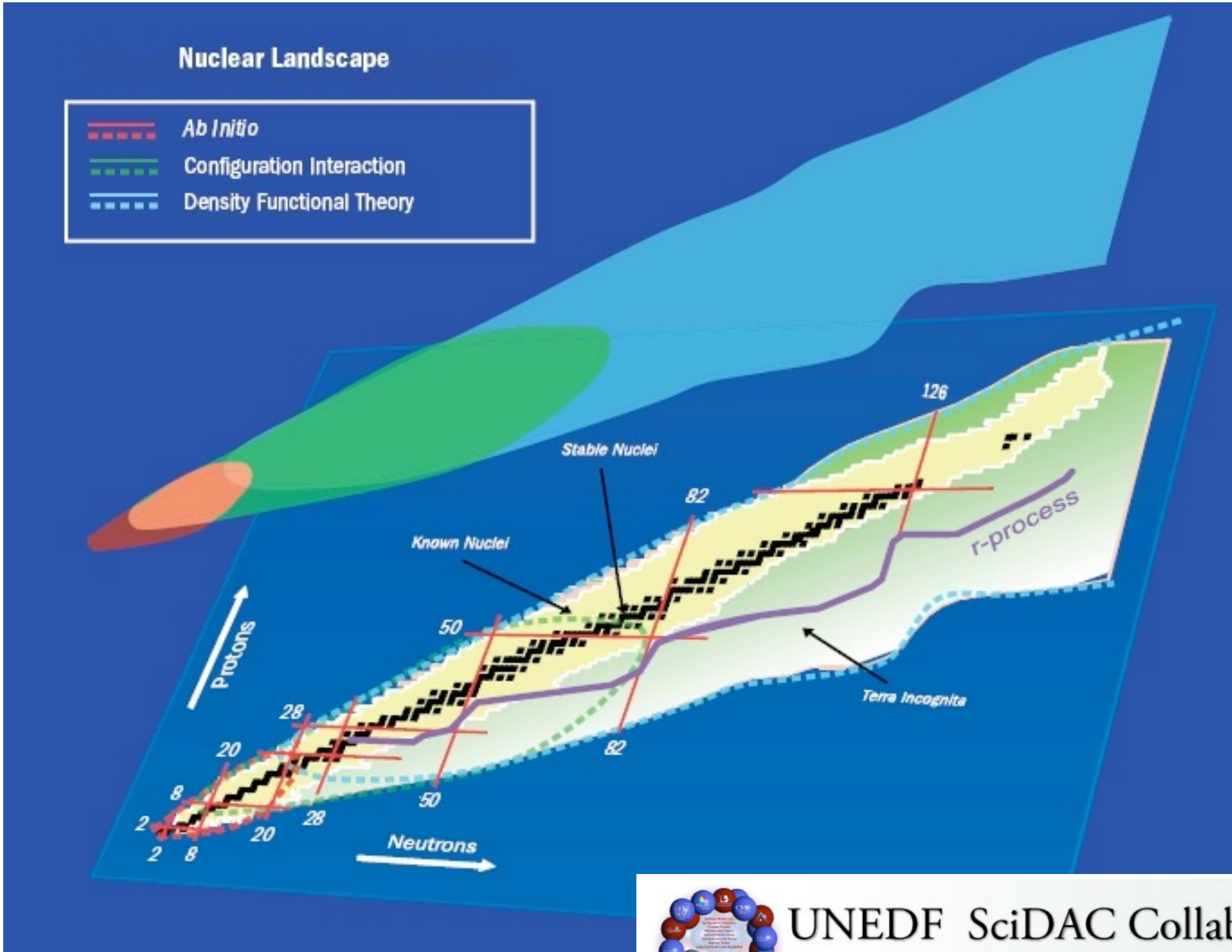
Nuclear Astrophysics

- How can our knowledge of nuclei and our ability to produce them benefit humankind? Life Sciences, Material Sciences, Nuclear Energy, Security

Applications of Nuclei

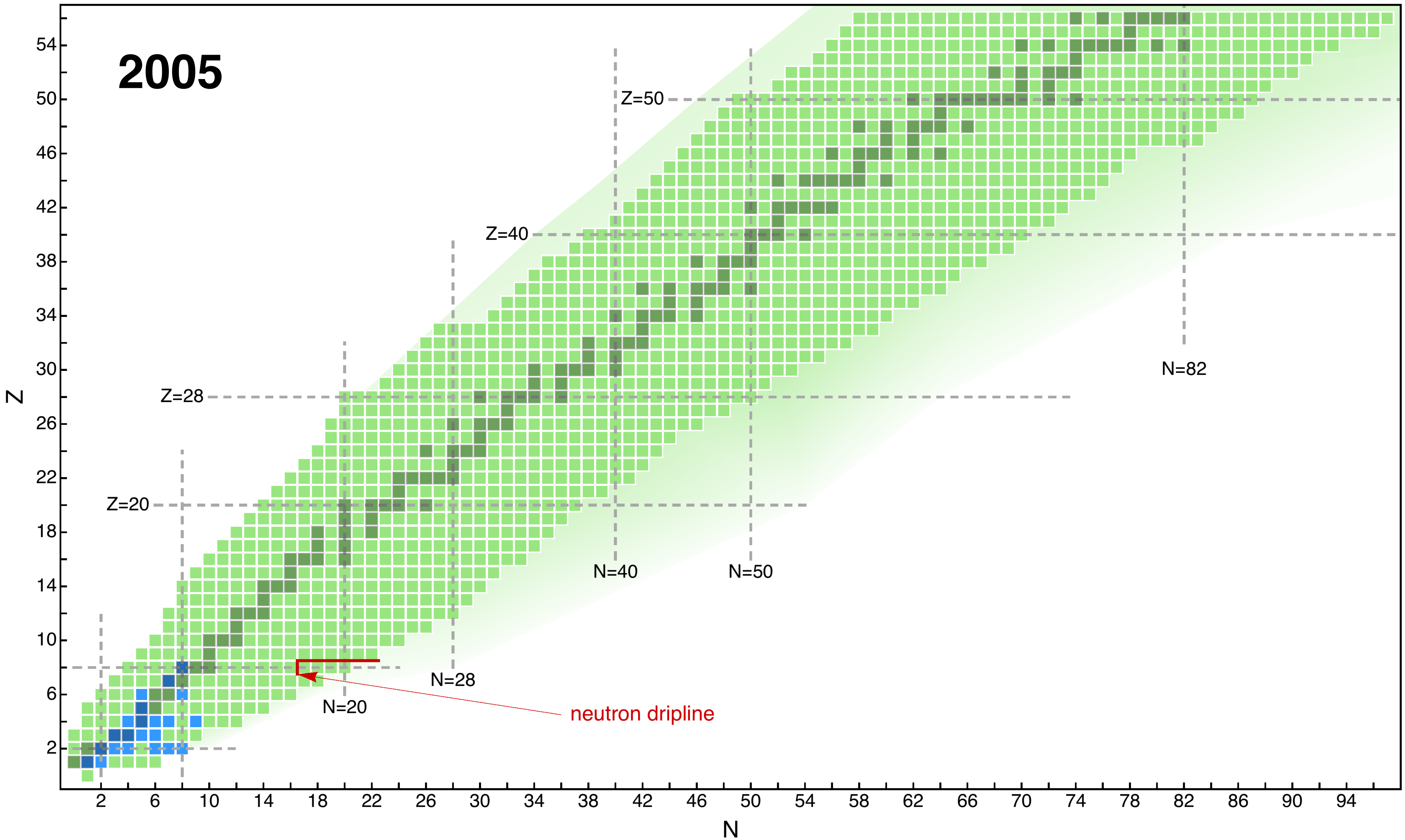
(Slide from a talk by Scott Bogner (MSU/NSCL))

