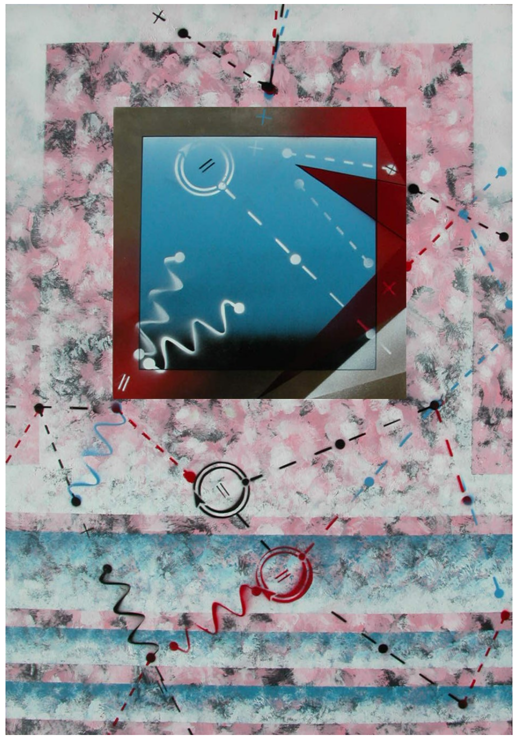
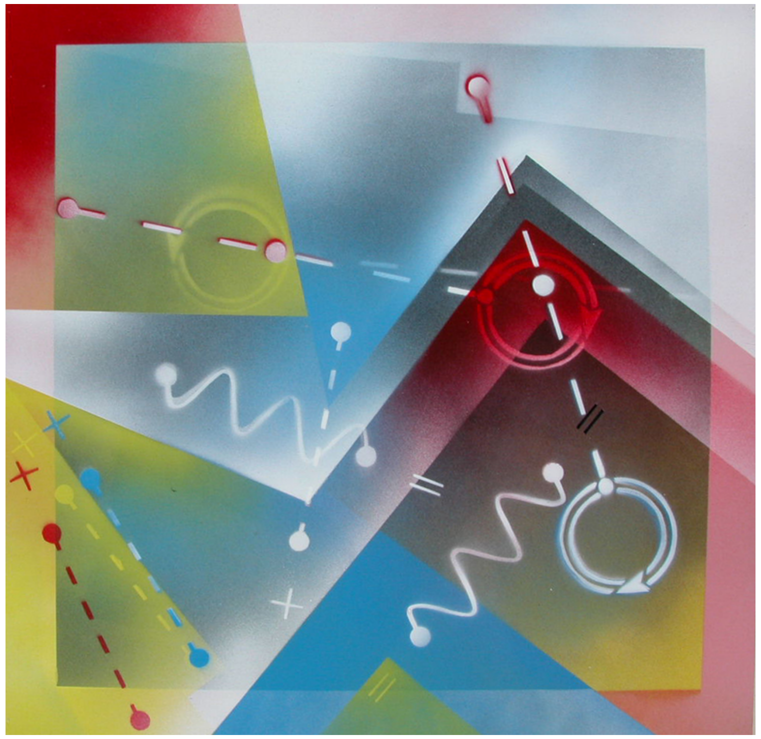
Recent progress in ab initio approaches to the nuclear many-body problem

Vittorio Somà
CEA Saclay / IRFU / Service de Physique Nucléaire



Forze nello spazio I



Forze nello spazio II

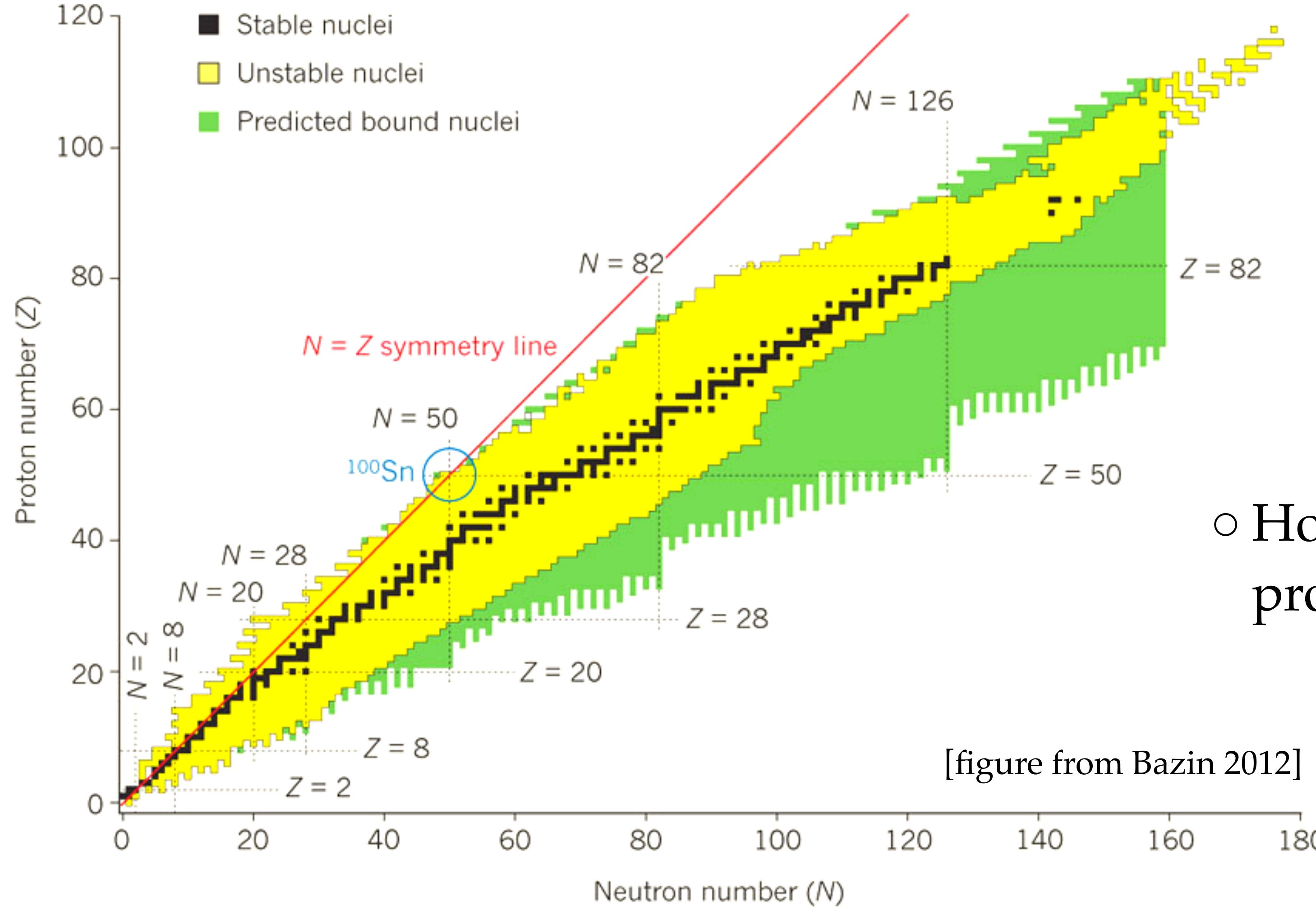
Meo Carbone (2014)

Progresses in algorithms and numerical tools for QCD
Orsay, 16 May 2017

Basic questions about nuclei

○ **How many** bound nuclei exist? (~6000-7000?)

○ **Heaviest** possible element?
Enhanced stability near Z=120?



[figure from Bazin 2012]

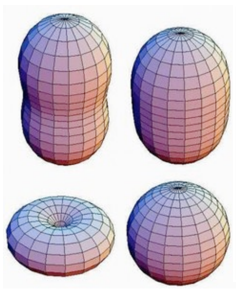
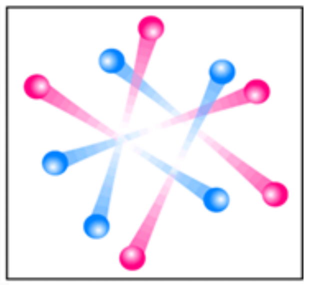
○ How nuclei have been produced in the universe?

○ Where is the neutron **drip-line** beyond Z=8?

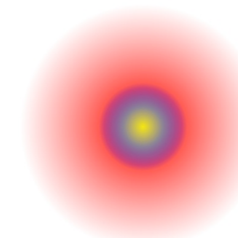
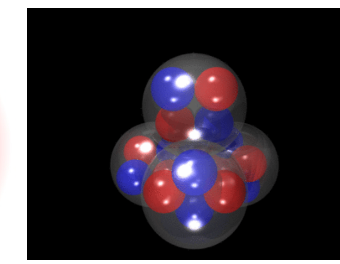
○ Are **magic numbers** the same for unstable nuclei?

Basic questions about nuclei

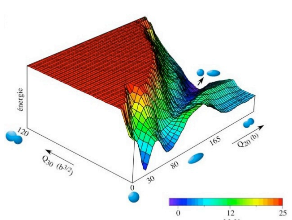
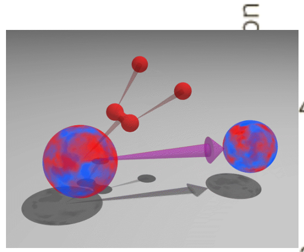
Ground state
Mass, size, deformation, superfluidity, …

