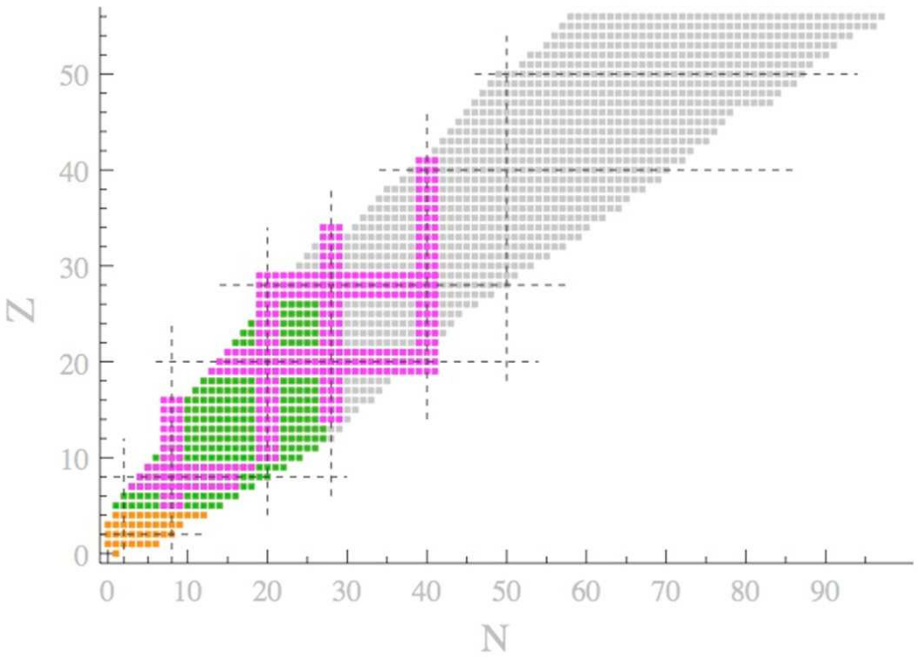
Ab initio calculations of open-shell mid-mass nuclei



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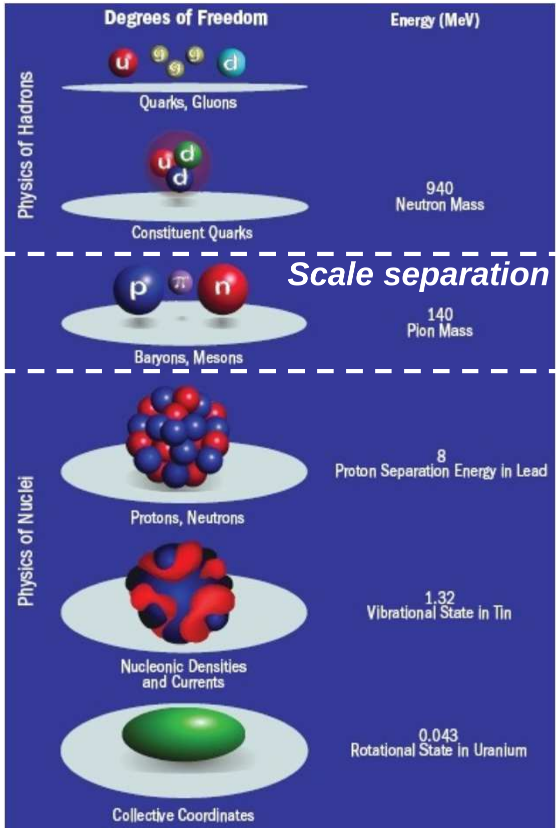
Joint LIA COLL-AGAIN, COPIGAL and POLITA workshop
LNS Catania, April 26-29 2016

Outline

- **Ab initio nuclear theory: context & state-of-the-art**
- Results in open-shell mid-mass nuclei: example of the Ca chain
- Some perspectives

Ab initio (=*in medias res*) *A*-body problem

More reductionist/elementary/"fundamental" description



Emergent phenomena amenable to effective descriptions

Ab initio view of the atomic nucleus

- Made of **structure-less nucleons** ($+\Delta_s$) + hyperons in S≠0
- Interacting via
  - Low energies → Pions + contact interactions ➡ *Pion-**ful** EFT*
  - Very low energies → Contact interactions ➡ *Pion-**less** EFT*
- Effective field theory (EFT)
  - Systematic construction of *A*N interactions (*A*=2, 3, …)
  - Symmetries of underlying theory built in
  - Coupling constants fixed by QCD (ideally) or data

Ab initio nuclear A-body problem viewpoint

- **Implement** in *A*-body sector → "ab initio" nuclear *A*-body problem

How does the rich nuclear phenomenology emerge from basic interactions between the nucleons?

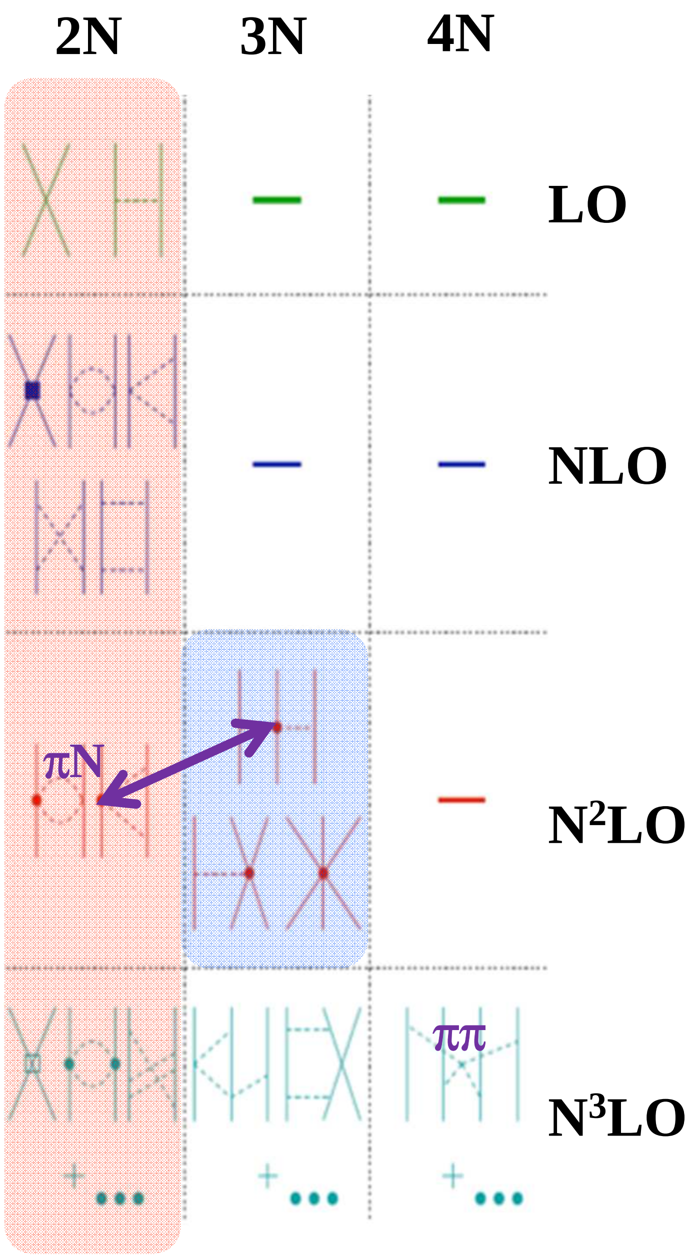
- **Solve** in *A*-body sector → emerging nuclear phenomena (= low-energy observables)

↓

Is there a natural limitation of such a description with A?

- **Benefits**: controlled extrapolations, assessment of errors, link to fundamental interactions

Link to QCD via pion-full EFT = current paradigm



Key features

- ✪ Separation of scales: DOFs are nucleons&pions (+ contact)
- ✪ Relevant **QCD information**: chiral symmetry (breaking)
- ✪ Weinberg PC: **NDA organizes Lagrangian** in $(Q_{low}/\Lambda_\chi)^\nu$
- ✪ **Natural hierarchy 2N>>3N>>4N>>…>>AN interactions**
- ✪ Fit LECs of BN operator on BN observables **via Schrod. Eq.**