Nuclear landscape vs. methods



UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

Entering a precision era in nuclear structure calculations…



courtesy of H. Hergert

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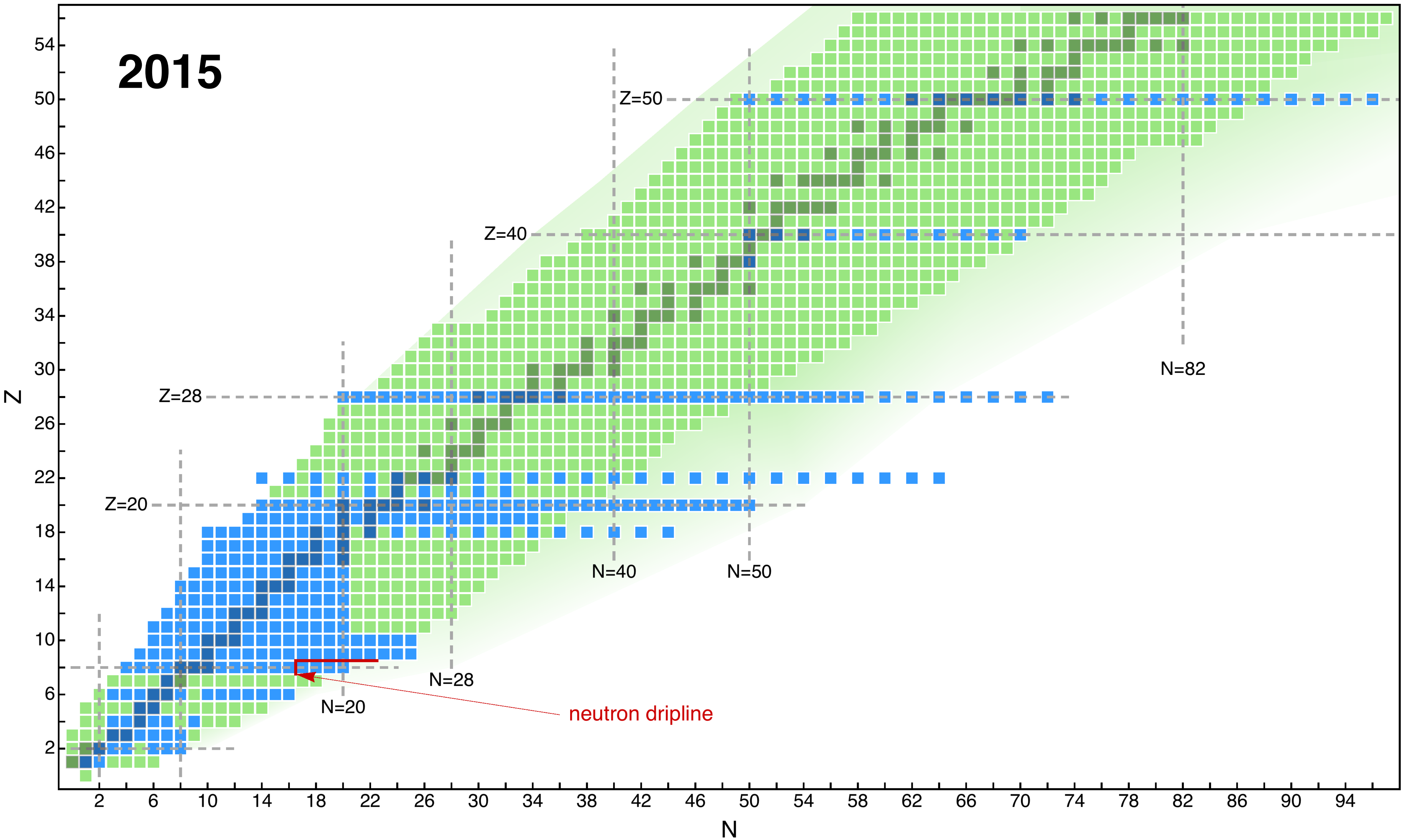