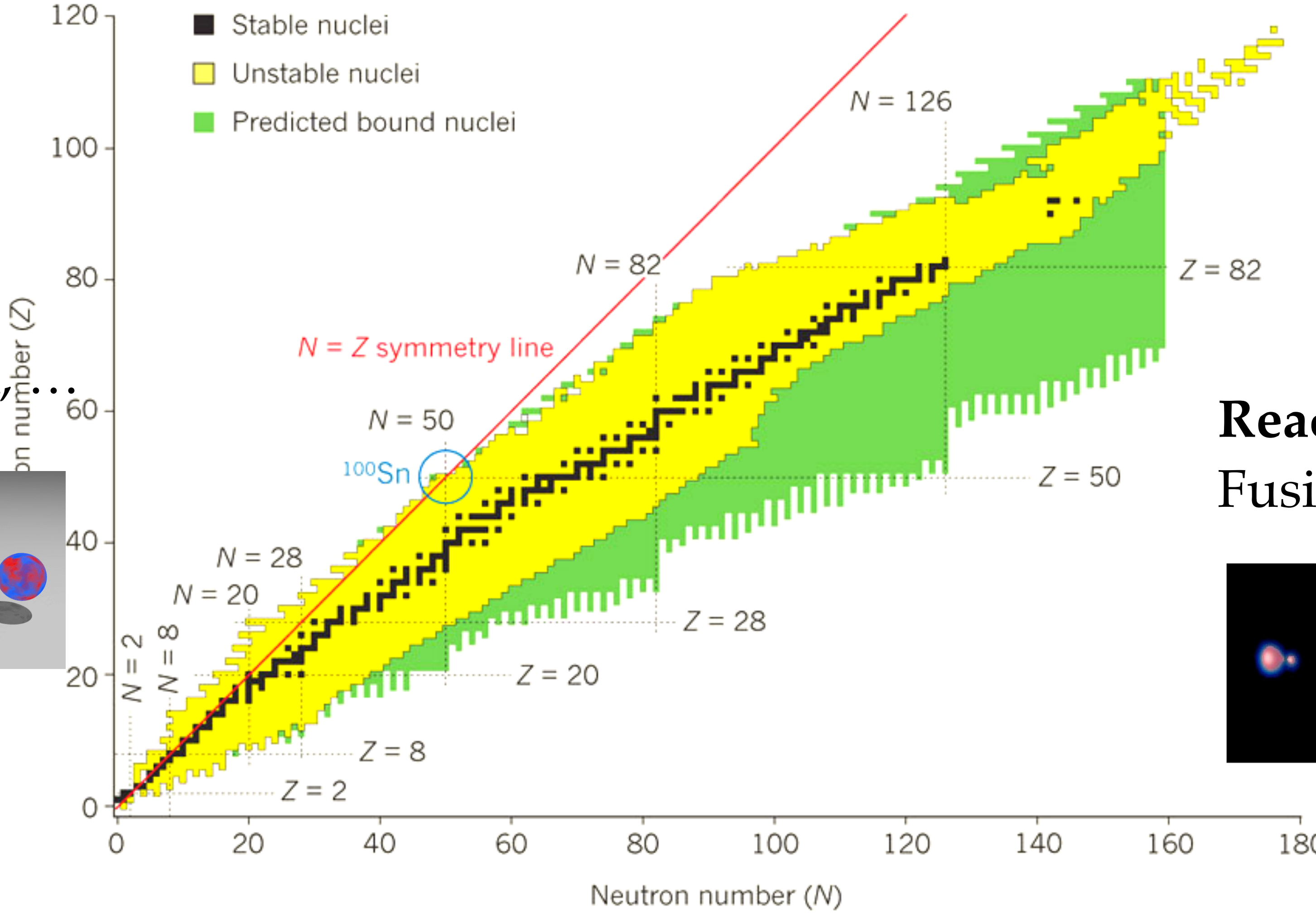



Exotic structures
Clusters, halos, …

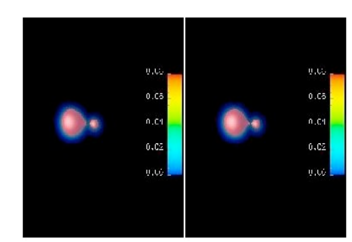
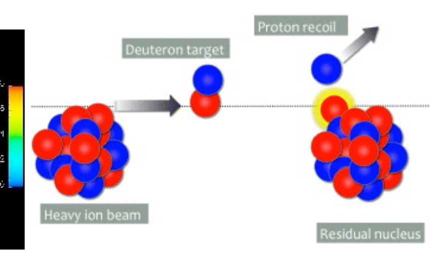



Radioactive decays
β, 2β, α, p, 2p, fission, …

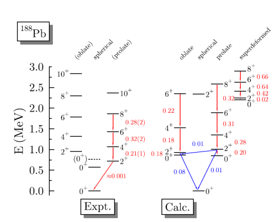



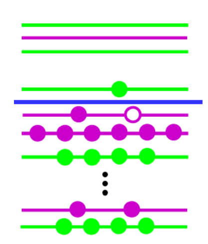
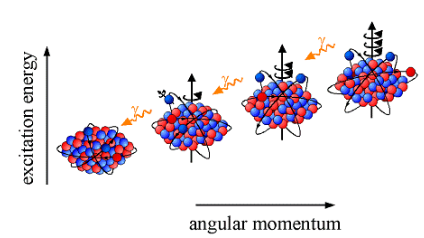


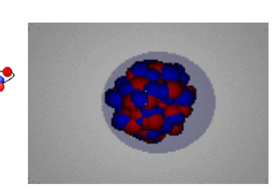
Reaction processes
Fusion, transfer, knockout, …

Spectroscopy
Excitation modes





Theory: ab initio vs effective

Ab initio approaches

$$H|\Psi\rangle = E|\Psi\rangle$$

- H describes NN system in vacuum
  - **Fit to NN scattering data & deuteron**
- Link to QCD is usually **present** (EFT)
- Require sophisticated many-body scheme
  - **Limited applicability in mass (A<100)**
  - **Limited to specific observables**
- Promise thorough theoretical errors

How far can this strategy be pushed?

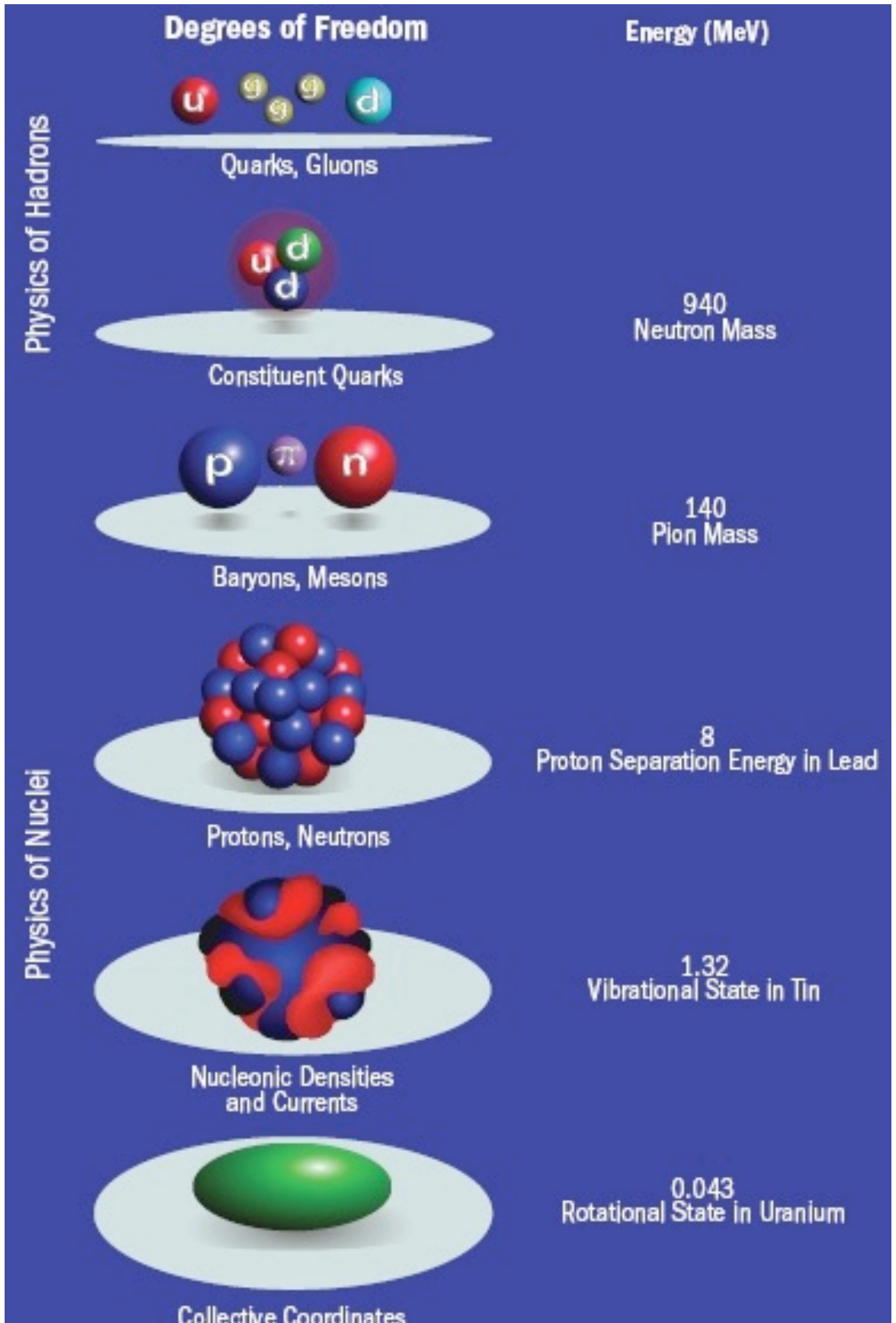
Effective approaches

$$H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$$

- H^{eff} incorporates in-medium correlations
  - **Fit to many-body observables**
- Link to QCD is usually **lost**
- Allow use of simple many-body scheme
  - **Applicable to whole nuclear chart**
  - **Access all nuclear properties**
- Systematic errors hard to assess

Can it be predictive?

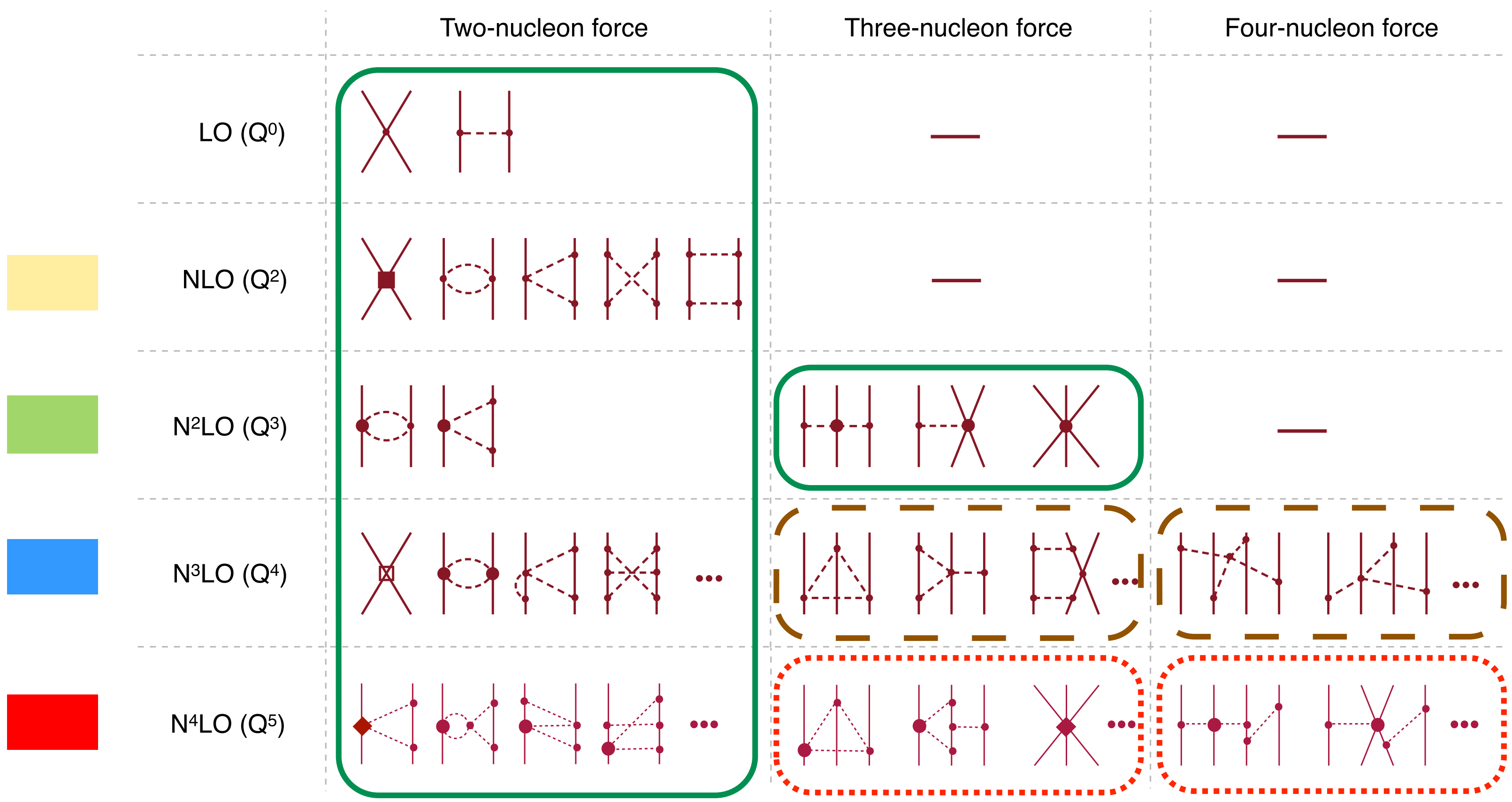
Chiral effective field theory (χEFT)