Unique promises

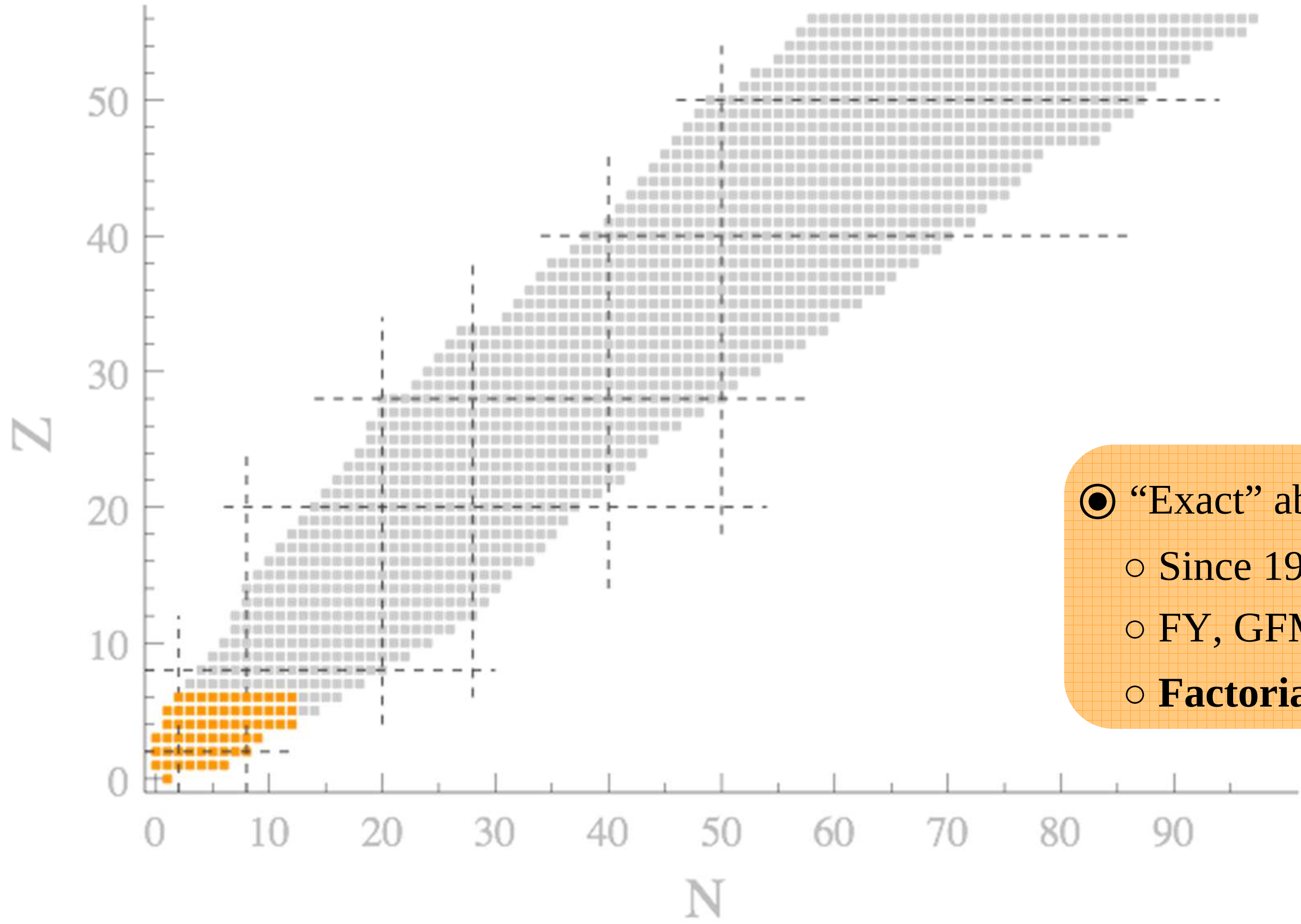
- ✪ **Consistent** $\pi\pi$ + πN + 2N, 3N, 4N… int. + electroweak op.
- ✪ **Systematic** (improvable) + provides error estimates

A-nucleon sector: fits the standard view of A-body problem

Two-step process

1. **Set up** H^ν **at order** ν
2. **Solve** $H^\nu|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ **to all orders**

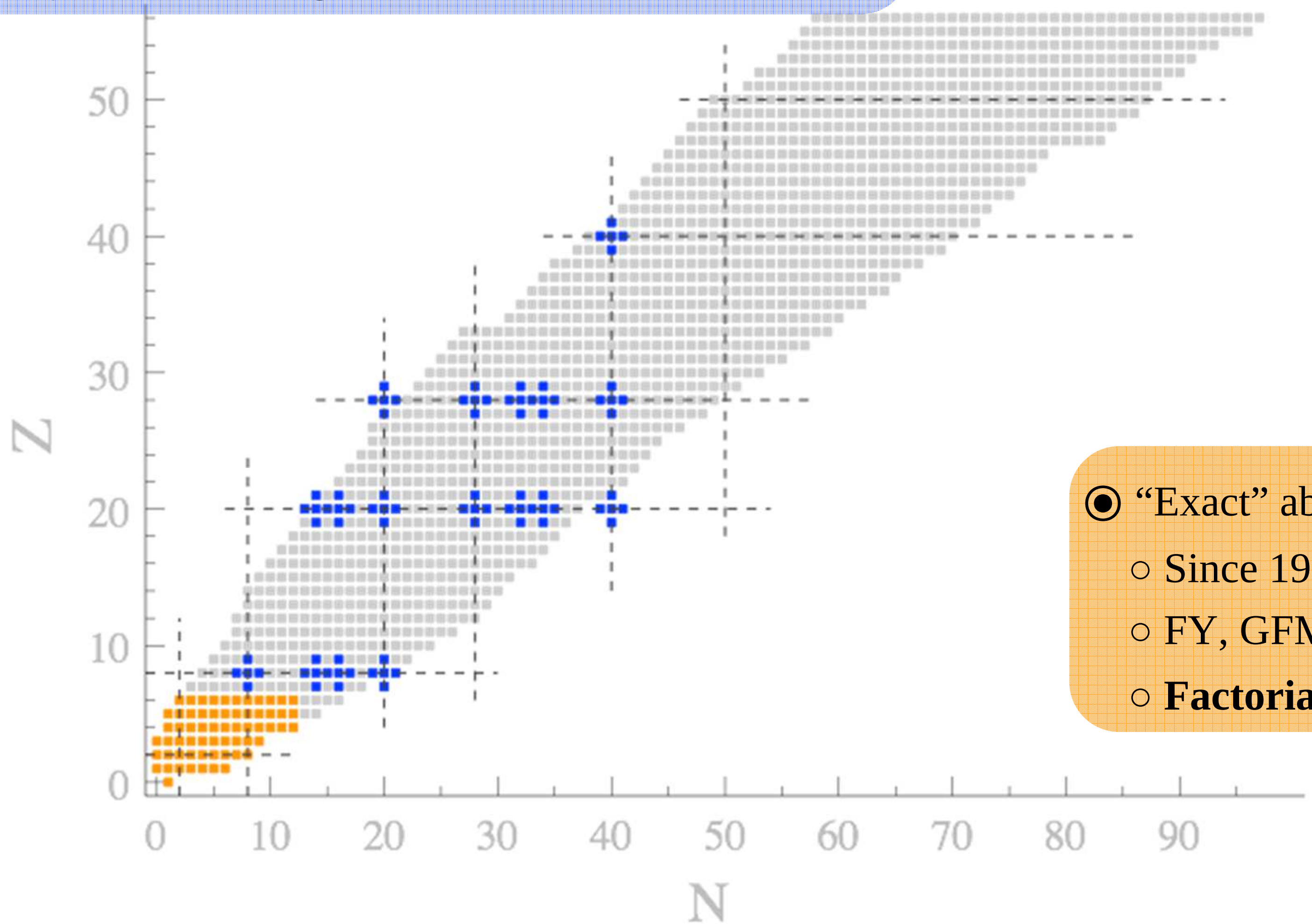
State-of-the-art of *ab initio* calculations in **2004**



- “Exact” ab initio approaches
  - Since 1980’s
  - FY, GFMC, NCSM, HH, …
  - **Factorial scaling**

State-of-the-art of *ab initio* calculations in **2010**

- Ab initio methods for **doubly closed-shell** nuclei
  - Since 2000’s
  - CC, DGF, IMSRG, … → cross-benchmarks
  - **Polynomial scaling**



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Landmark result of *ab initio* methods

◉ **Binding energy of ^{A}O**

- IMSRG, IT-NCSM, DGF, CC
- E_{max} = 15 HO shells ; E_{3max} = 14

Input

Original 3N mandatory

Correct dripline location

◉ Inter-nucleon interactions

- Chiral **2N** (N^3LO ; Λ_{2NF} = 500 MeV/c)

[D.R. Entem, R. Machleidt, PRC 68, 041001 (2003)]

- Chiral **3N** (N^2LO ; Λ_{3NF} = 400 MeV/c)

[P. Navratil, FBS 41, 117 (2007)]

- SRG evolved down to λ = 1.9 fm^{-1}

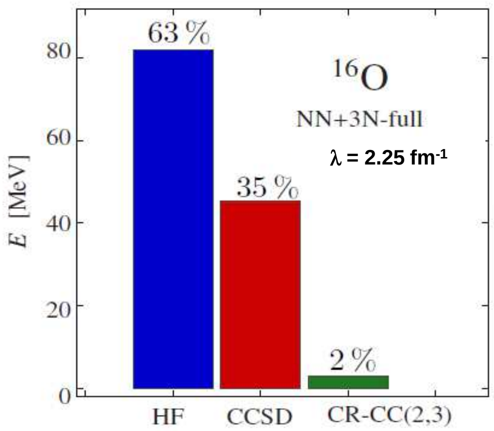
[S.K. Bogner et al., PPNP65, 94 (2010)]