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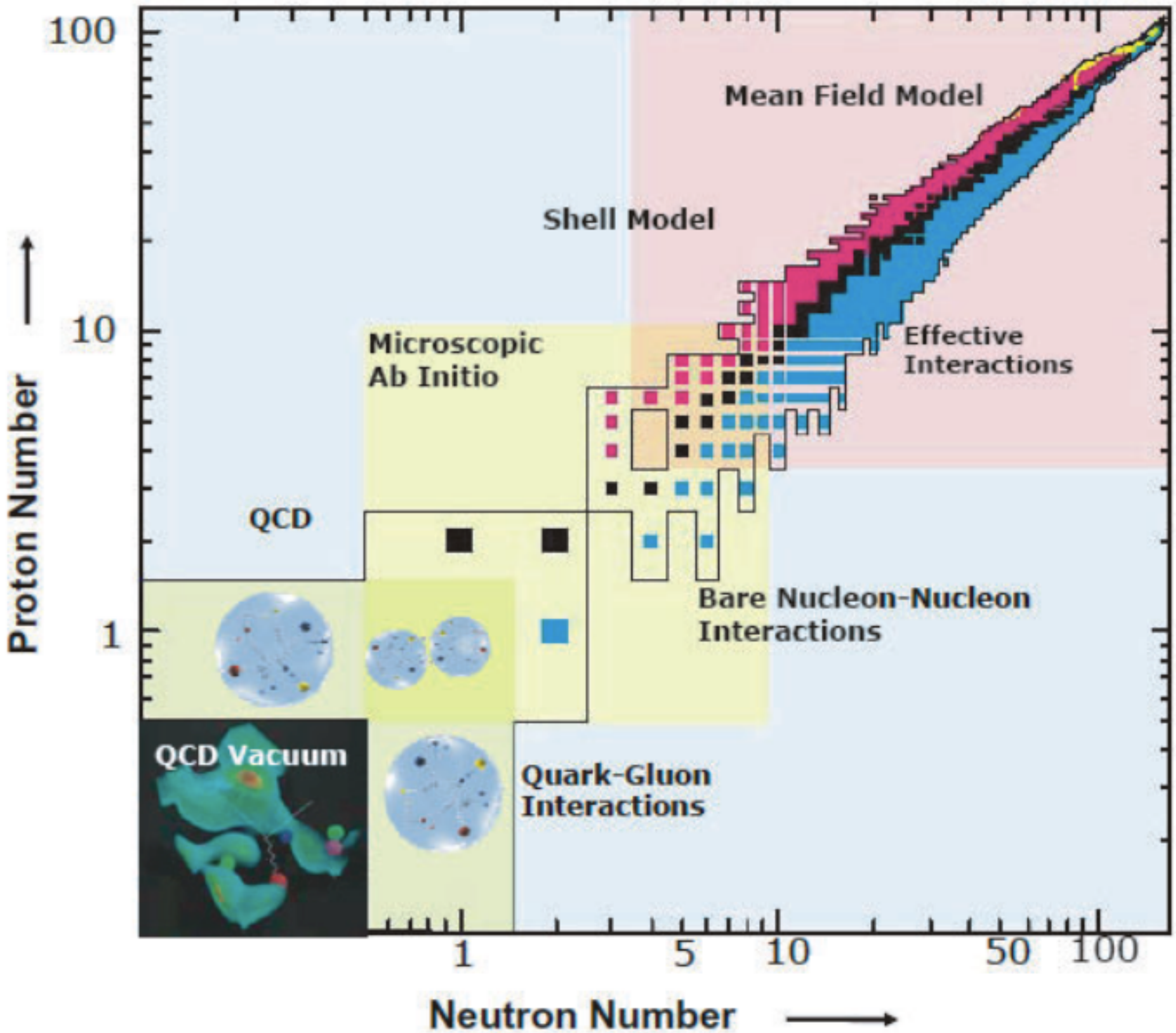
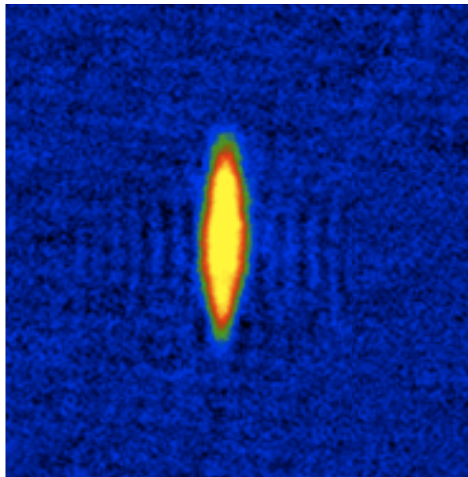
Physics and degrees of freedom