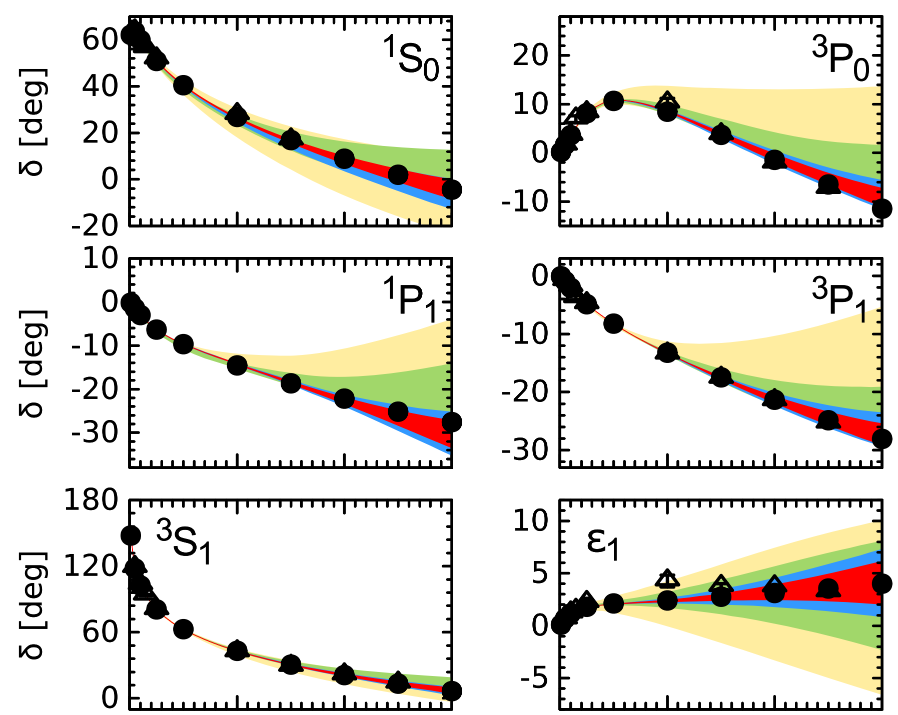


- **EFT: exploit separation of scales**
  - Relevant DOFs are nucleons and pions
  - Nucleons interact via pions + contact terms
- **Knowledge of QCD (symmetries) inherited**
  - In particular chiral symmetry (breaking)
- **Lagrangian organised to select dominant processes**
  - Systematic, many-nucleon forces emerge naturally
  - Provides means to estimate theoretical errors
- **Parameters ("low-energy constants")**
  - Today, X-nucleon forces adjusted to X-nucleon data
  - In the future, computed from (lattice) QCD

Chiral EFT & many-body problem

- **Chiral effective field theory** as a systematic framework to construct *A*N interactions (*A*=2, 3, …)
  - Hierarchy dictated by power counting
  - Hope that 2N & 3N forces are sufficient
  - Hope that few orders in the chiral expansion are sufficient





[Meißner 2016]

- **Ideally**, perform order-by-order many-body calculations with **propagated uncertainties**

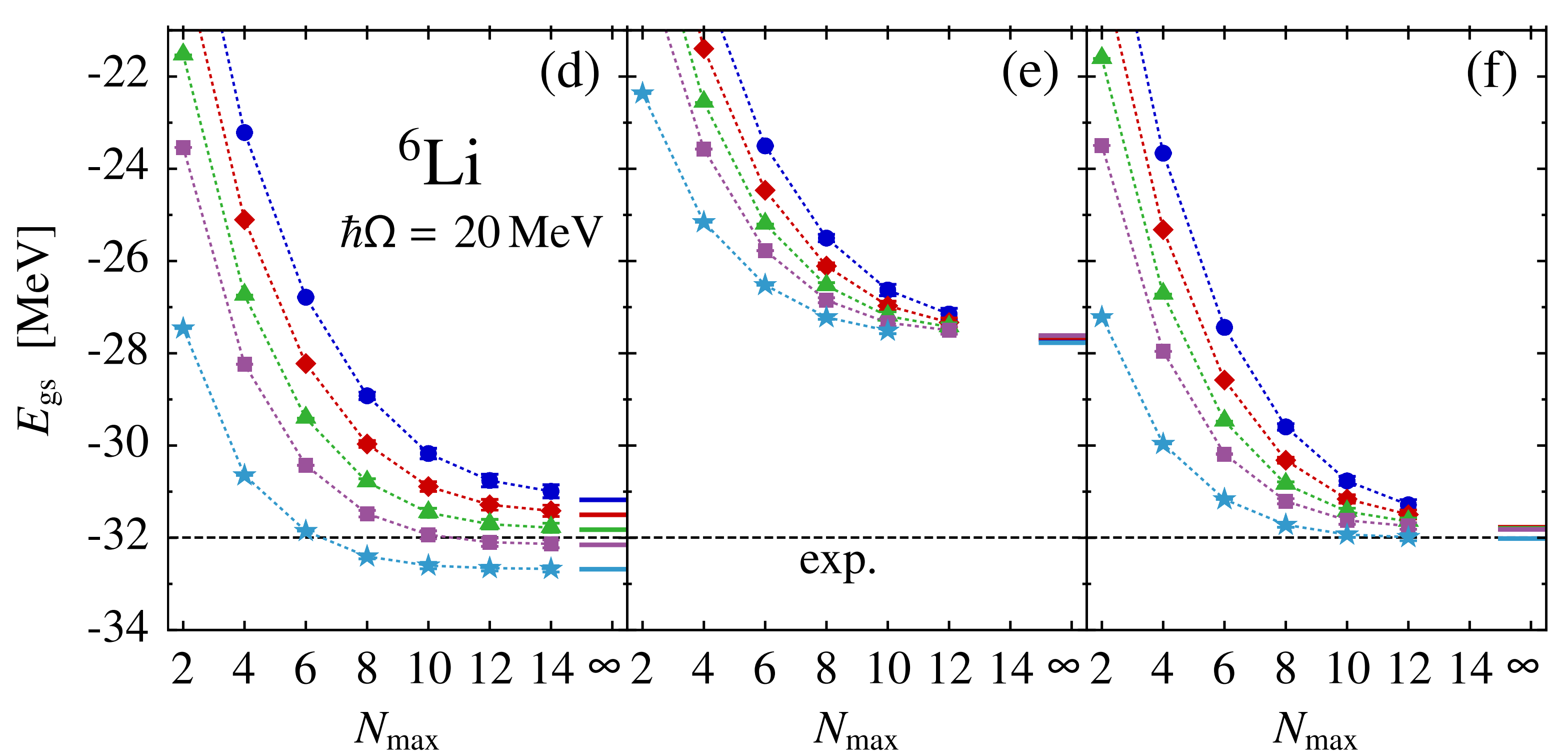
Exact method: no-core shell model (CI)

- **Solve many-body Schrödinger equation in a finite-dimensional Hilbert space**
  - Expand wave functions in (finite set of) basis states
  - Express Hamiltonian in basis
  - Diagonalise Hamiltonian

$$H|\Psi\rangle = E|\Psi\rangle$$

- **One is interested in lowest eigenvalues and associated eigenvectors of Hamiltonian operator**
  - Use of Krylov projection techniques (Lanczos, LOBPCG, …)

- **Finite basis (= model space) must be large enough to allow extrapolations to infinite basis**

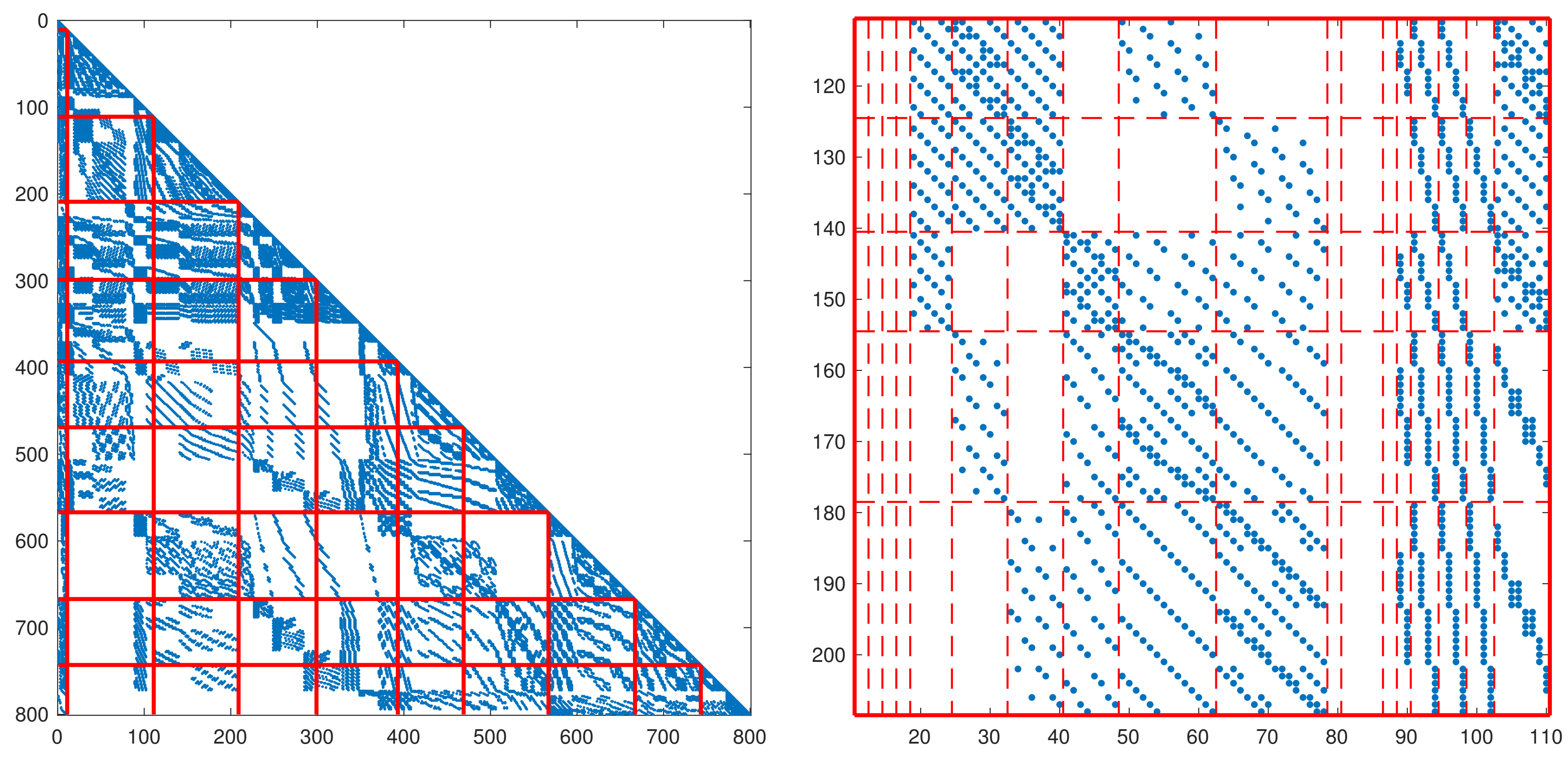


[Roth *et al.*, 2011]

- **Cost of diagonalisation grows factorially with A**

Exact method: no-core shell model (CI)