◉ A-body methods

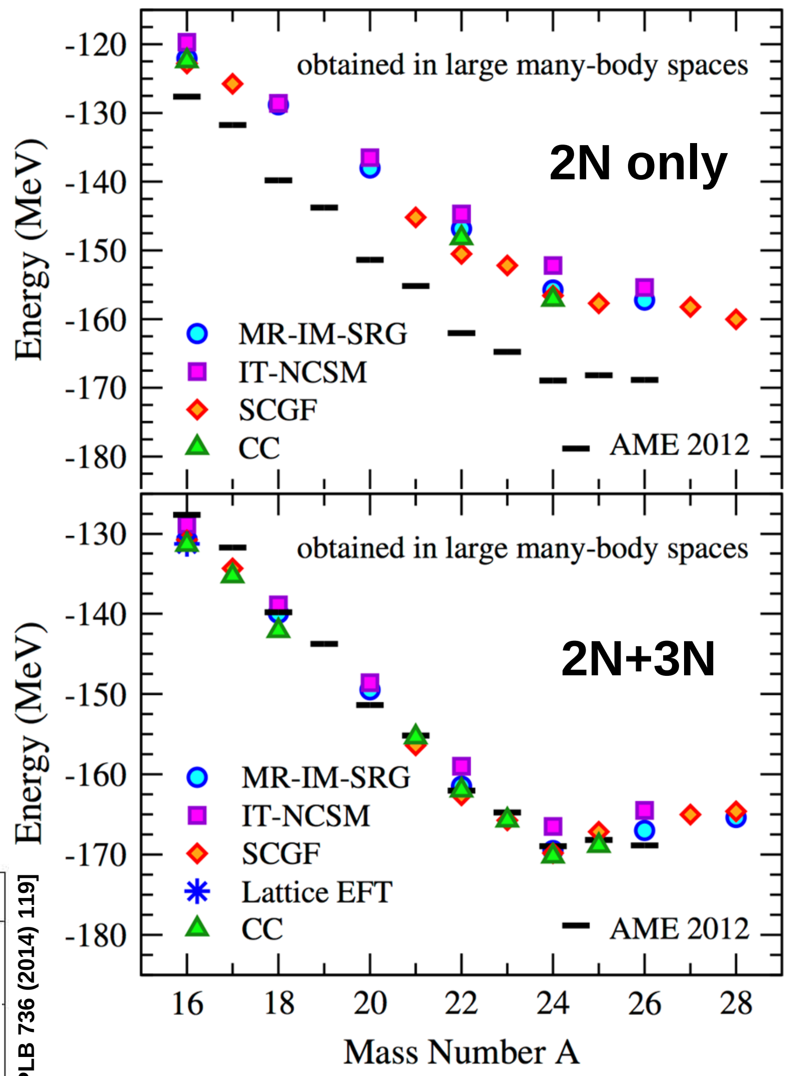
- **Excellent cross benchmark**
- Converging expansions to ~2%
- **Various systematic errors ~2%**

Omitted induced BN forces for B>3

Basis truncations: SRG, 3NF, NO2B



[S. Binder et al., PLB 736 (2014) 119]



[K. Hebeler *et al.*, Ann. Rev. Nucl. Part. Sci., in press]

Polynomially-scaling Ab initio methods for open-shell nuclei

◉ **Standard expansion schemes fail** when dealing with, e.g., pairing and quadrupole instabilities

➟ Idea: exploit **symmetry breaking**, e.g. particle number to account for pairing

$$H|\Psi_k^{\mathrm{A}}\rangle = E_k^{\mathrm{A}}|\Psi_k^{\mathrm{A}}\rangle$$

$$|\Psi_0^{\mathrm{A}}\rangle = \Omega_0|\Phi\rangle$$

where both Ω_0 and $|\Phi\rangle$ break symmetries

$$E_0^{\mathrm{A}} = \frac{\langle\Phi|H\Omega_0|\Phi\rangle}{\langle\Phi|\Omega_0|\Phi\rangle}$$

◉ **Gorkov self-consistent Green functions (GGF)**
[Somà, Duguet, Barbieri 2011]

◉ Multi-reference IMSRG
[Hergert *et al.* 2013]

◉ **Bogoliubov coupled-cluster (BCC)**
[Signoracci *et al.* 2015]

◉ **Symmetry-restored BCC**
[Duguet 2015; Duguet, Signoracci 2016]

◉ Revisit basic/investigate new questions from an ***ab initio* perspective**

○ **Emergence of magic numbers** and their evolution

○ **Limits of stability** on neutron-rich side beyond Z=8

○ **Mechanism for nuclear superfluidity**

○ Emergence and evolution of quadrupole collectivity

○ Role and validation of AN forces

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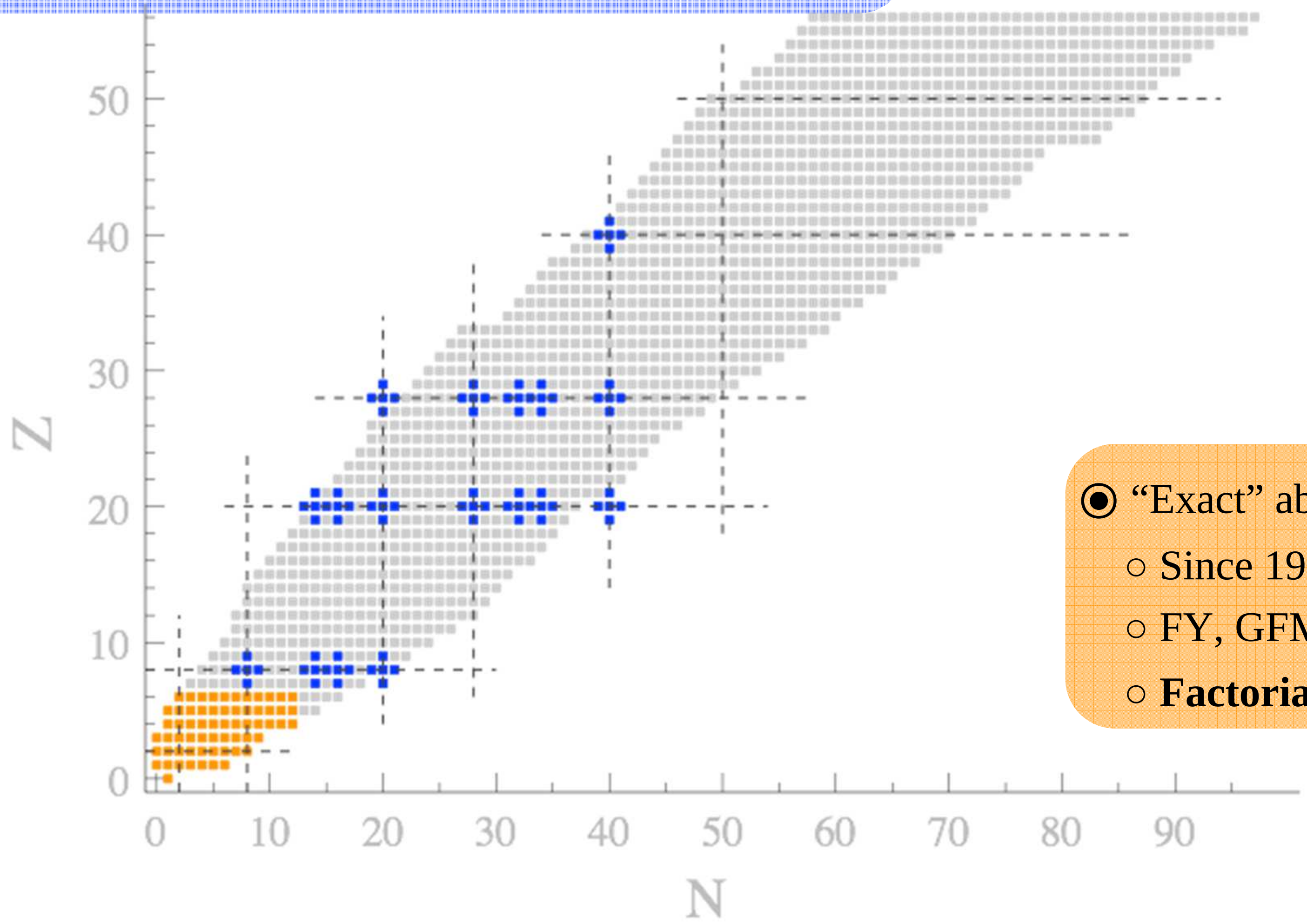