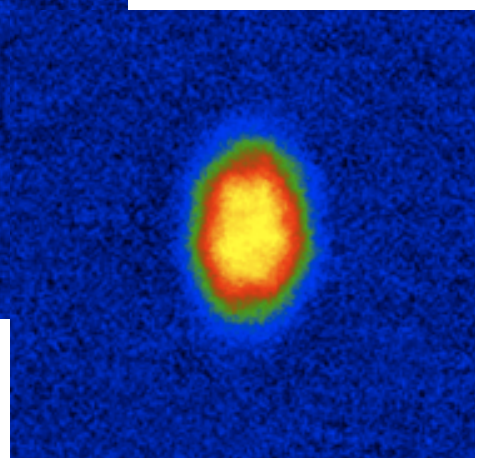


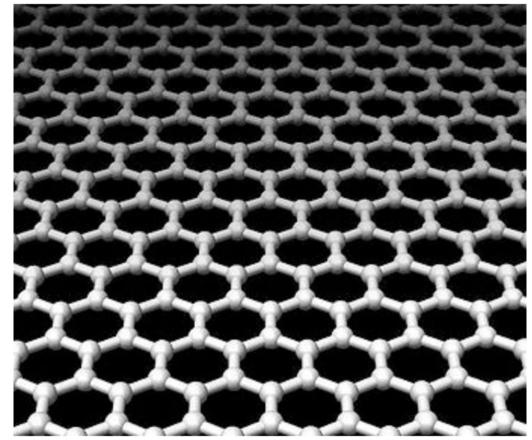
Ultracold Gases

Condensed Matter Physics



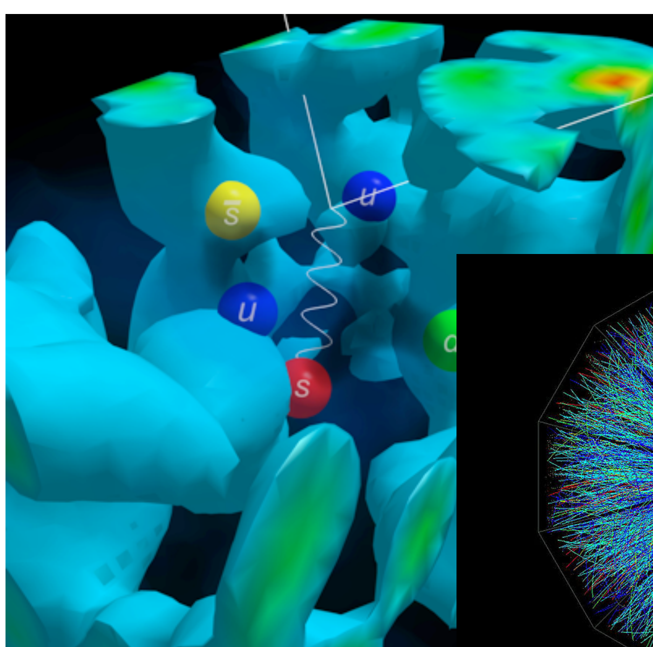
JETLab (NCSU)