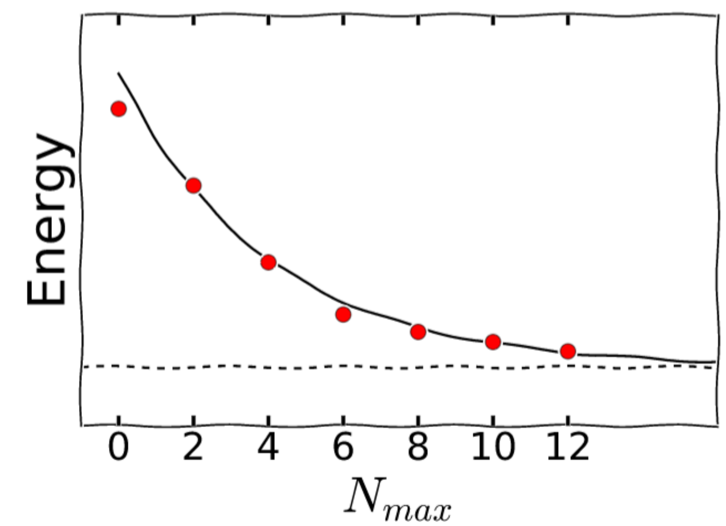
- **Non-trivially optimisable numerical problem**
  - Parallel computing, accelerators, vectorisation, …
  - Sparsity of the Hamiltonian matrix heavily exploited
  - Optimisation of the basis, transformation on the Hamiltonian, …

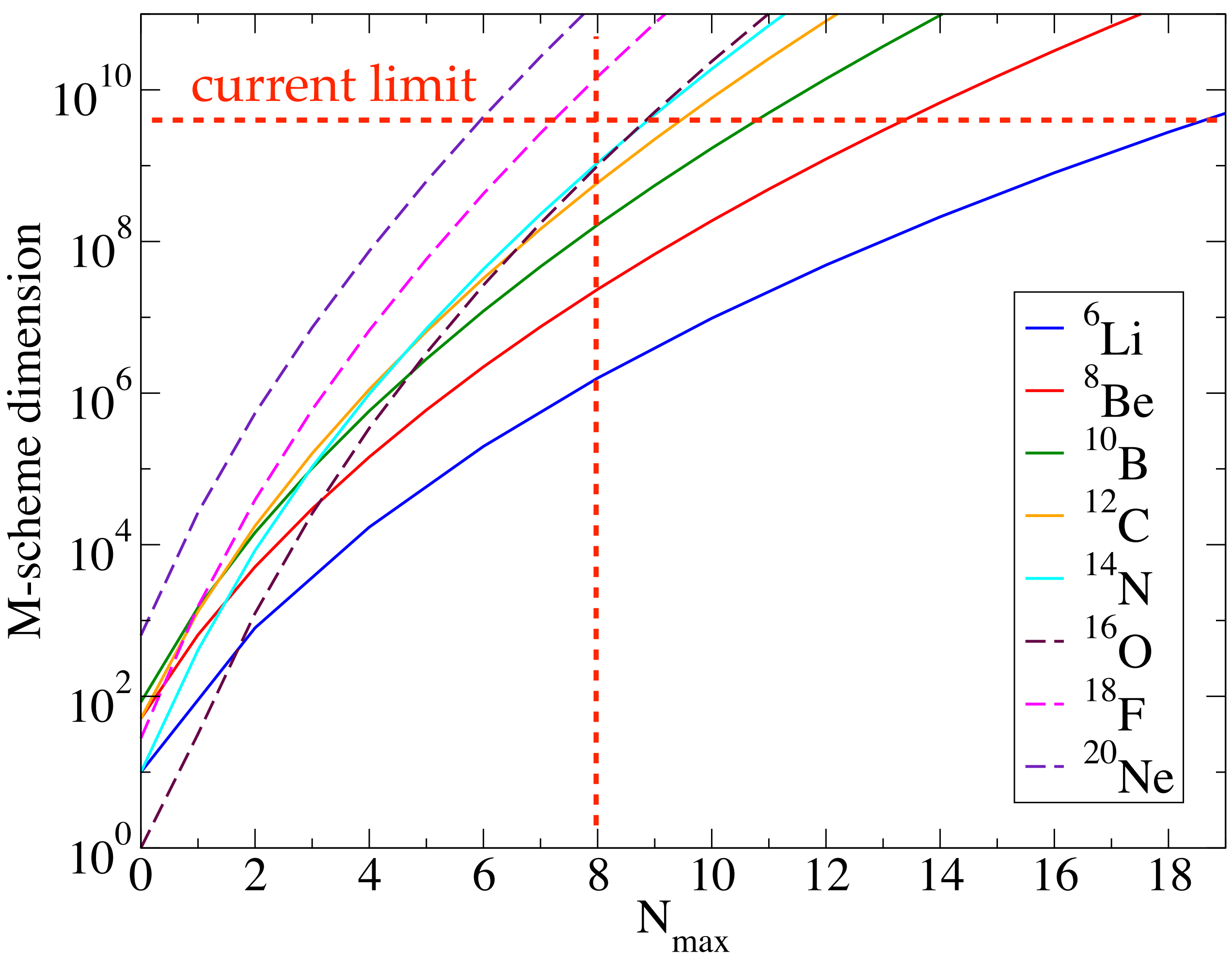


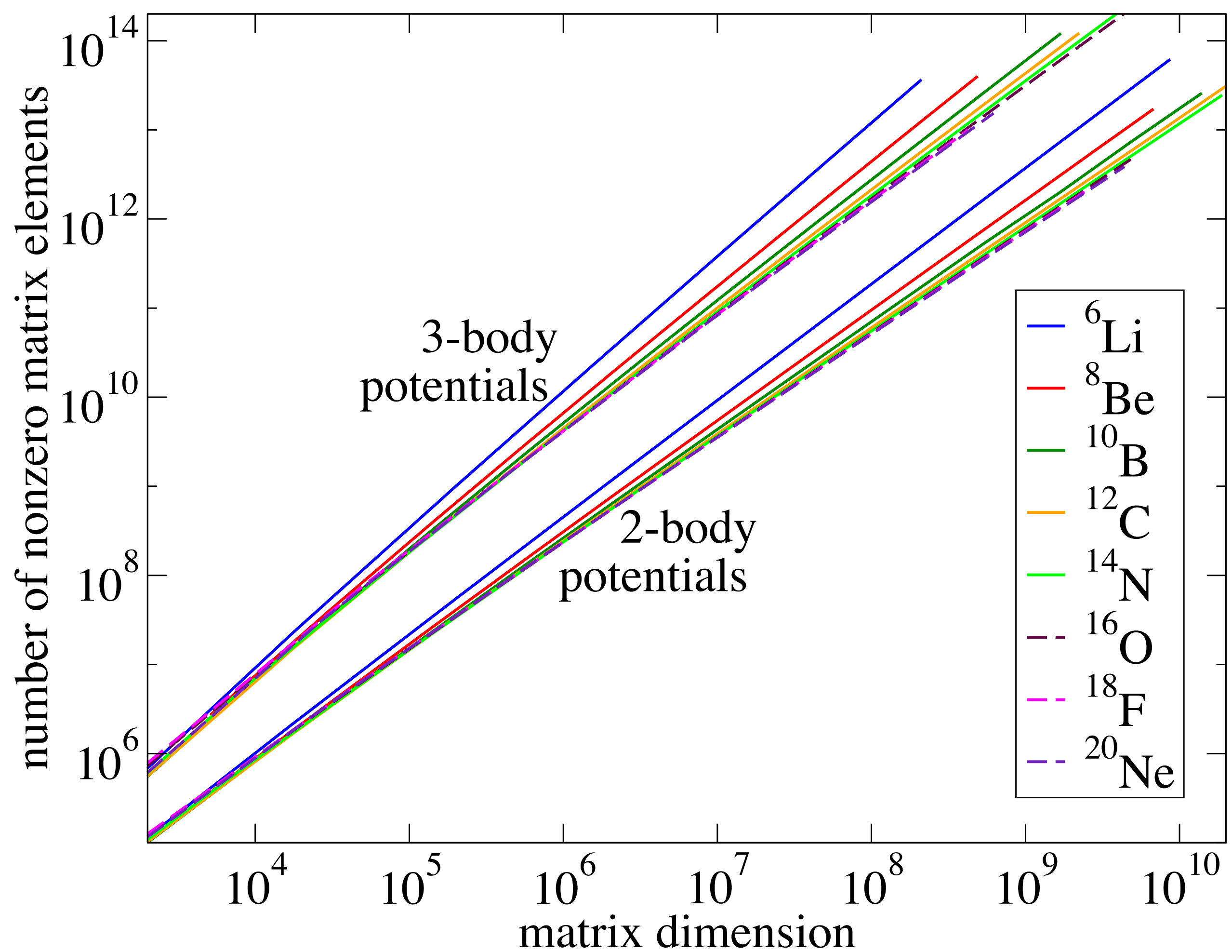
- **Large collaborations including physicists, mathematicians and computer scientists**
  - Yearly allocation of the order of 100M CPU hours

Exact method: no-core shell model (CI)

- **Main limitation: aggregate memory**
  - 10^{14} nonzero matrix elements → 800 TB
  - At least $N_{max} = 8$ to perform reliable extrapolations
  - Progress relies on "Moore's law"







Approximate methods

- **Trade exactness of the solution for more favourable scaling with A**
  - Express the problem in perturbation → truncate → resum (non perturbative)

1. Self-consistent Green's function theory (SCGF)

- Rewrite many-body Schrödinger equation in terms of G and Σ → Dyson equation

$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

2. Coupled-cluster theory (CC)

- Computes the similarity-transformed normal-ordered Hamiltonian

$$\overline{H} \equiv \mathrm{e}^{-T} H_N \mathrm{e}^{T} \qquad\qquad E = \langle \phi | \overline{H} | \phi \rangle$$

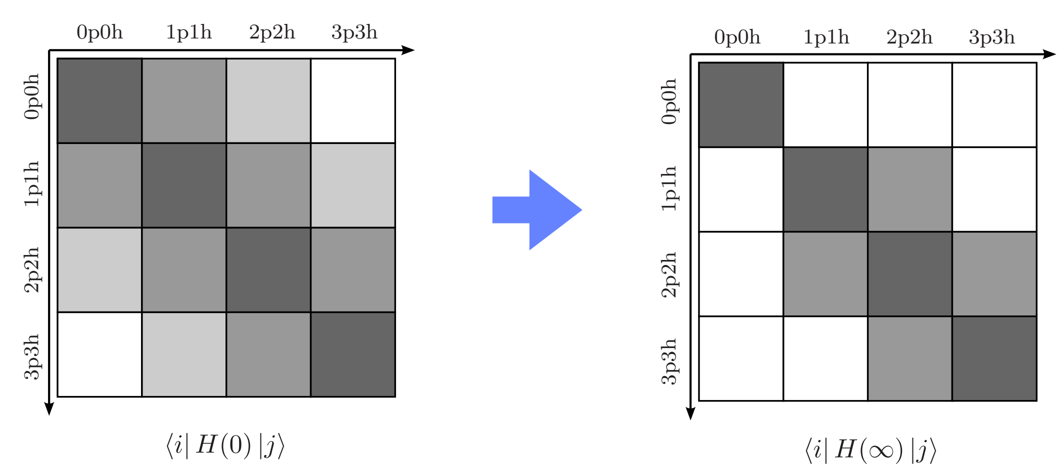
3. In-medium similarity renormalisation group (IM-SRG)

- Employs a continuous unitary transformation of H to decouple g.s. from excitations