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  - GGF, MR-IMSRG, BCC
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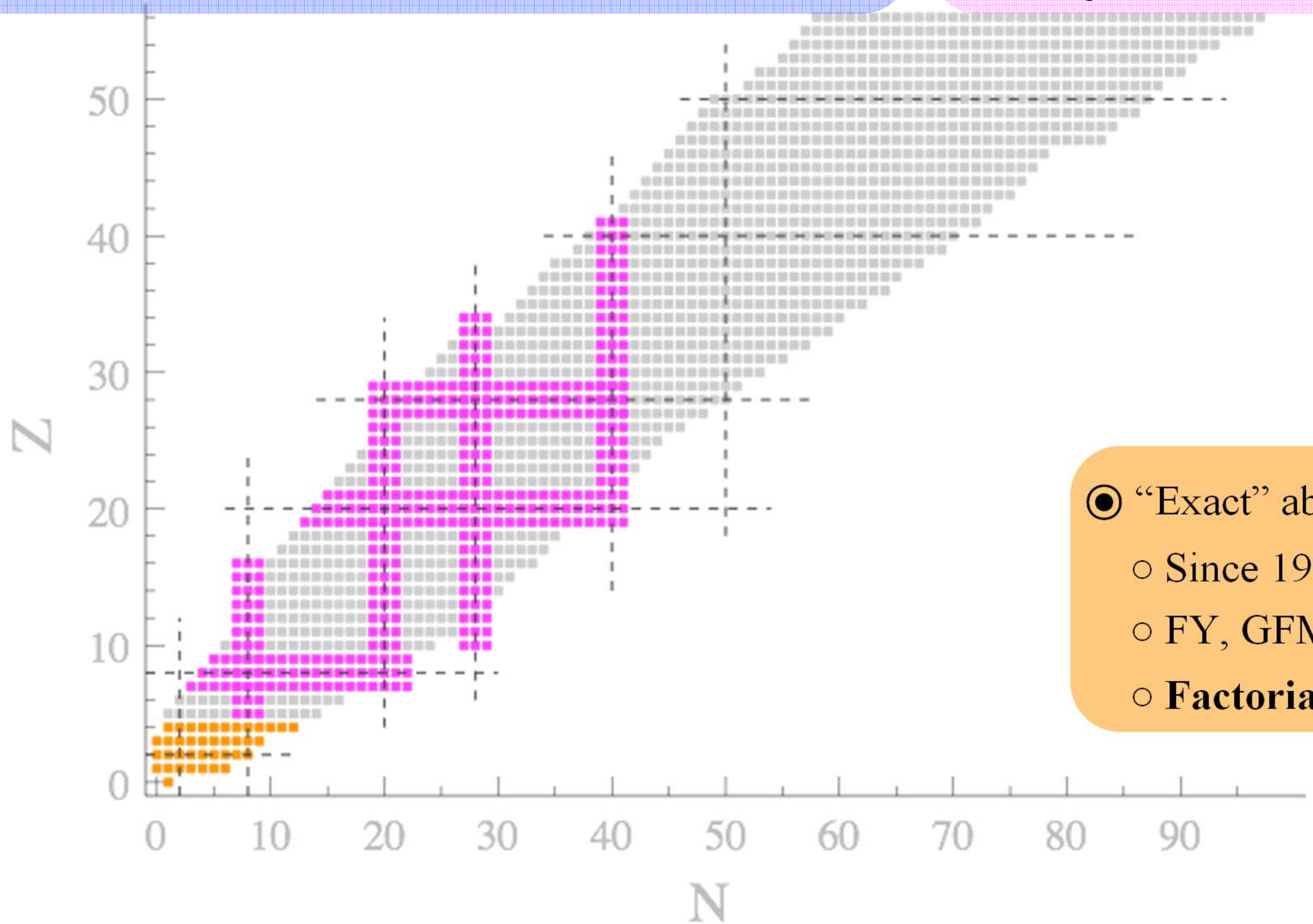

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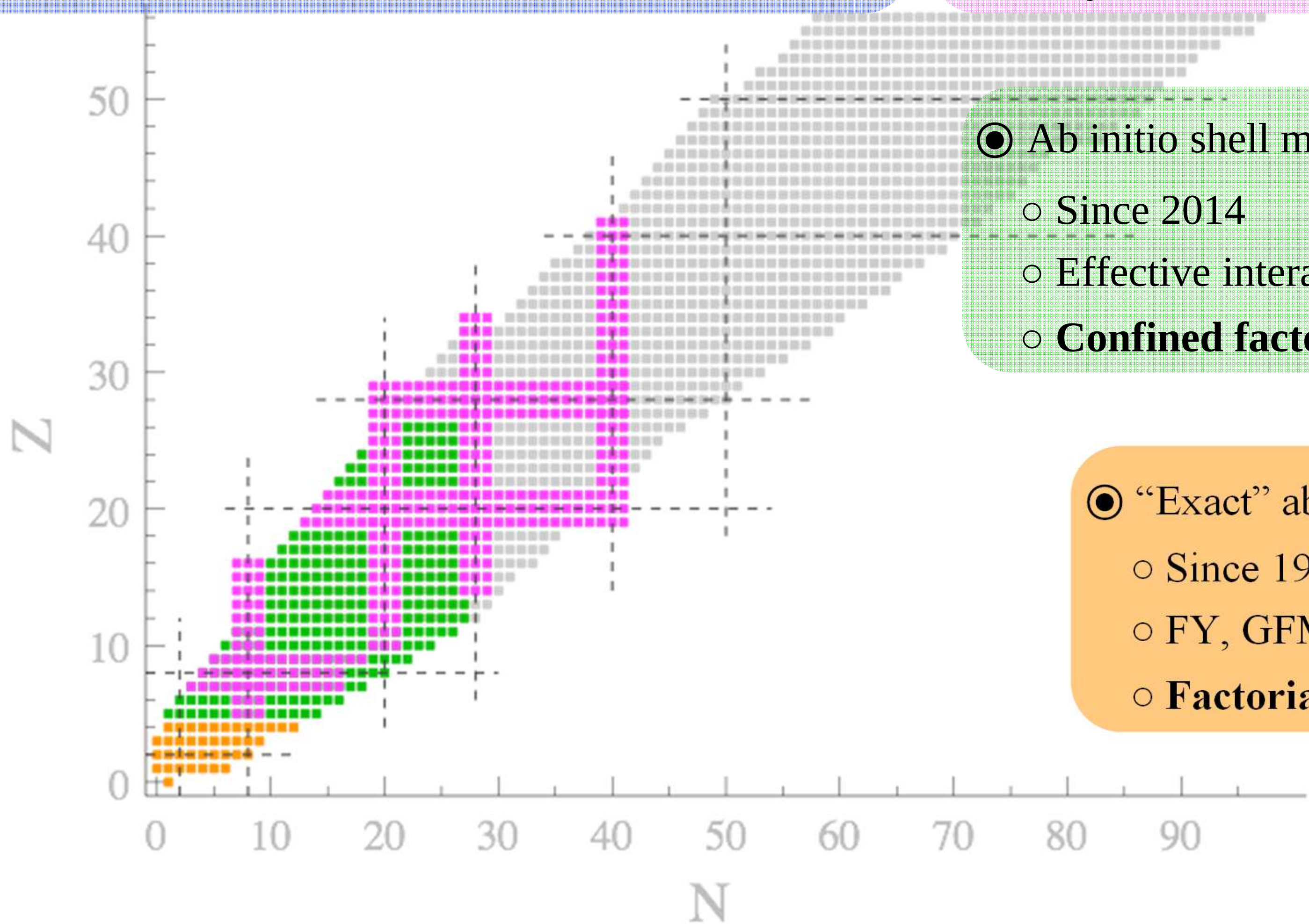

◉ Ab initio shell model for **open-shell**
- Since 2014
- Effective interaction via CC/IMSRG
- **Confined factorial scaling**

◉ "Exact" ab initio approaches
- Since 1980's
- FY, GFMC, NCSM, HH, …
- **Factorial scaling**

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Two sets of 2N+3N pion-full EFT interactions

✪ **N^{3}LO 2N** (NLR - 500MeV) + **N^{2}LO 3N** (LR - 400MeV) **= « EM »**

¤ SRG-evolved down to 1.88-2.0 fm^{-1} [Entem, Machleidt 2003; Navrátil 2007; Roth *et al.* 2012]

EM

- ❑ **Sequential** optimization of 2N and 3N
- ❑ LECs fitted on **A=2,3,4**

Conventional

NNLO$_{sat}$

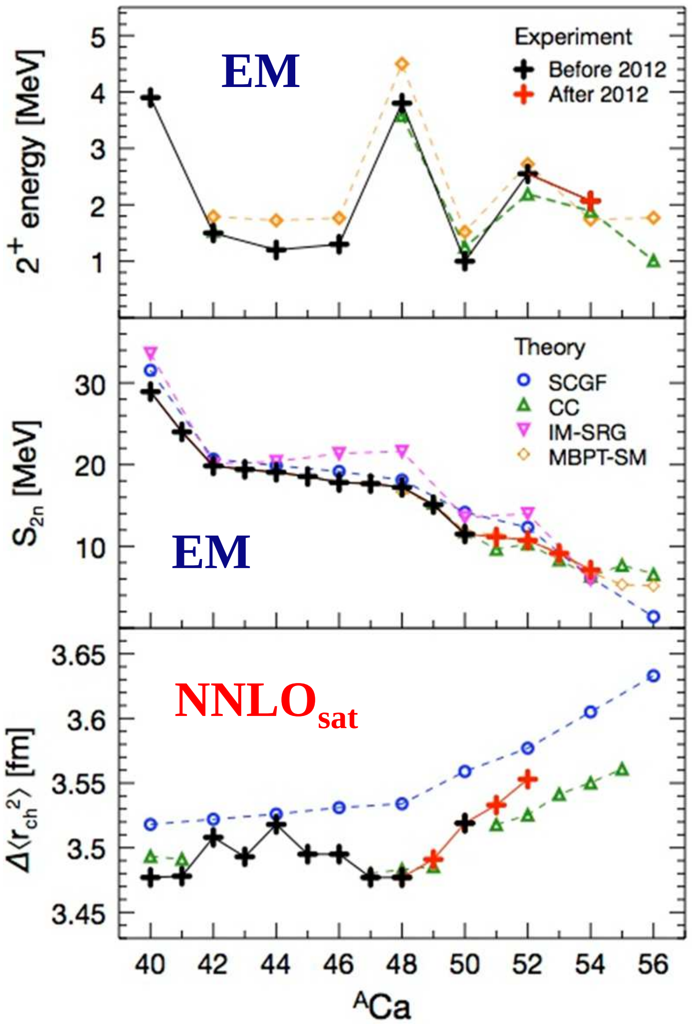
- ❑ **Simultaneous** optimization of 2N and 3N
- ❑ LECs fitted on **A≤25**