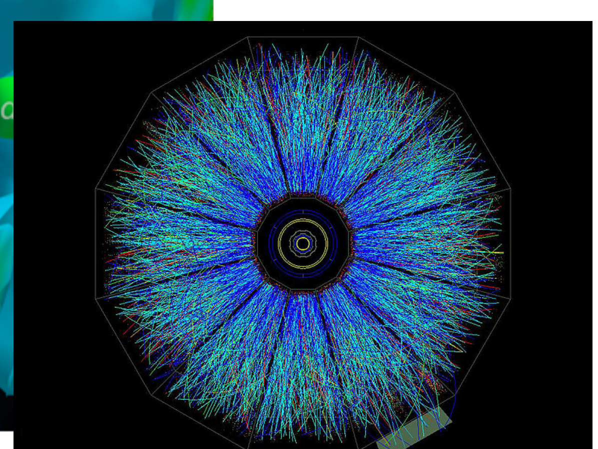




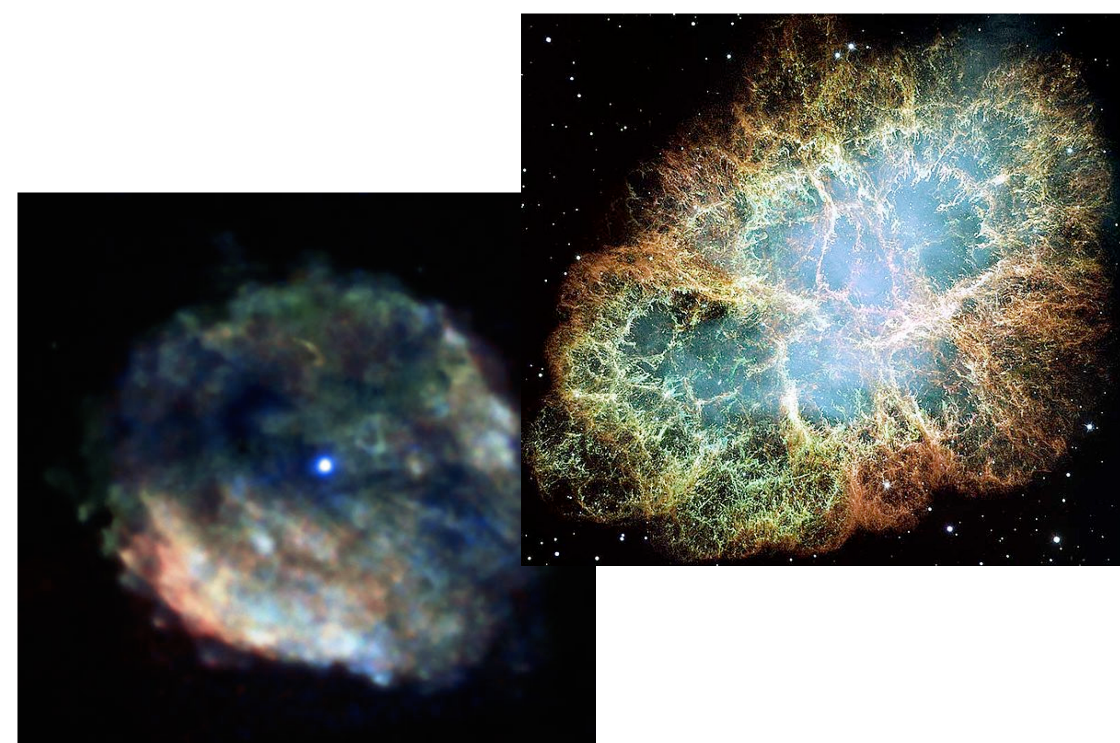
Materials Science

High-Energy Physics, QCD, Low-Energy NP

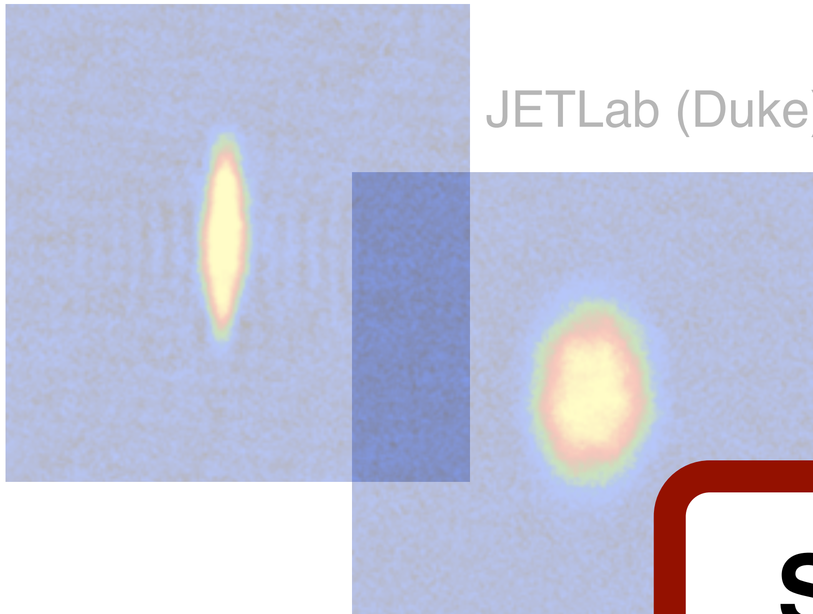




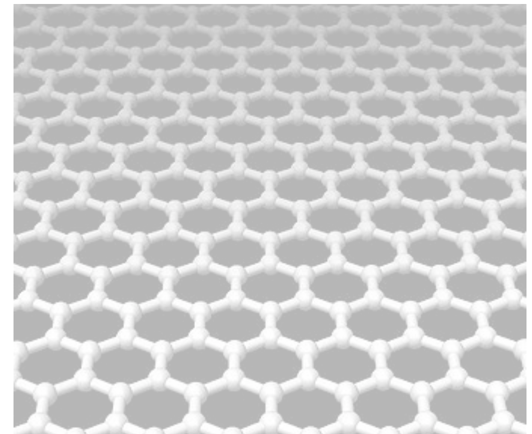
Astrophysics



Ultracold Gases


JETLab (Duke)

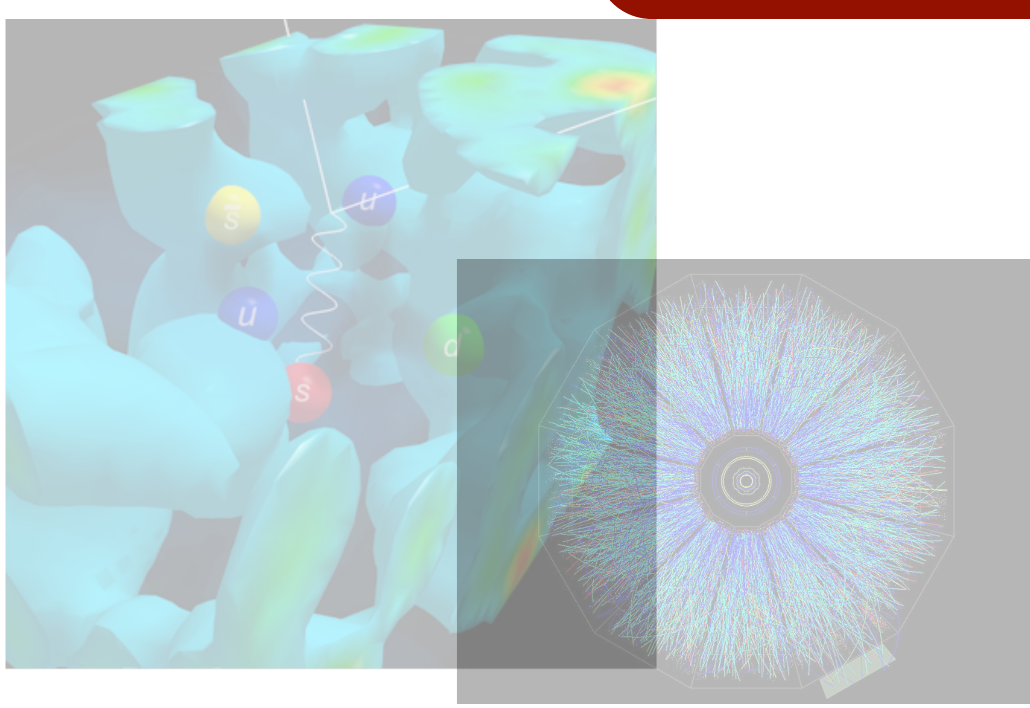
Condensed Matter Physics



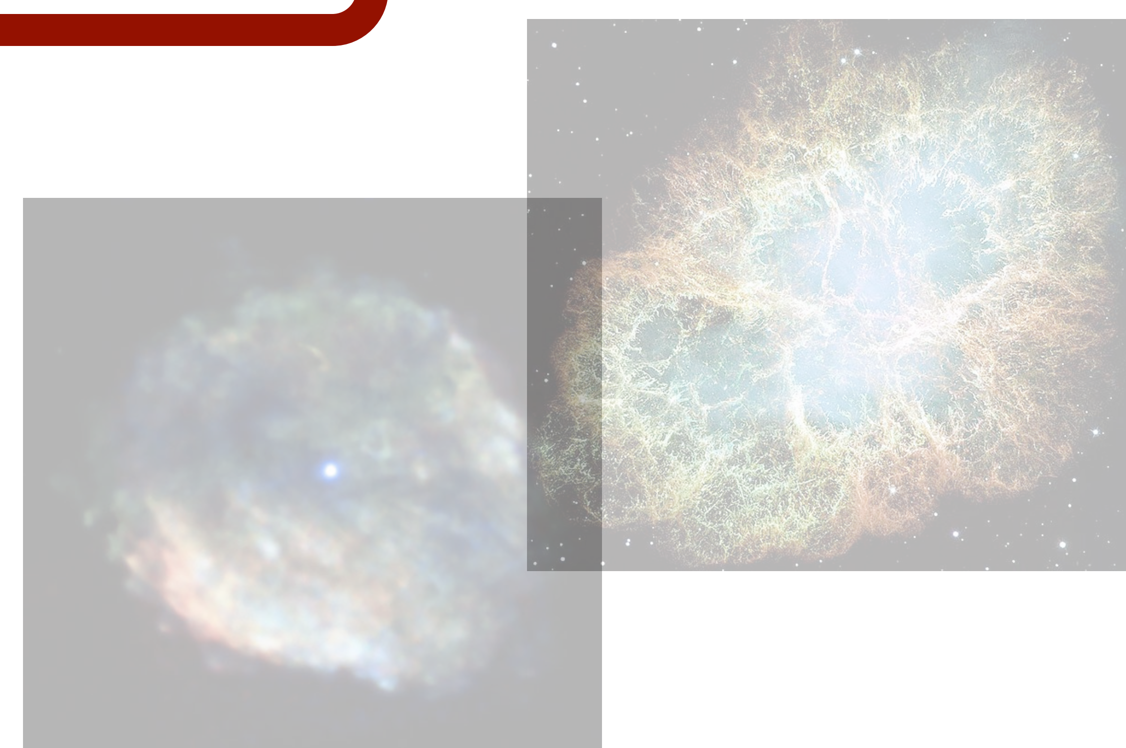
Materials Science

Strongly correlated quantum many-body systems

High-Energy Pl
QCD, Low-Ene



strophysics
ly neutron stars)



Thermodynamics
and
Statistical Mechanics

Fundamental thermodynamic identity

$$dE = TdS - PdV + \mu dN$$

"In equilibrium, there exists a function…"

Internal energy $E = E(S, V, N)$

S, V, N *extensive* variables

The *intensive* variables (independent from system size) are therefore

$$T = \left(\frac{\partial E}{\partial S}\right)_{V,N} \qquad -P = \left(\frac{\partial E}{\partial V}\right)_{S,N} \qquad \mu = \left(\frac{\partial E}{\partial N}\right)_{S,V}$$

This formulation is useful to study *isentropic* processes, but in many cases we are more interested in *isothermal* processes.