Flow equation

$$\frac{d}{ds} H(s) = [\eta(s), H(s)]$$

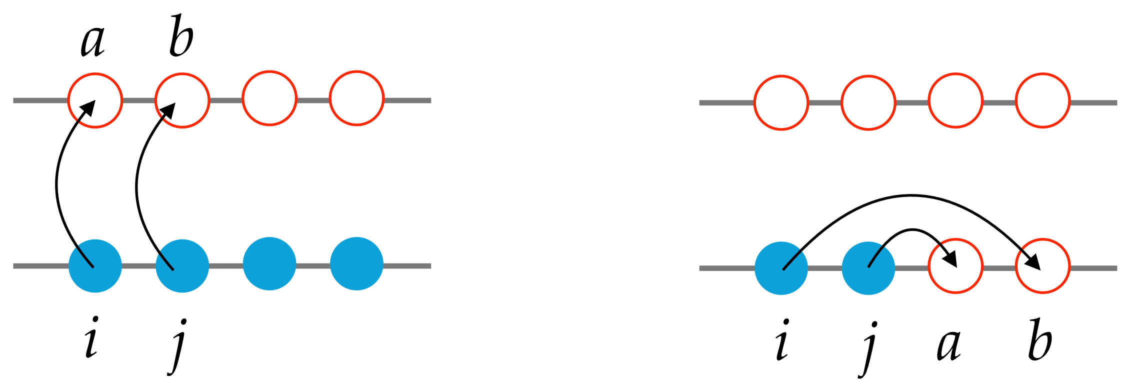
truncated at rank n at each step



Approximate methods

- Approximate/truncated methods capture correlations via an expansion in **ph excitations**
- Open-shell nuclei are **(near-)degenerate** with respect to ph excitations

closed-shell



open-shell

○ E.g. consider MBPT(2)
$$\Delta E^{(2)} = \frac{1}{4}\sum_{abij}\langle ij|\hat{v}|ab\rangle \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

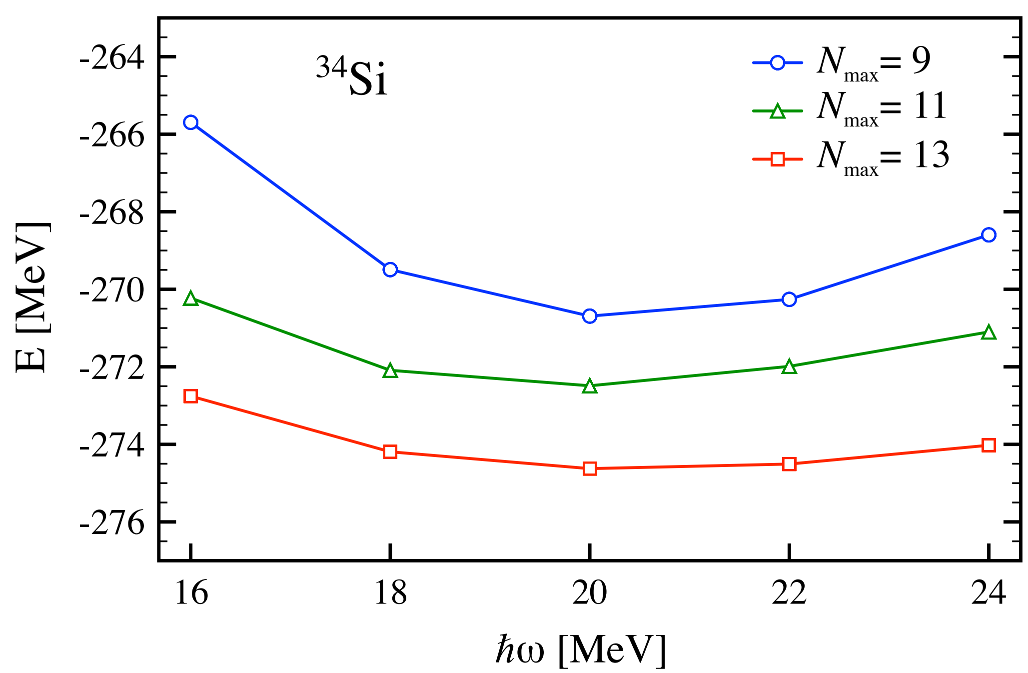
when $\epsilon_i + \epsilon_j = \epsilon_a + \epsilon_b$ the expansion breaks down

- Way out: formulate the expansion around a **symmetry-breaking** reference state
  - ○ Symmetry-breaking solution allows to **lift the degeneracy**
  - ○ GF theory extended to particle-number breaking scheme (Gorkov formalism) [Gorkov 1958]
  - ○ Implementation for semi-magic nuclei developed in Saclay & Surrey [Somà, Duguet & Barbieri 2011]
  - ○ Symmetries must be eventually restored

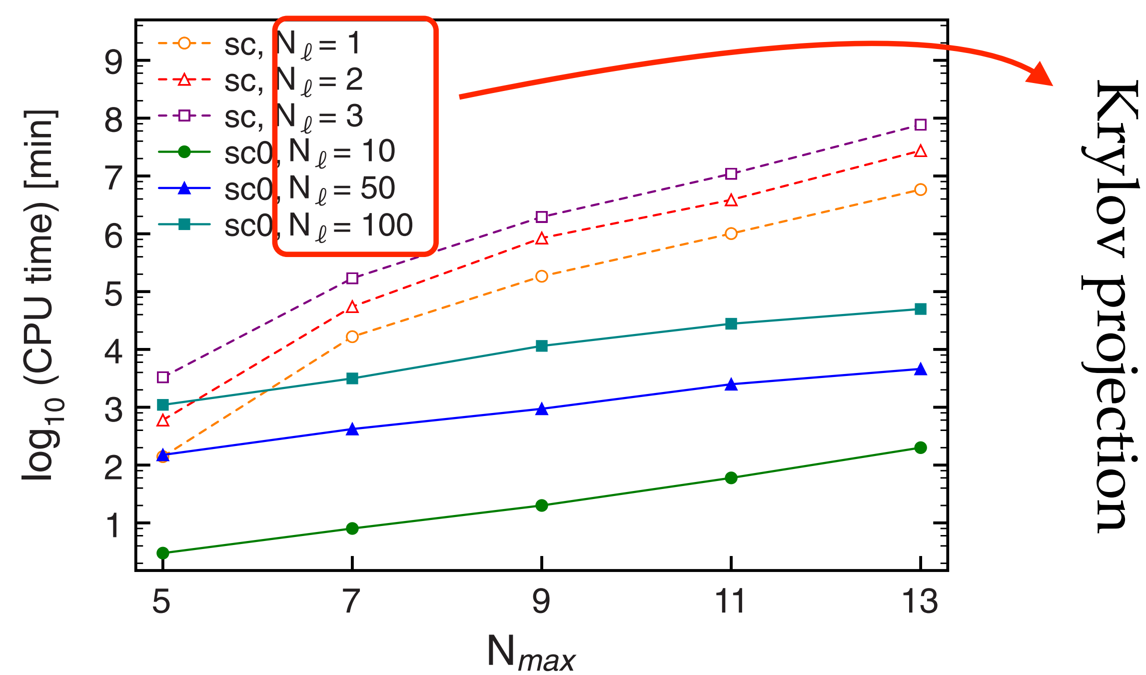
Approximate methods

- **Calculations typically assume spherical symmetry**
  - Eigenvalue problem of reduced dimensionality
  - N_{max} = 14 or 15 in state-of-the-art calculations
  - Similar algorithms & tricks as for exact methods, but still room for optimisation

Model space convergence



Self-consistency & CPU cost

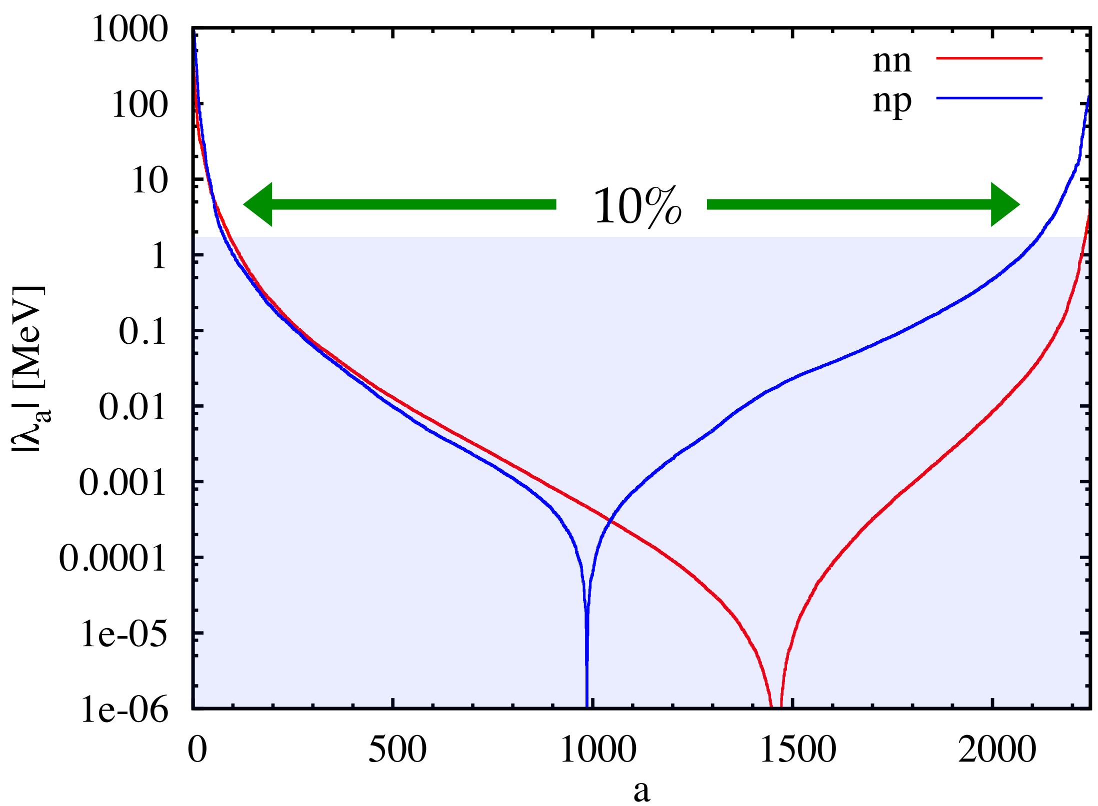


- **Main limitation: size of 3N matrix elements**
  - Cuts on $N3_{max}$ hinder convergence
  - Currently file sizes of 50-100 GB can be handled

$N3_{max}$	14	16	18
memory [GB]	5	25	100+

Factorised matrix elements

- Interaction matrix elements: **low information content** compared to the **size**
  - *How can one reduce the size without losing important information?*
- **Two-body forces** can be factorised as $v_{ijkl} = \sum_a \lambda_a \, g^a_{ik} \, g^a_{jl}$ (→ Singular Value Decomposition)



[Lesinski 2013]