Unconventional

✪ **N^{2}LO 2N+3N** (NLR - 450MeV) **= « NNLO$_{sat}$ »**

¤ Bare [Ekstrom *et al.* 2015]

Status of ab initio calc. vs recent exp. in Z=20 isotope chain



NuPPEC LRP 2016 (fig. prepared by V. Somà)

First 2$^+$ excitation energy

- ○ Good description with EM (probably less with NNLO$_{sat}$)
- ○ **High value on ^{48}Ca emerges from 3NF**
- ○ ^{52,54}Ca as sub-shell closures (prediction for ^{54}Ca)

Absolute binding energies (not shown)

- ○ **Systematic overbinding with EM (^{A}O were good)**
- ○ Corrected with NNLO$_{sat}$
- ○ Trend correct requires 3NF

Two nucleon separation energies

- ○ Good reproduction with EM and NNLO$_{sat}$
- ○ 3NF significantly influences drip-line location
- ○ **N=28 magicity emerges from 3NF (and correct N=20)**

Charge radii

- ○ **Too low [~12% (0.4fm)] with EM (not shown)**
- ○ **Corrected by NNLO$_{sat}$ (^{16}O input in fit)**
- ○ Calc. not fully converged

Conclusions

- ○ **Emergence of magicity/3NF essential**
- ○ **Put χ interactions / χ-EFT strongly to the test**
- ○ Need more accuracy, observables, nuclei, errors…

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Extensions of polynomially scaling *ab initio* methods

Doubly open-shell nuclei

- ○ All methods **limited to spherical nuclei**
- ○ Break rotational SU(2) symmetry
- ○ **Access nuclei beyond semi-magic (=all)**

GGF □□□ BCC □□□ IMSRG □□□

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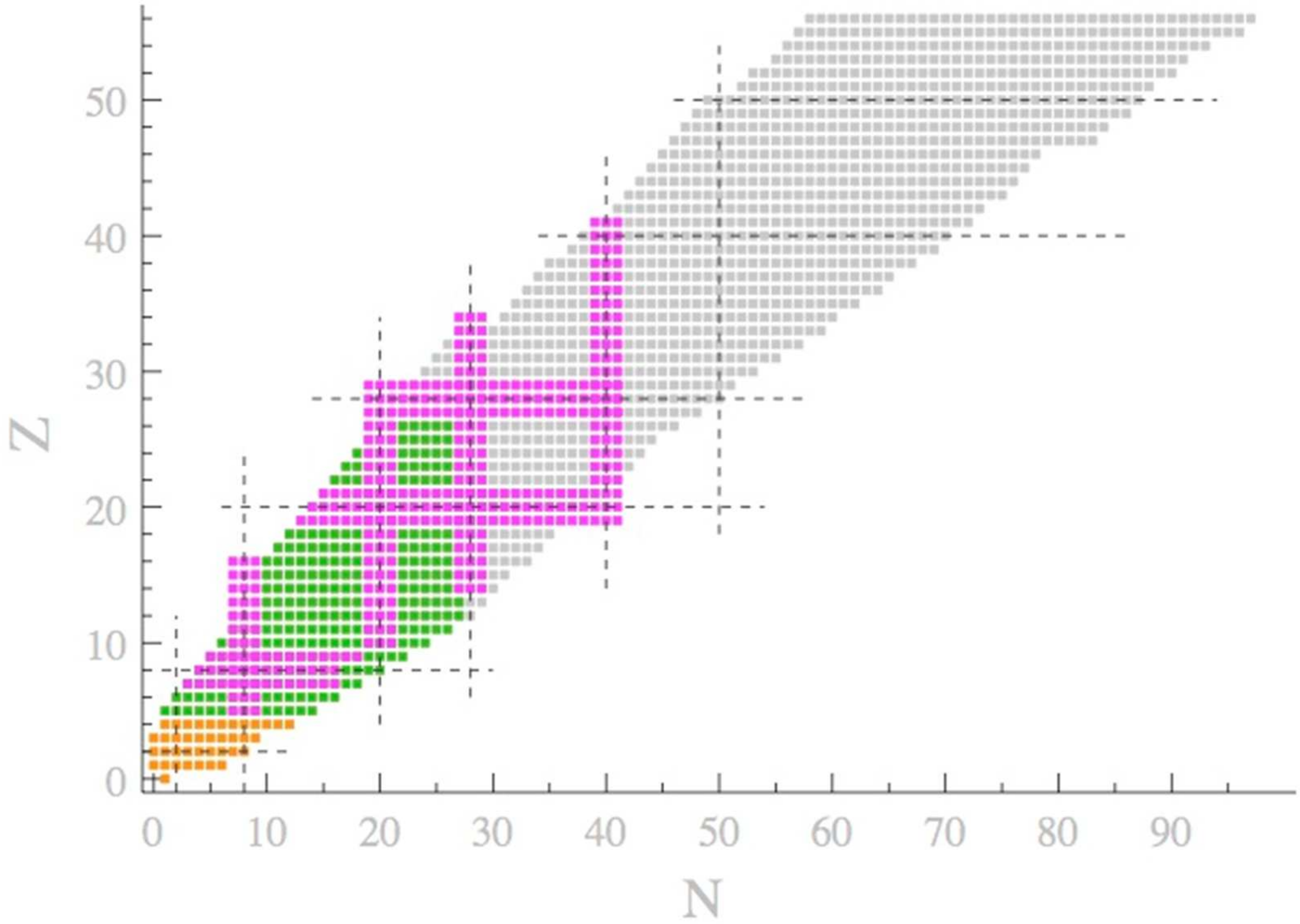

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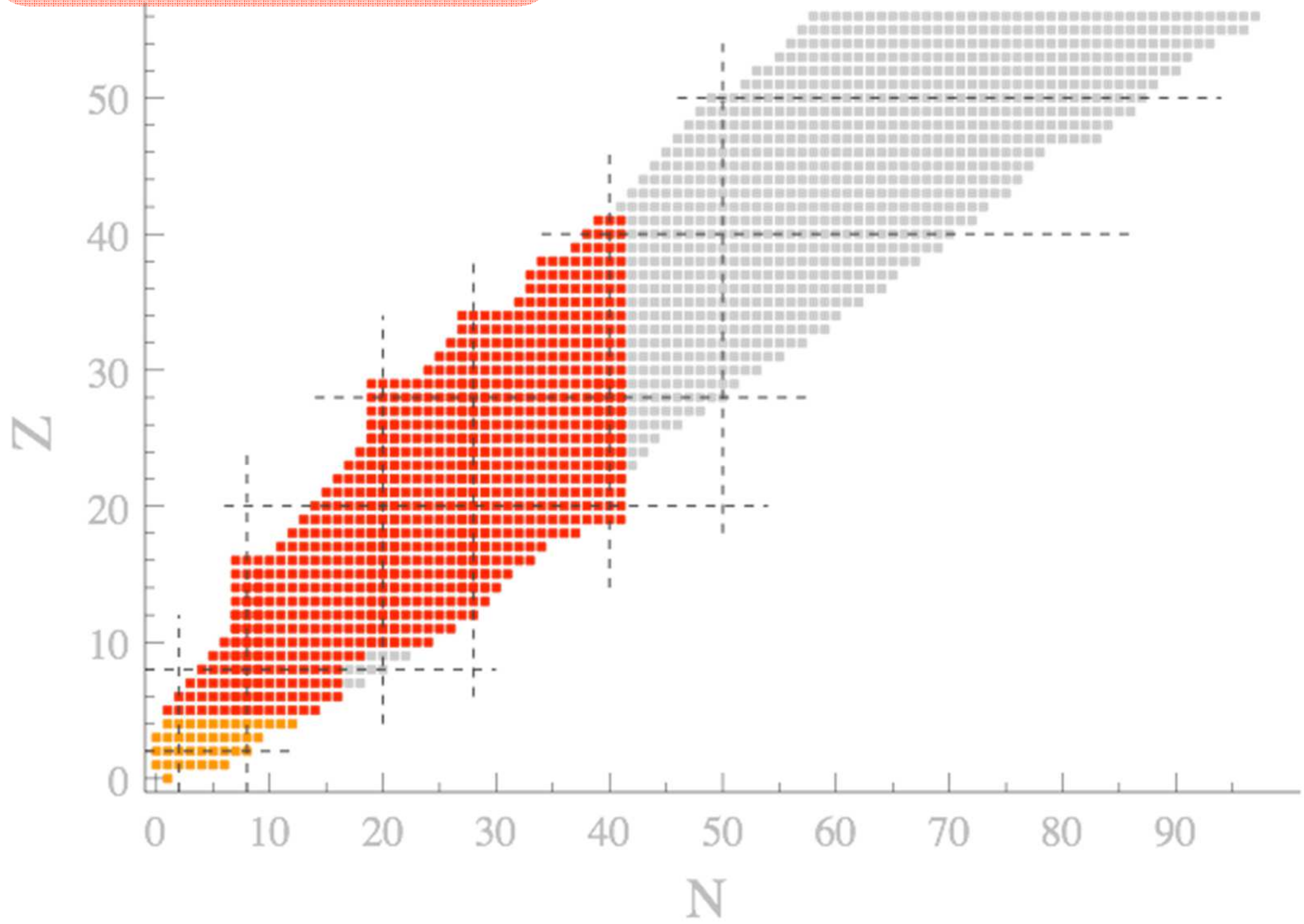