Legendre transforms

Helmholtz free energy

$$F = E - TS$$

$$T = \left(\frac{\partial E}{\partial S}\right)_{V,N}$$

$$dF = -SdT - PdV + \mu dN$$

$$F = F(T, V, N)$$

Gibbs free energy

$$G = E - TS + PV$$

$$-P = \left(\frac{\partial E}{\partial V}\right)_{S,N}$$

$$dG = -SdT + VdP + \mu dN$$

$$G = G(T, P, N)$$

To do: Familiarize yourself with the geometric meaning of the Legendre transform, if you don't know this already.

Legendre transforms

Helmholtz free energy

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$$F = F(T, V, N)$$

Gibbs free energy

$$G = E - TS + PV$$

$$-P = \left(\frac{\partial E}{\partial V}\right)_{S,N}$$

$$dG = -SdT + VdP + \mu dN$$

$$G = G(T, P, N)$$

All of these are valid and useful thermodynamic potentials.
The most important one for us, however, will be the
grand thermodynamic potential

$$\Omega(T, V, \mu) = F - \mu N = E - TS - \mu N$$

$$d\Omega = -SdT - PdV - Nd\mu$$

Extensive variables, homogeneity, and the Gibbs-Duhem relation

All thermodynamic potentials are extensive; they are *homogeneous functions* of the extensive variables:

$$E(\lambda S, \lambda V, \lambda N) = \lambda E$$

Differentiate w.r.t. λ and set $\lambda = 1$ to show that

$$E = TS - PV + \mu N$$

Clearly,

$$F = -PV + \mu N \qquad G = \mu N \qquad \Omega = -PV$$

This is all OK, but our goal is to obtain this thermodynamic description from the **microscopic variables**…

Statistical mechanics: canonical ensemble

Hamiltonian

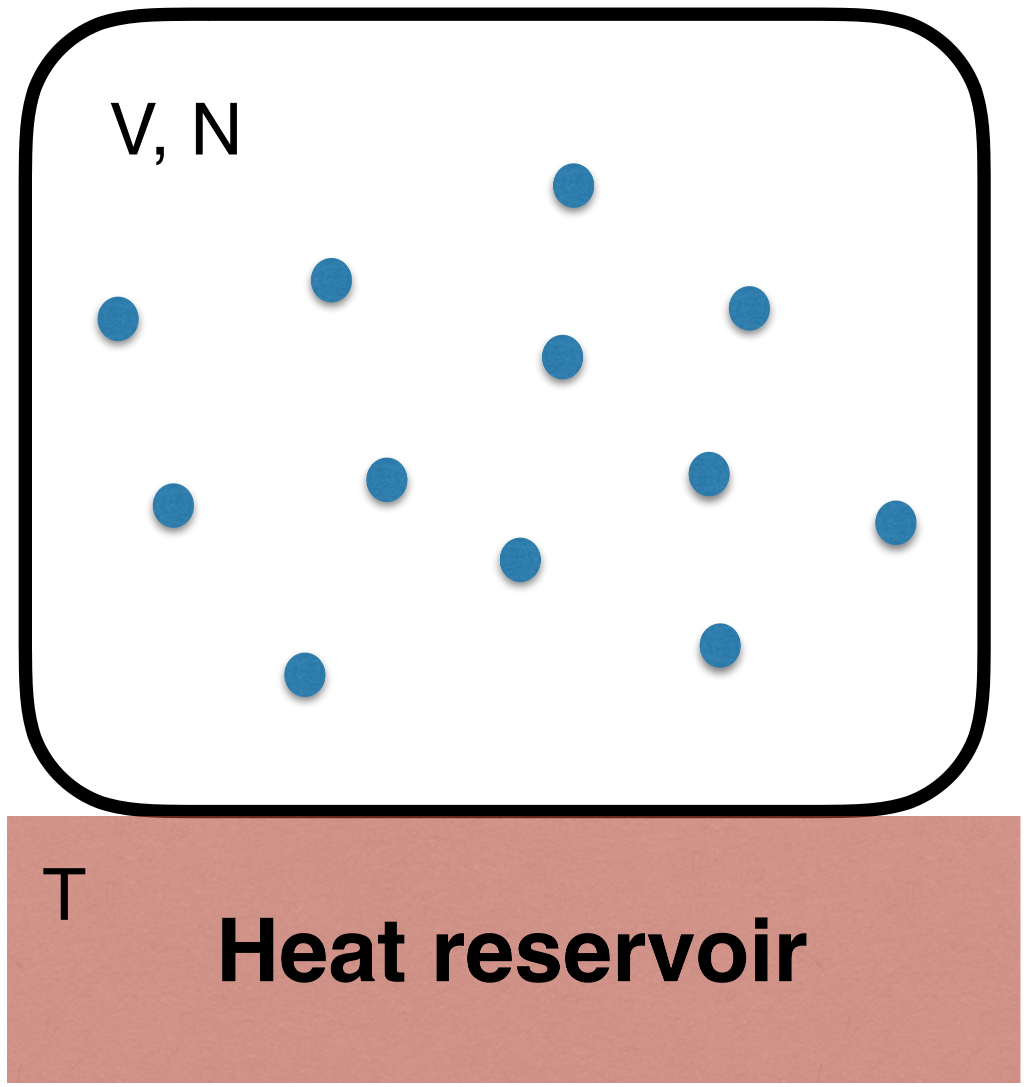
$\hat{H}$

Particle number

$\hat{N}$

Other conserved charges

“Canonical ensemble”