Gain #1: **size** (→ storage and memory needs)

$$\sum_{kl} v_{ijkl} = \sum_a \lambda_a \sum_k g^a_{ik} \sum_l g^a_{jl}$$

N² m (N + N) = **mN**

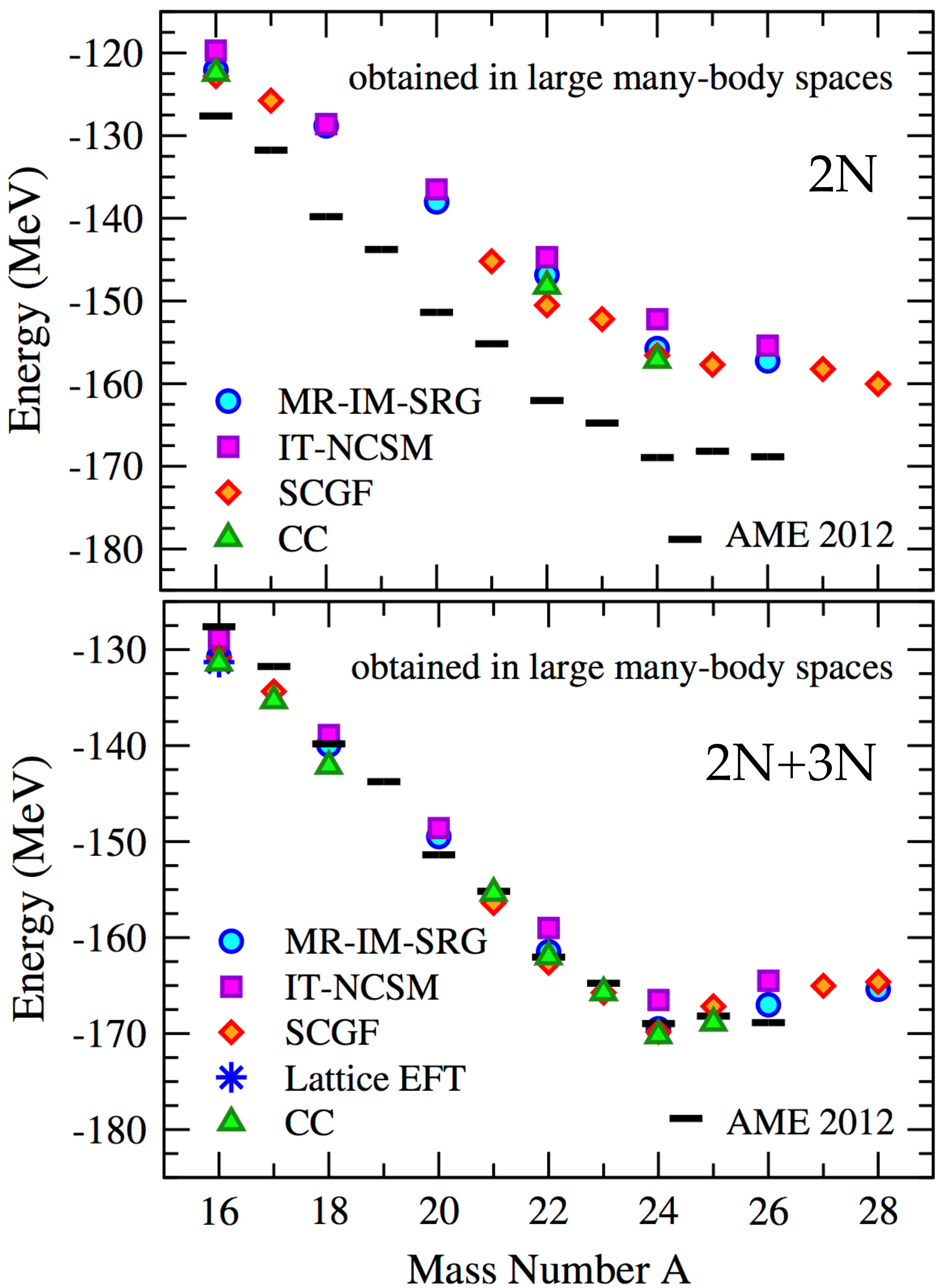
Gain #2: **CPU speed-up**

HF test calculation: 10% of the matrix elements → **0.003% error** and **factor 10 speed-up**

- **Three-body forces**
  - Exploit recent development from applied maths: Higher-Order SVD
  - Even **larger gain** → size of 3B matrix elements (~100 GB - 1 TB) current bottleneck

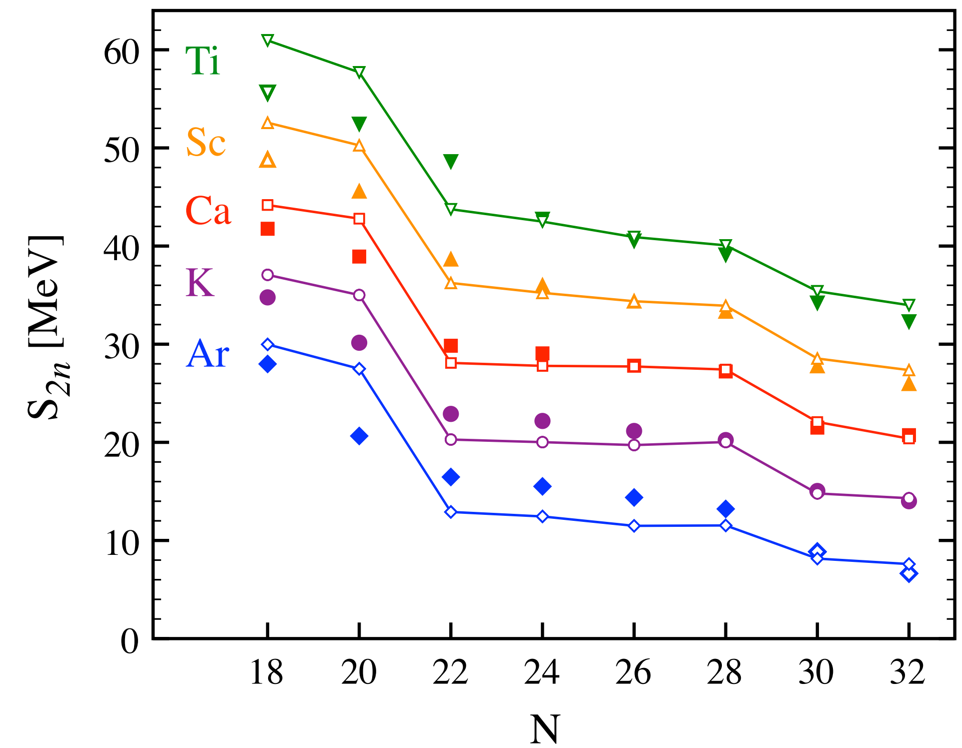
Approximate methods

A~20

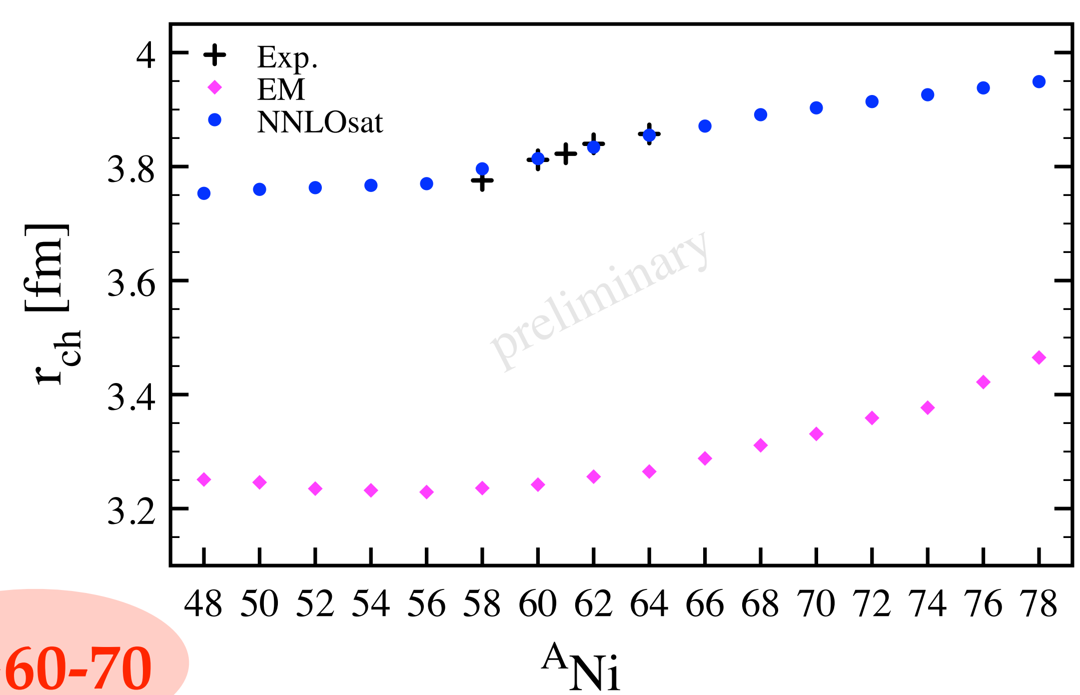


[Hebeler *et al.* 2015]

A~40-50



[Somà *et al.* 2014]



A~60-70

[Somà *et al.* unpublished]

Hybrid methods (valence-space)

Configuration interaction

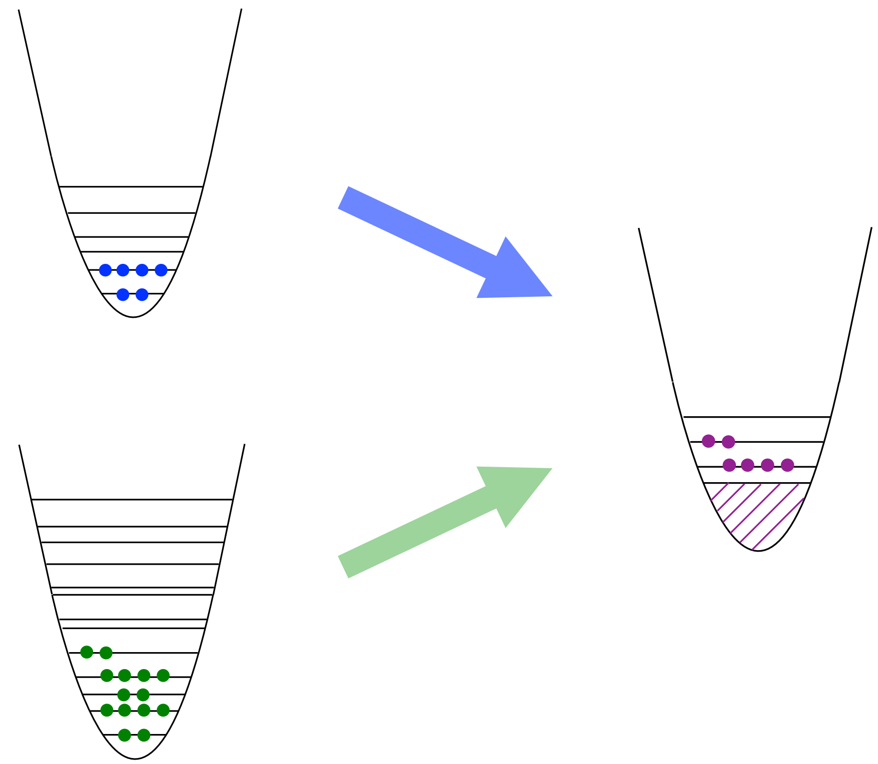
✓ Exact

✗ Unfavourable scaling

Many-body expansion

✗ Approximate

✓ Favourable scaling



(Ab initio) shell model

✓ Exact within a valence space

✓ Not-so-unfavourable scaling

- **Ab initio version of traditional shell model**
  - Valence-space interaction derived with a many-body expansion approach
  - Diagonalisation performed in a reduced Hilbert space → larger model spaces can be accessed

- **Main limitations: size of 3N matrix elements & size of diagonalisation**
  - Faces combined issues of the other two types of approaches