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Continuum coupling

○ **Particle continuum discretized in HO**

○ Couple HO with Berggren or Bessel basis

○ **Dripline + some applications to reactions**

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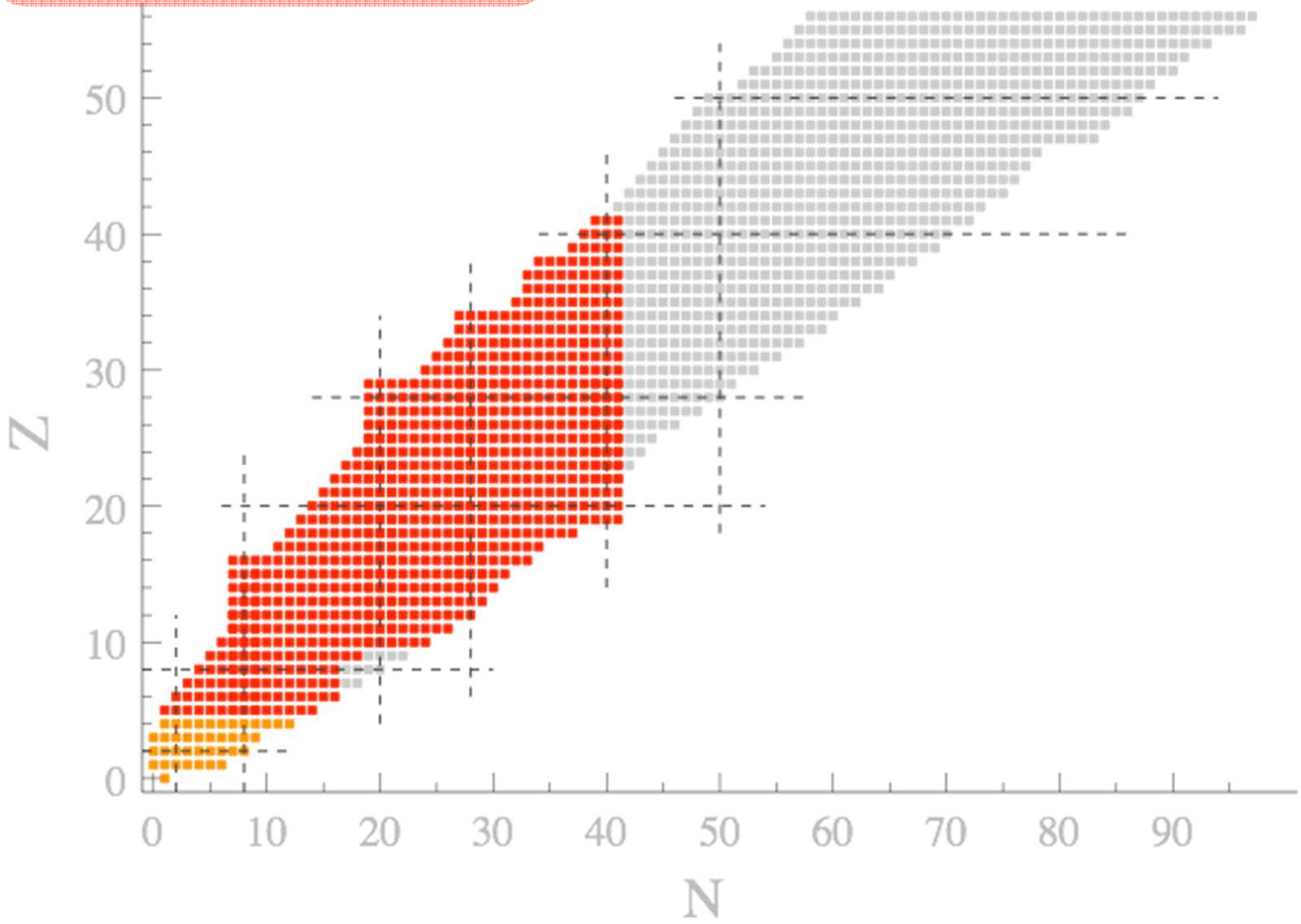

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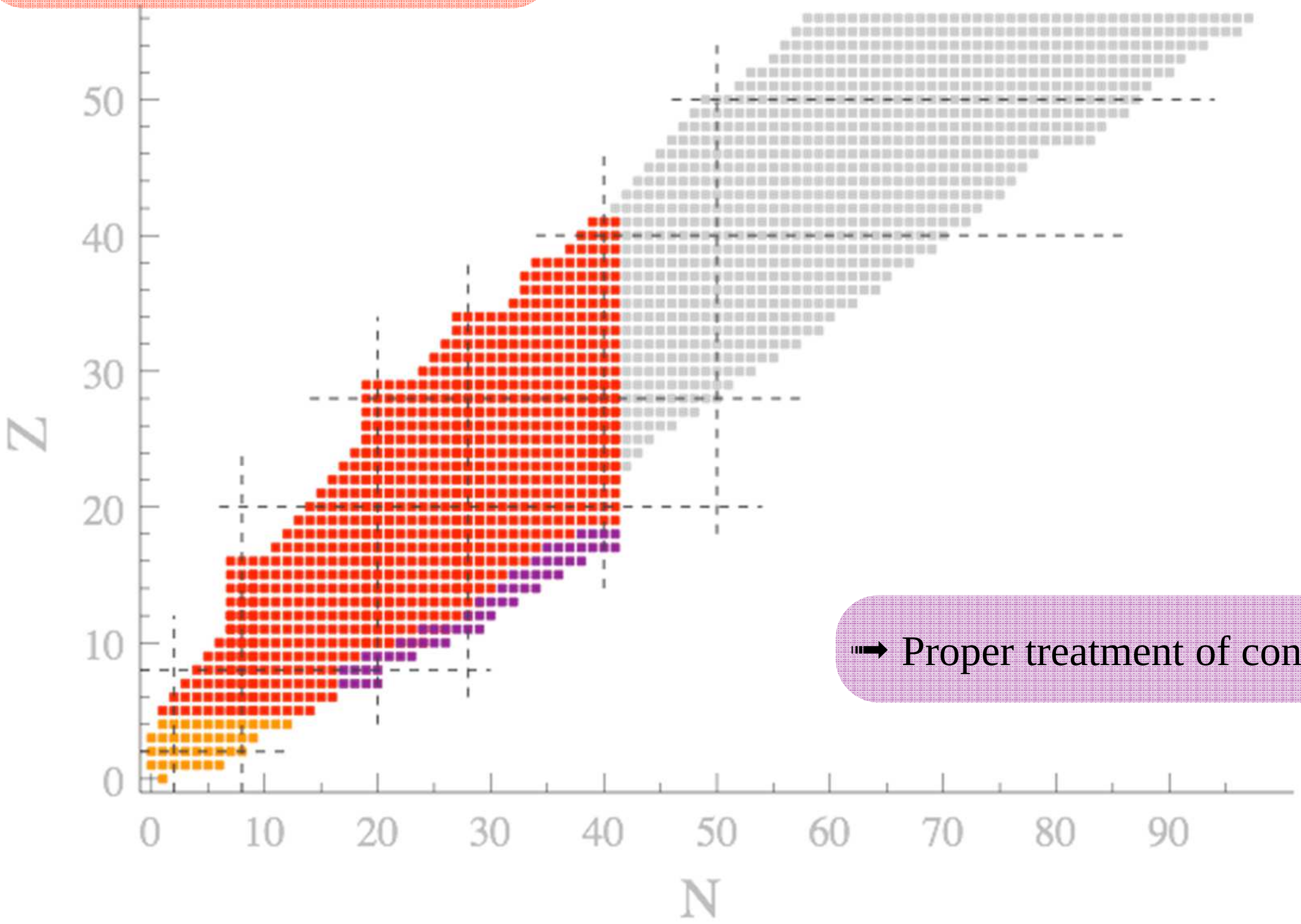

➟ Proper treatment of continuum

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GGF ☐☐☐ BCC ☐☐☐ IMSRG ☐☐☐

Heavy nuclei

- Calculation **limited by size of 3NF input file**
- Terabyte or petabyte files beyond A~100
- Need breakthrough to reduce **memory load**