Statistical mechanics: grand-canonical ensemble

Hamiltonian

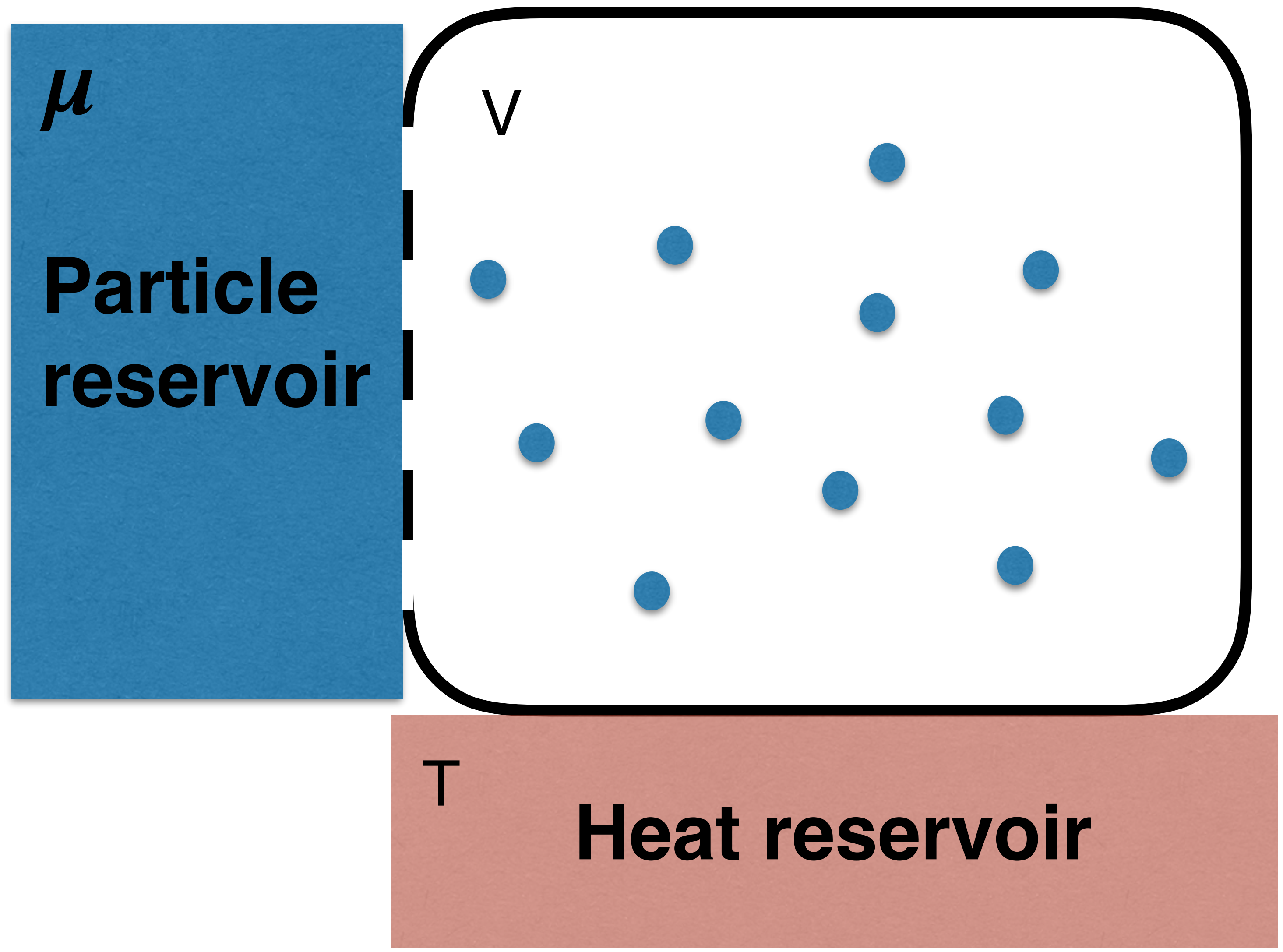
$\hat{H}$

Particle number

$\hat{N}$

Other conserved charges

“Grand-canonical ensemble”



Statistical mechanics: connection to thermodynamics

Canonical ensemble

partition function

$$\mathcal{Q}_N = \mathrm{tr}_N \left[e^{-\beta \hat{H}} \right] = \sum_j e^{-\beta E_j(N)}$$

"inverse temperature"

$$\beta = \frac{1}{k_B T}$$

Grand-canonical ensemble

partition function

$$\mathcal{Z} = \mathrm{tr} \left[e^{-\beta(\hat{H} - \mu \hat{N})} \right] = \sum_N \sum_j e^{-\beta(E_j(N) - \mu N)} = \sum_N z^N \mathcal{Q}_N$$

"fugacity"

$$z = e^{\beta \mu}$$

Connection to thermodynamics

$$-\beta F(T, V, N) = \ln \mathcal{Q}_N \qquad -\beta \Omega(T, V, \mu) = \ln \mathcal{Z}$$

Statistical mechanics: expectation values

Two equivalent ways to think about this:

1.- Define the *statistical operator*

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathcal{Z}}$$

Then the ensemble average of a given operator is

$$\langle\hat{O}\rangle = \mathrm{tr}\left[\hat{\rho}\ \hat{O}\right] = \frac{\mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\hat{O}\right]}{\mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]}$$

Statistical mechanics: expectation values

Two equivalent ways to think about this:

2.- Insert a *source* in the partition function

$$\mathcal{Z} \to \mathcal{Z}[j(x)] = \mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N}-X[j(x)])}\right]$$

$$X[j(x)] = \int d^d x\; j(x)\hat{O}(x)$$

Then the ensemble average we want is

$$\langle\hat{O}\rangle = \frac{1}{\beta}\frac{\delta \ln \mathcal{Z}[j(x)]}{\delta j(x)}\bigg|_{j\to 0}$$

Try it!