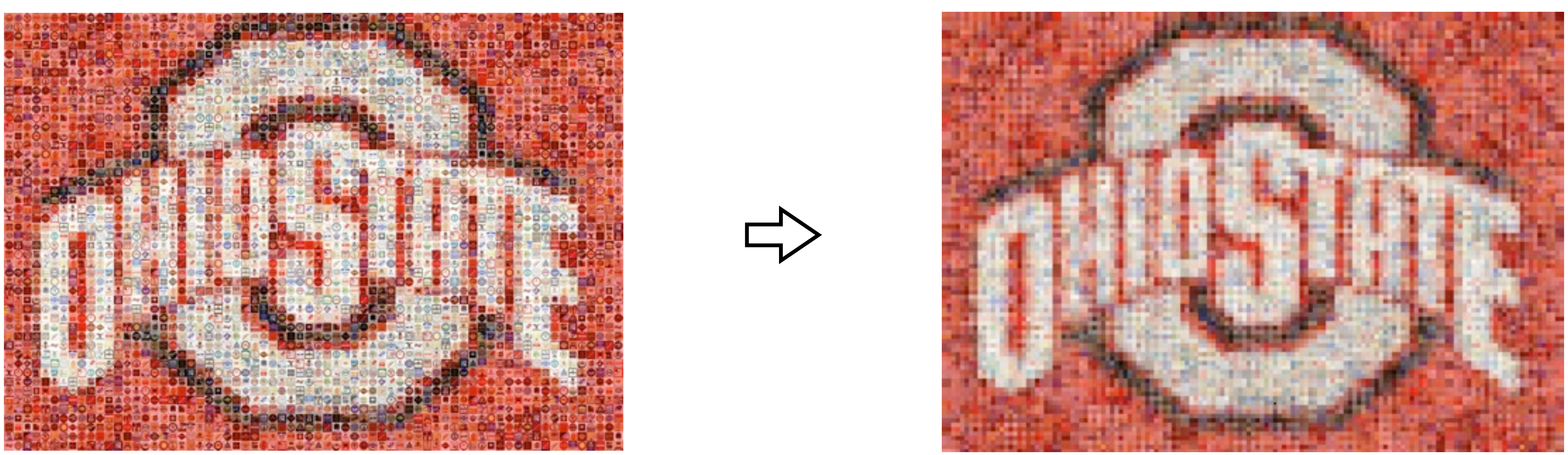
Renormalisation-group techniques for nuclear forces

- **Coupling between low and high momenta** are present in NN potentials
  - Large model spaces needed to converge $\rightarrow$ applicability limited to light nuclei
- Are high momenta, i.e. high resolution, necessary to compute **low-energy observables**?

➟ Small-distance details are irrelevant when we are interested in the long-wavelength information

➟ Strategy: **change the resolution** and “integrate out” unnecessary information

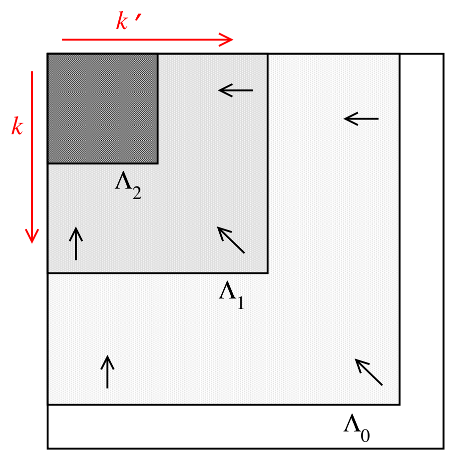
[figures from K. Hebeler]

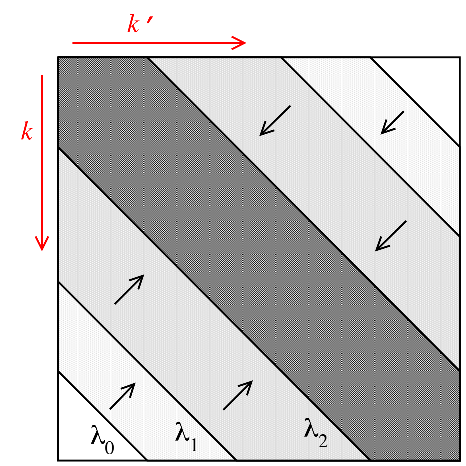


Renormalisation-group techniques for nuclear forces

- Renormalisation group techniques for 2N and 3N forces
  - (Unitary) transformation to **lower the resolution scale** of the original Hamiltonian

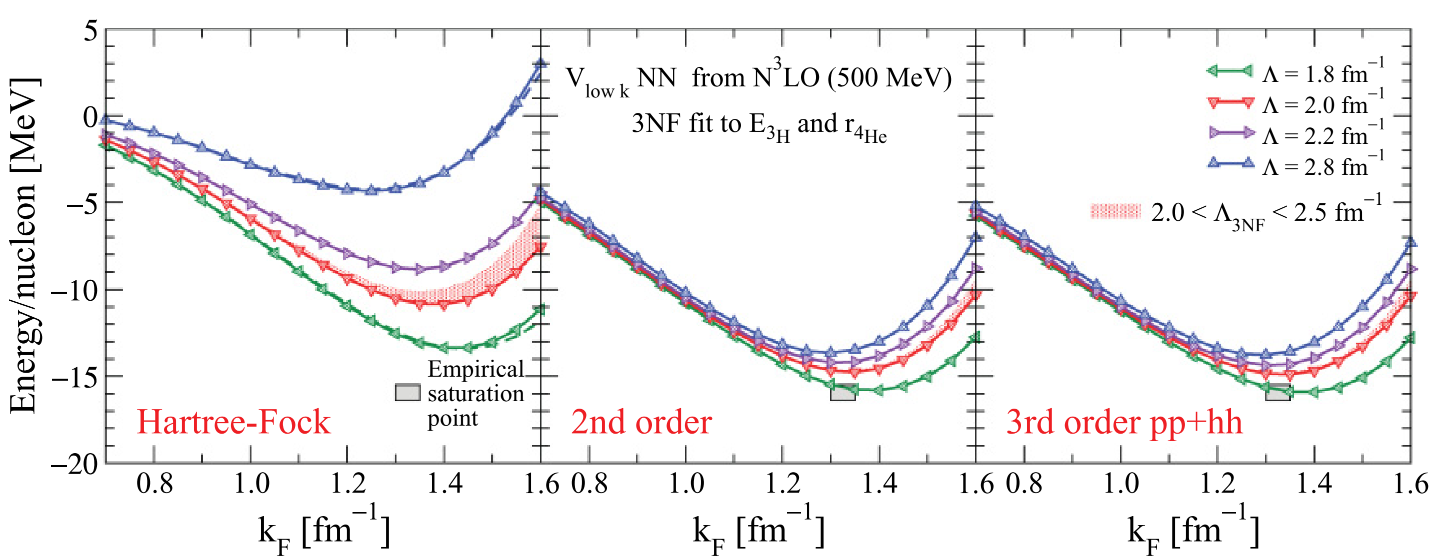
$V_{\text{low-k}}$



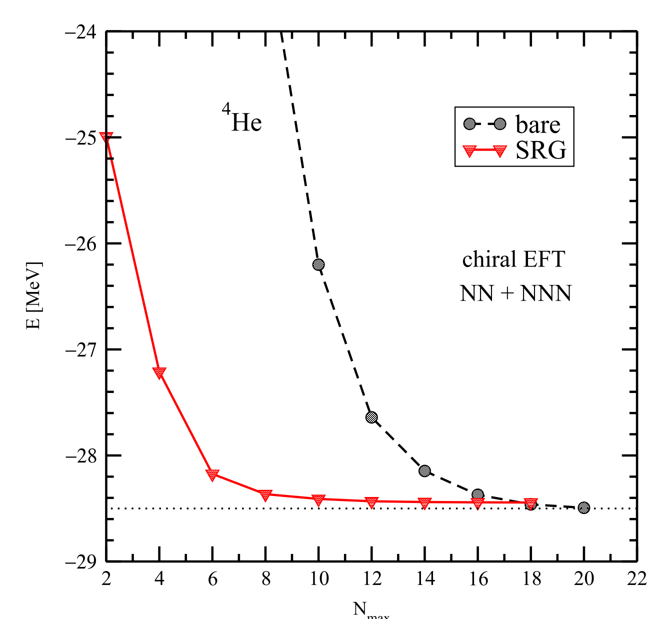


V_{SRG}

- Improved convergence of many-body calculations
  - Less refined **many-body truncations** & smaller **model spaces** needed

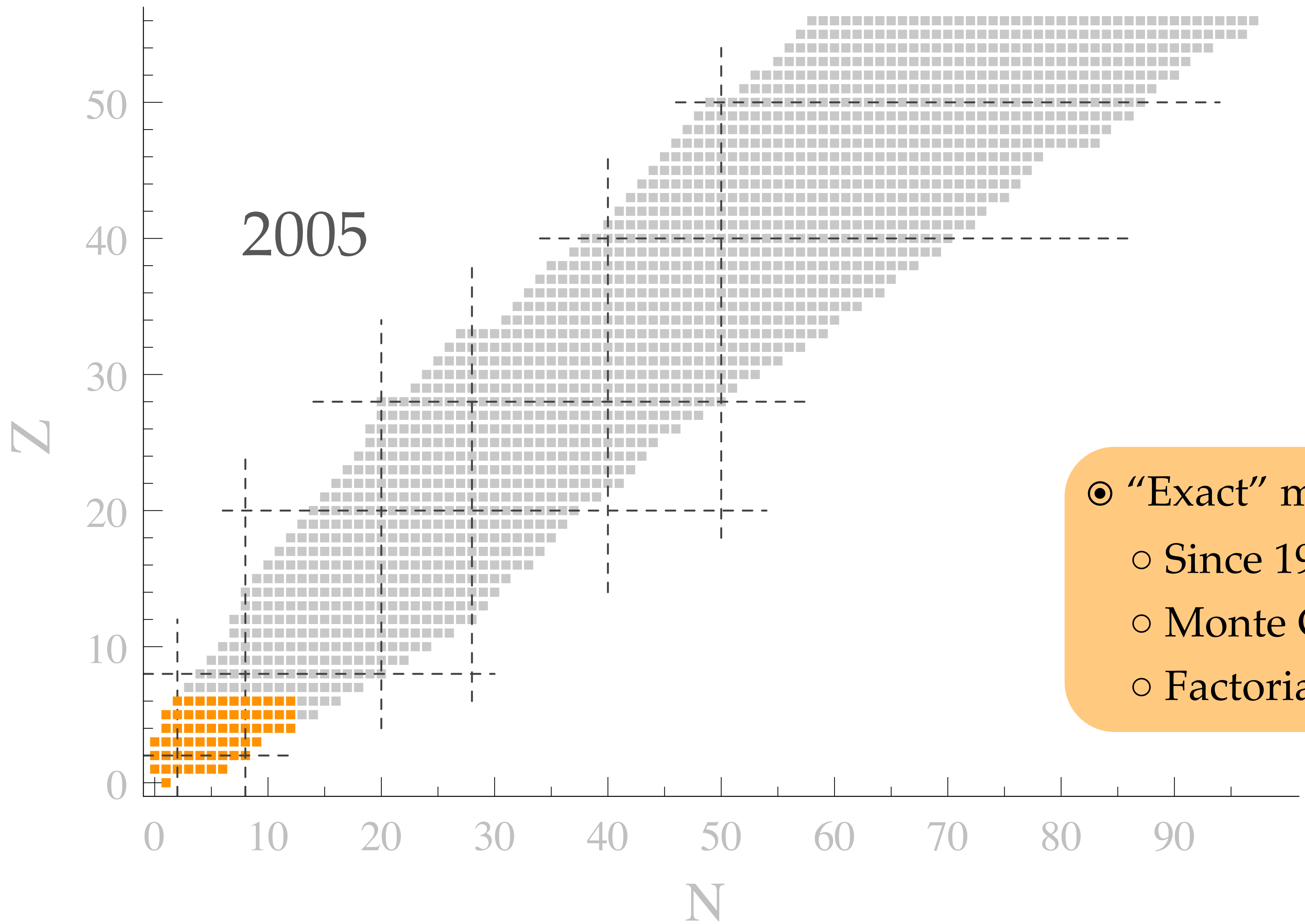


[Hebeler *et al.* 2011]



[Jurgenson, Navratil & Furnstahl 2013]