DGF ☐☐☐ CC ■■■ IMSRG ☐☐☐

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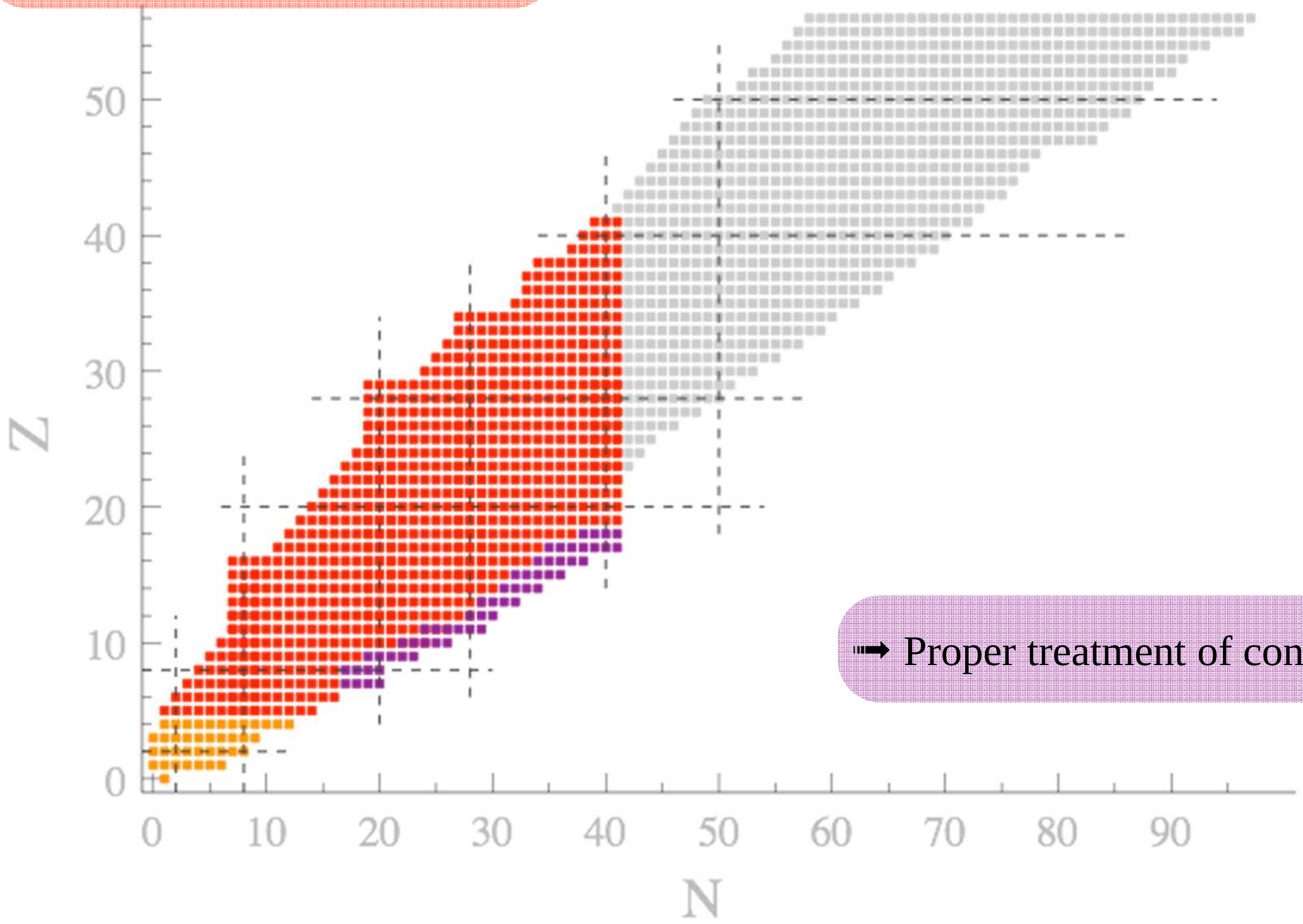
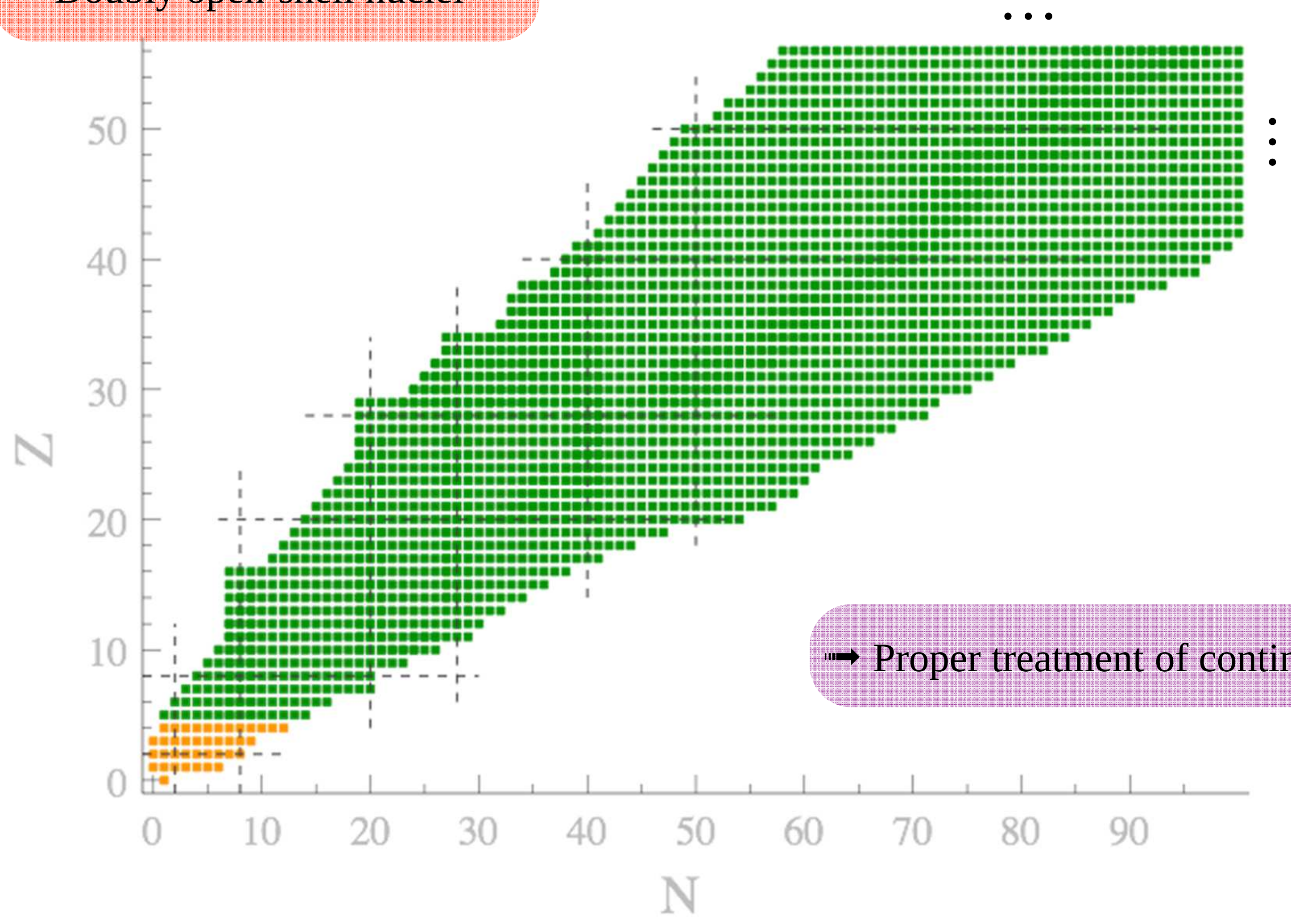


➟ Proper treatment of continuum

Extensions of polynomially scaling *ab initio* methods

➟ Handle of 3-body matrix elements

➟ Doubly open-shell nuclei



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DGF CC IMSRG

GGF BCC IMSRG

Higher orders in the many-body expansion

○ Current GGF **limited in precision**

○ Develop and implement ADC(3)

○ Affect gs observables, spectroscopy, pairing…

DGF CC IMSRG

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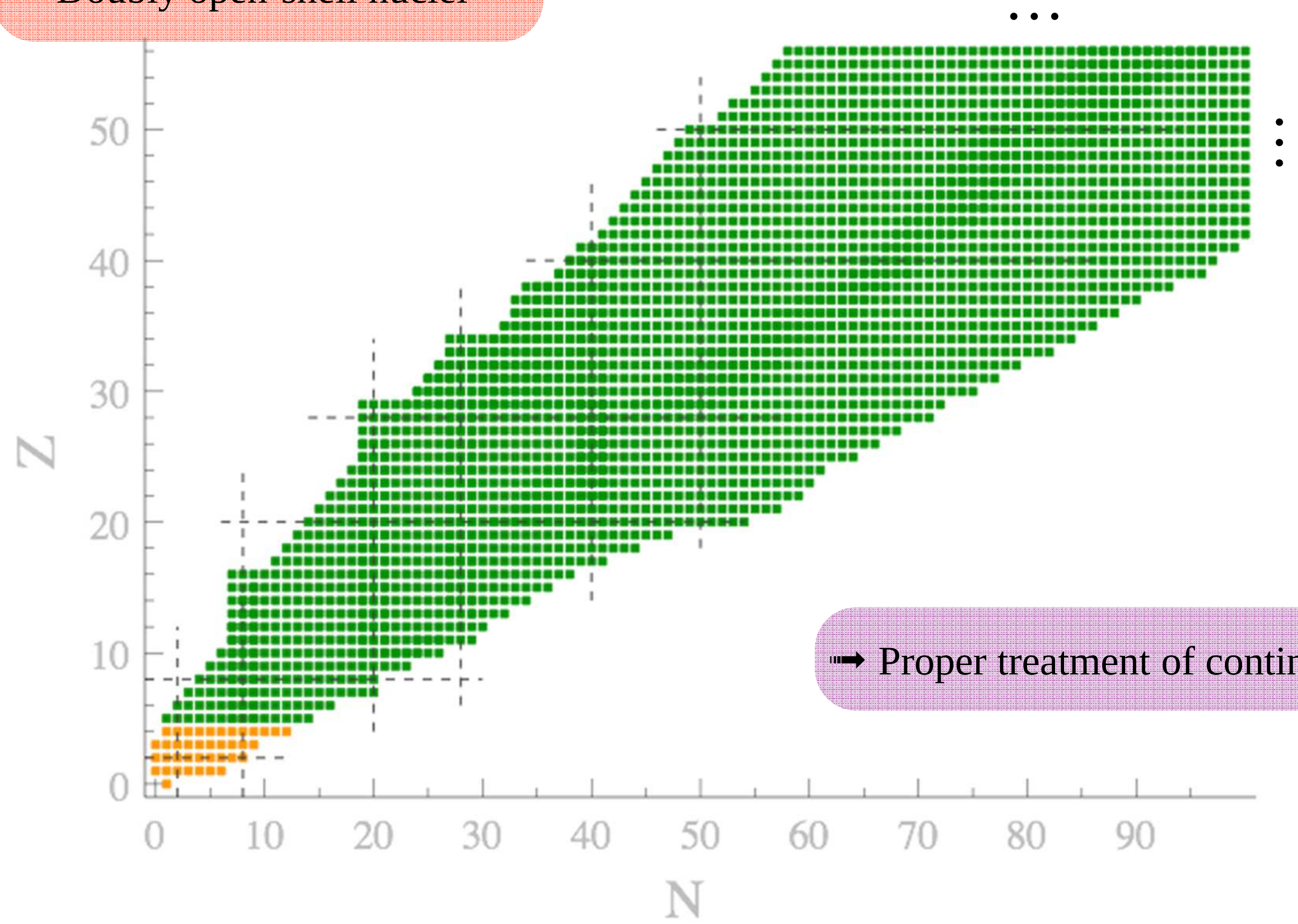

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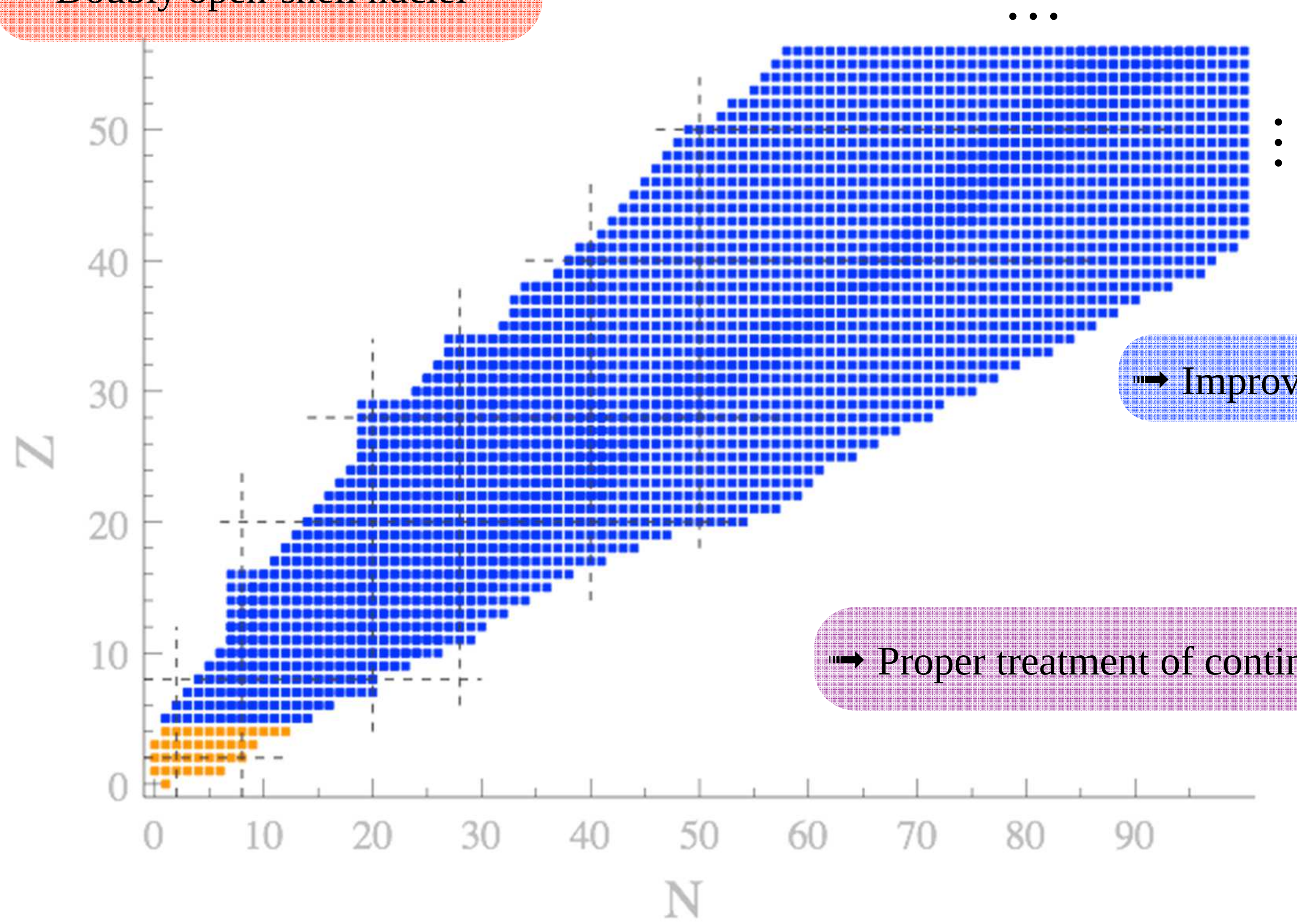
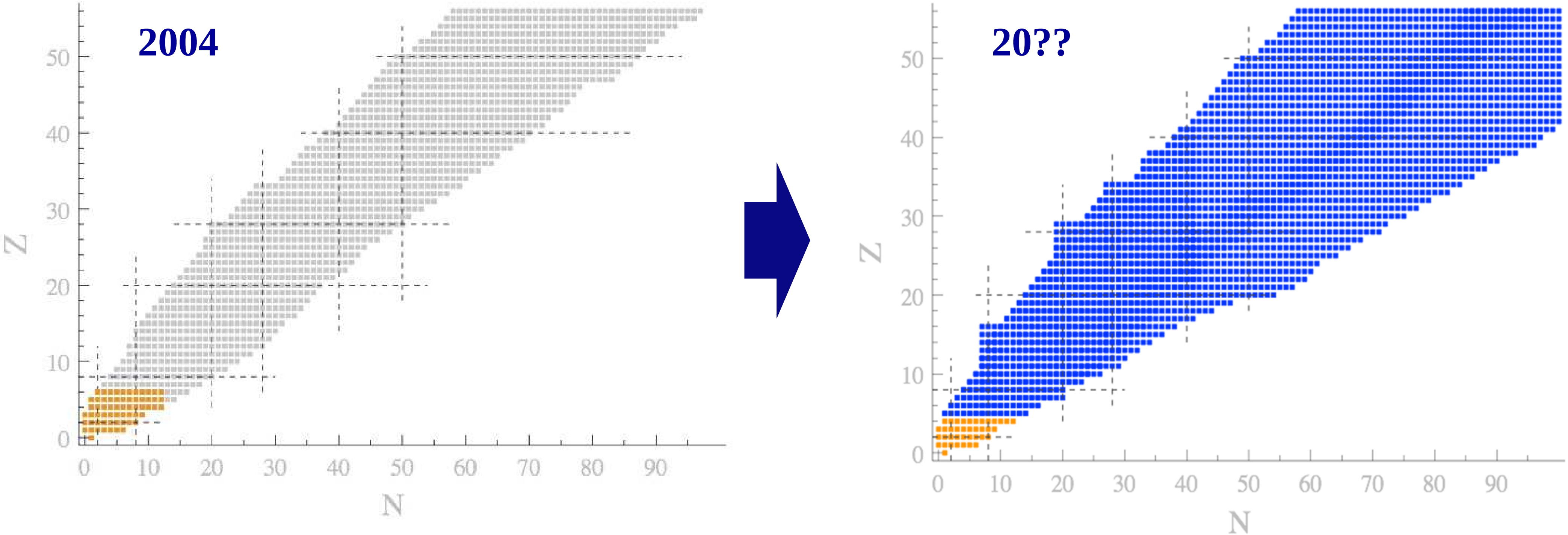


➡ Improved convergence

➡ Proper treatment of continuum

Long-term perspectives



Emergence of nuclear phenomena from nucleons and their interactions?

- ○ Binding, size, limit of existence, collectivity, superfluidity, decays…
- ○ Limits of such a description with A/in accuracy?
  - ○ Modified A-body ab initio effective theory when A increases?
  - ○ More effective but explicitly connected approaches?

Detailed, quantitative and systematic description of nuclei of interest