Simplest examples:

$$\langle\hat{N}\rangle = ? \qquad\qquad \langle\hat{H}\rangle = ?$$

Second quantization

Repackaging of many-body quantum mechanics

Symmetry and anti-symmetry properties of the many-body wavefunction are encoded in operator algebra of creation/annihilation operators

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$$

Bosons

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}$$

Fermions

$$\hat{a}_j^\dagger|0\rangle = |000001_j0000\rangle \longrightarrow \varphi_j(x)$$

$\hat{a}_j^\dagger \hat{a}_j$ counts occupation of state j

Quantum Gases

Statistical mechanics of non-interacting quantum gases

Hamiltonian

$$\hat{H} = \hat{H}_0 = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}}$$

Single-particle states

Continuum
box

$$\sum_{\mathbf{p}} \to \frac{L^d}{(2\pi)^d} \int d^d p$$

Statistical mechanics of non-interacting quantum gases

Hamiltonian

$$\hat{H} = \hat{H}_0 = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}}$$

Single-particle states

Continuum box

$$\sum_{\mathbf{p}} \to \frac{L^d}{(2\pi)^d} \int d^d p$$

Lattice box

$$\mathbf{p} = (p_1, p_2, \ldots, p_d)$$

PBC $\quad p_j : \dfrac{2\pi}{L} n_j, \qquad n_j = -L/2, \ldots, L/2$

HWBC $\quad p_j : \dfrac{\pi}{L} n_j, \qquad n_j = 1, \ldots, L$

Statistical mechanics of non-interacting quantum gases

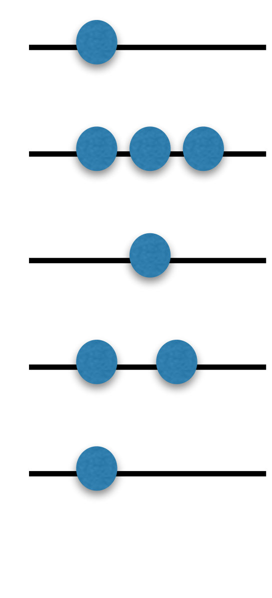
Grand-canonical partition function

Summing over all possible states amounts to summing over all possible **occupations** of the single-particle states.

$$\mathcal{Z} = \mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]$$

$$\mathcal{Z} = \sum_{n_1, n_2, \ldots, n_\infty} e^{-\beta\left(\frac{p_1^2}{2m}-\mu\right)n_1} \ldots e^{-\beta\left(\frac{p_\infty^2}{2m}-\mu\right)n_\infty}$$

$$= \prod_{i=1}^{\infty} \sum_{n_i} e^{-\beta\left(\frac{p_i^2}{2m}-\mu\right)n_i}$$



Statistical mechanics of non-interacting quantum gases

Grand-canonical partition function: Fermions

$$\mathcal{Z}_F = \prod_{i=1}^{\infty} \left[1 + e^{-\beta\left(\frac{p_i^2}{2m} - \mu\right)} \right]$$

$$-\beta\Omega_F = \ln \mathcal{Z}_F = \sum_{i=1}^{\infty} \ln \left[1 + e^{-\beta\left(\frac{p_i^2}{2m} - \mu\right)} \right]$$

$$\langle \hat{N} \rangle = \frac{\partial(-\beta\Omega_F)}{\partial(\beta\mu)} = \sum_{i=1}^{\infty} \frac{e^{-\beta(\epsilon_i - \mu)}}{1 + e^{-\beta(\epsilon_i - \mu)}} \qquad \epsilon_i = p_i^2/2m$$

Statistical mechanics of non-interacting quantum gases

Grand-canonical partition function: Fermions

$$\langle \hat{N} \rangle = \frac{\partial(-\beta\Omega_F)}{\partial(\beta\mu)} = \sum_{i=1}^{\infty} \frac{e^{-\beta(\epsilon_i - \mu)}}{1 + e^{-\beta(\epsilon_i - \mu)}}$$

How would you calculate this in practice?

What would you plot?

What are the variables?

Statistical mechanics of non-interacting quantum gases

Grand-canonical partition function: Bosons

$$\mathcal{Z}_B = \prod_{i=1}^{\infty} \left[1 - e^{-\beta\left(\frac{p_i^2}{2m} - \mu\right)} \right]^{-1}$$

$$-\beta\Omega_B = \ln \mathcal{Z}_B = \sum_{i=1}^{\infty} - \ln \left[1 - e^{-\beta\left(\frac{p_i^2}{2m} - \mu\right)} \right]$$

$$\langle \hat{N} \rangle = \frac{\partial(-\beta\Omega_B)}{\partial(\beta\mu)} = \sum_{i=1}^{\infty} \frac{e^{-\beta(\epsilon_i - \mu)}}{e^{-\beta(\epsilon_i - \mu)} - 1} \qquad \epsilon_i = p_i^2/2m$$

Statistical mechanics of non-interacting quantum gases

Grand-canonical partition function: Bosons

$$\langle \hat{N} \rangle = \frac{\partial(-\beta\Omega_B)}{\partial(\beta\mu)} = \sum_{i=1}^{\infty} \frac{e^{-\beta(\epsilon_i-\mu)}}{e^{-\beta(\epsilon_i-\mu)}-1}$$

Suggested exercises

- Use the expressions we derived to calculate the **particle number density** and **energy density** on the lattice…
- Calculate for fermions and bosons in 1D, with periodic and hard-wall boundaries.
- Repeat the above in higher dimensions.

Suggested exercises

- Use the expressions we derived to calculate the **particle number density** and **energy density** on the lattice…
- Calculate for fermions and bosons in 1D, with periodic and hard-wall boundaries.
- Repeat the above in higher dimensions.
- How would you compute other properties?

$$\hat{\mathcal{O}} = O_{pp'}\hat{a}^\dagger_p \hat{a}_{p'} \qquad\qquad \hat{\mathcal{O}} = O_{xx'}\hat{\psi}^\dagger_x \hat{\psi}_{x'}$$

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \mathrm{tr}\left[\hat{\mathcal{O}} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right]$$

References

- H. B. Callen, *Thermodynamics and an introduction to thermostatistics.*
- Fetter & Walecka, *Quantum theory of many-particle systems.*