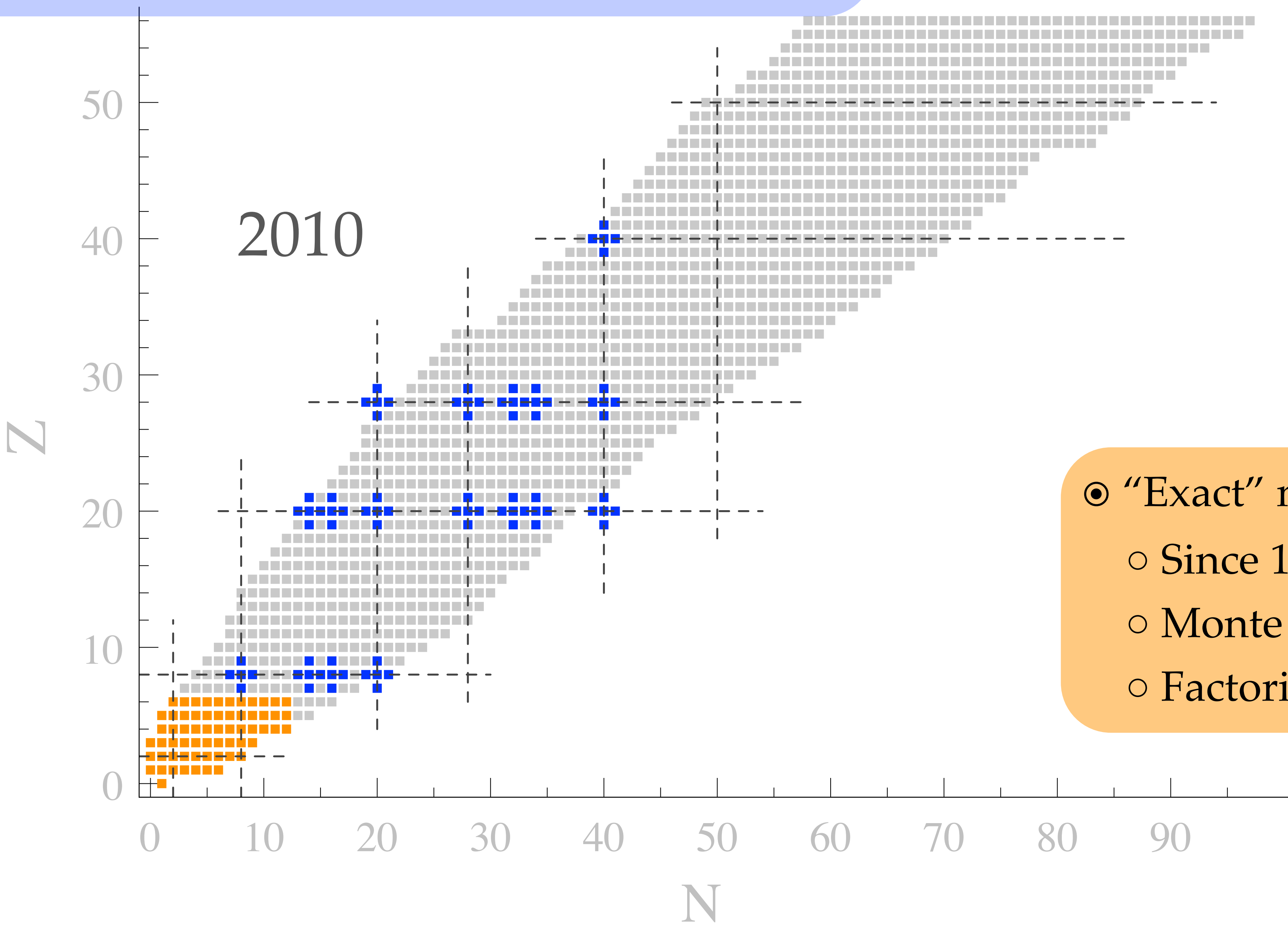
Evolution of ab initio nuclear chart



- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

Evolution of ab initio nuclear chart

- Approximate methods for closed-shells
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling



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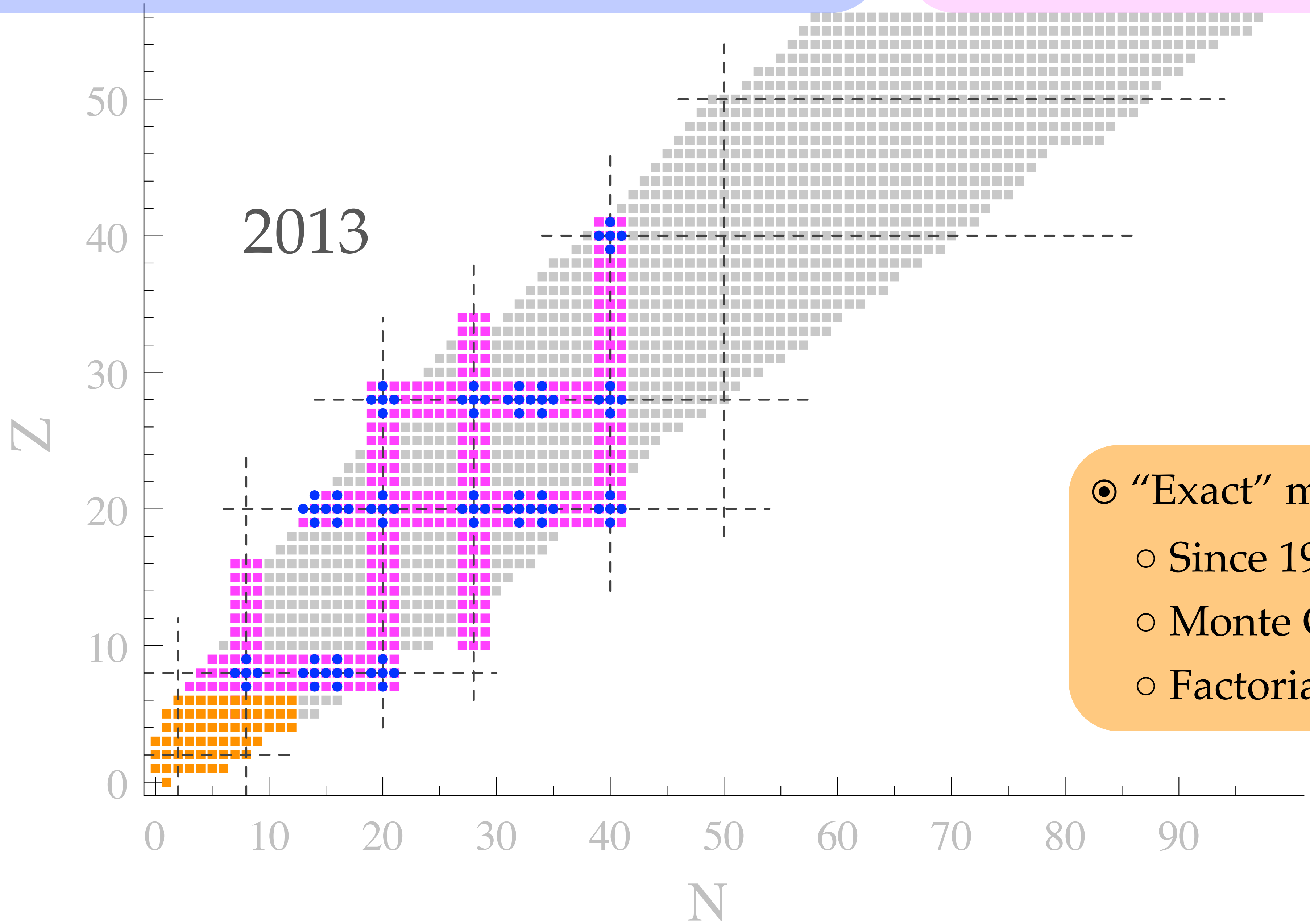
  - Polynomial scaling

- Approximate methods for open-shells
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling



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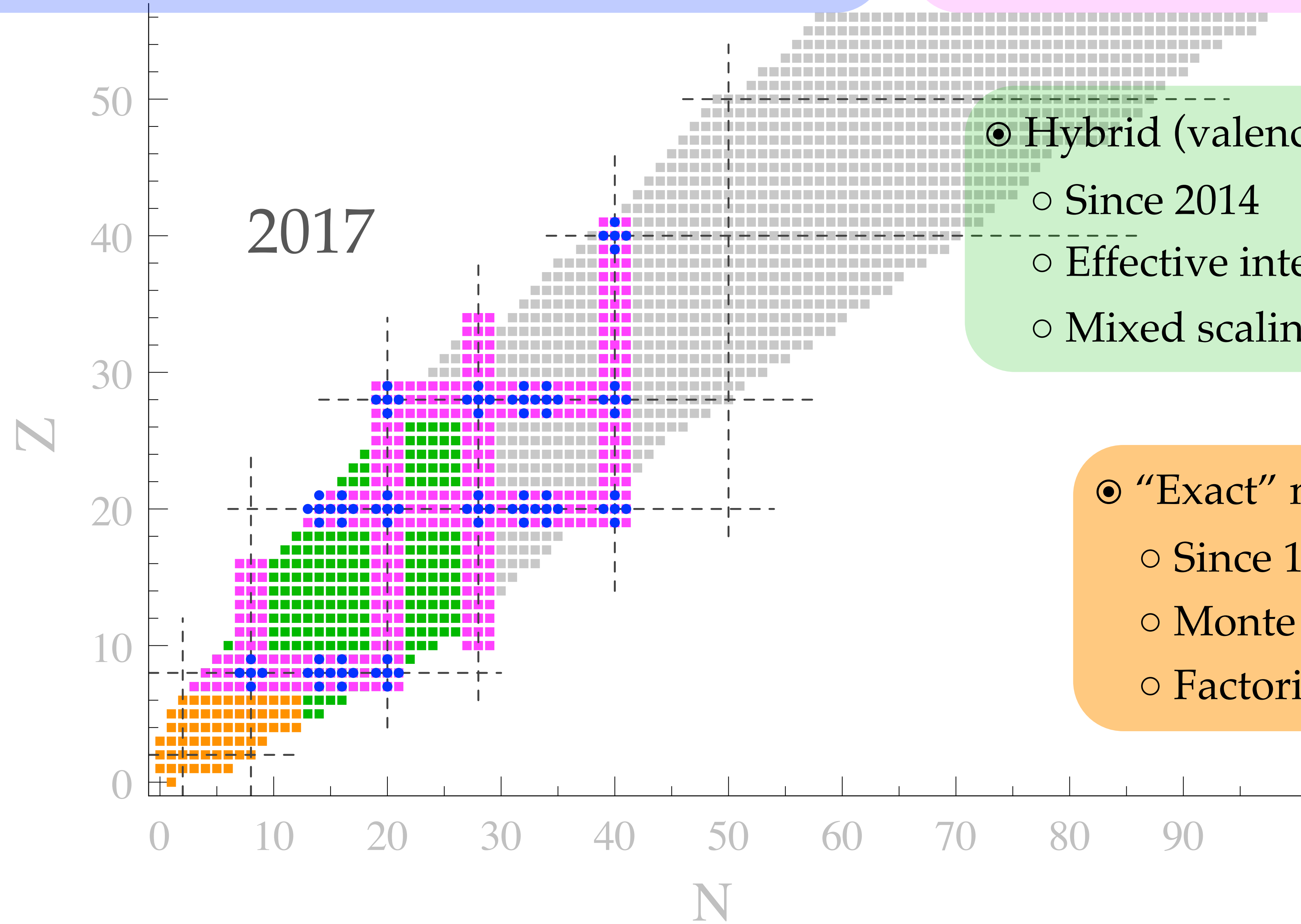

- Hybrid (valence-space) methods
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling