Potential interplay between ab-initio and energy density functional approaches

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PND2-2 workshop, October 14-17 2014, Bruyères Le Chatel, France

Introduction

Microscopic theoretical approaches

Ab-initio **many-body theories**

- **Based on *elementary* interactions**
- ***Complete*** **and disjointed error estimate**

Limited **reach**
Controlled **extrapolations**

Test fundamental interactions
Do not focus on accuracy at first

Extended **reach**
Uncontrolled **extrapolations**

Do not probe fundamental interactions
Aims at high accuracy around known data

Effective **many-body theories**

- **Based on *effective* interactions**
- ***Partial*** **and composite error estimate**

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Status of *ab-initio* many-body theories

***Ab-initio* many-body theories**
- Effective structure-less nucleons
- 2N + 3N + … inter-nucleon interactions
- Solve A-body Schrödinger equation
- Thorough assessment of errors needed

→ **Controlled extrapolations**
Limited applicability domain

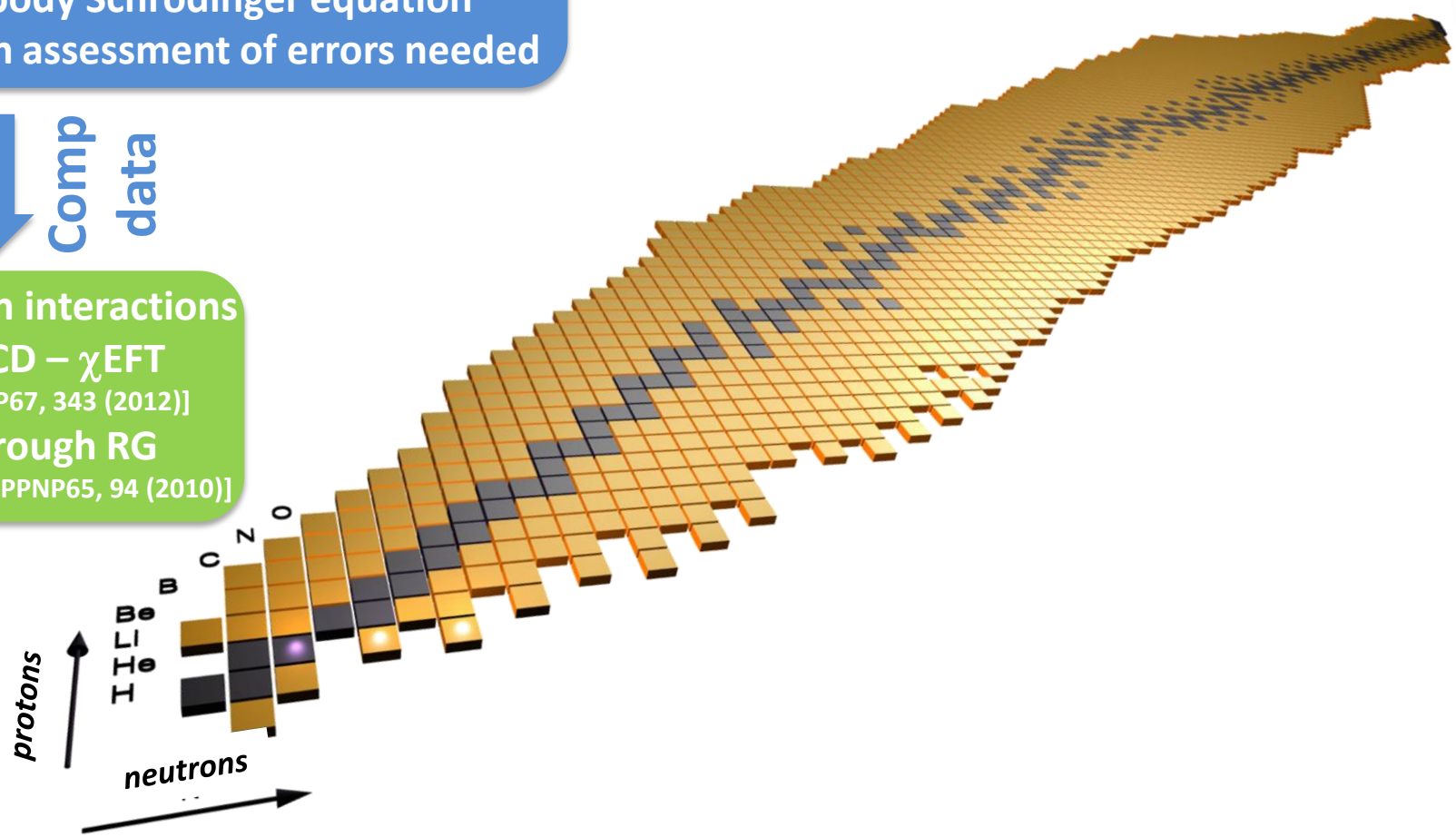
Input

Comp data

Inter-nucleon interactions
- Link to QCD – χEFT

[E. Epelbaum, PPNP67, 343 (2012)]
- Soften through RG

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



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1972-2014
EDF approach
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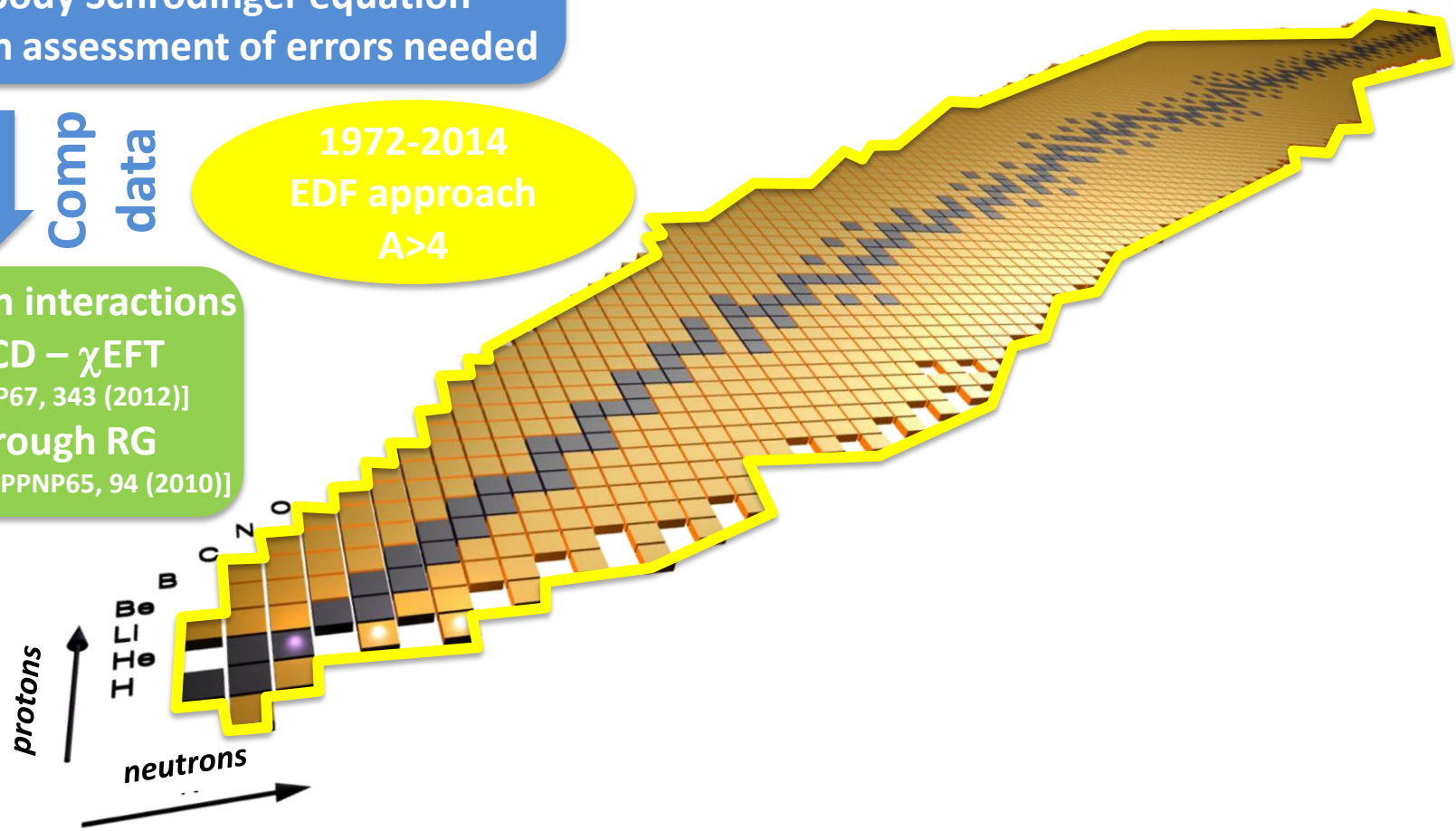

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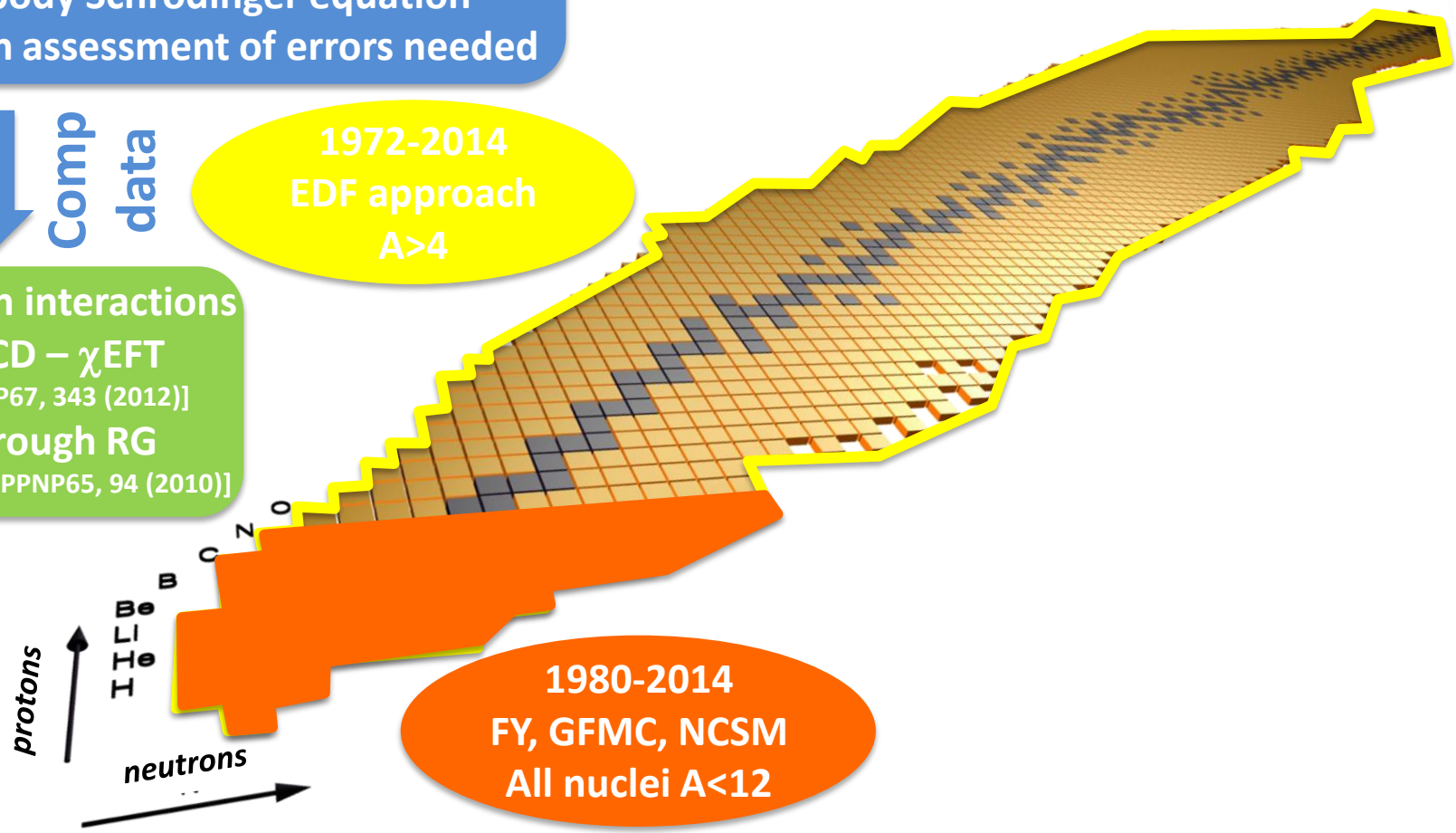

1980-2014
FY, GFMC, NCSM
All nuclei A<12

[Carlson, Pieper, Wiringa]
[Barrett, Vary, Navratil, Ormand]

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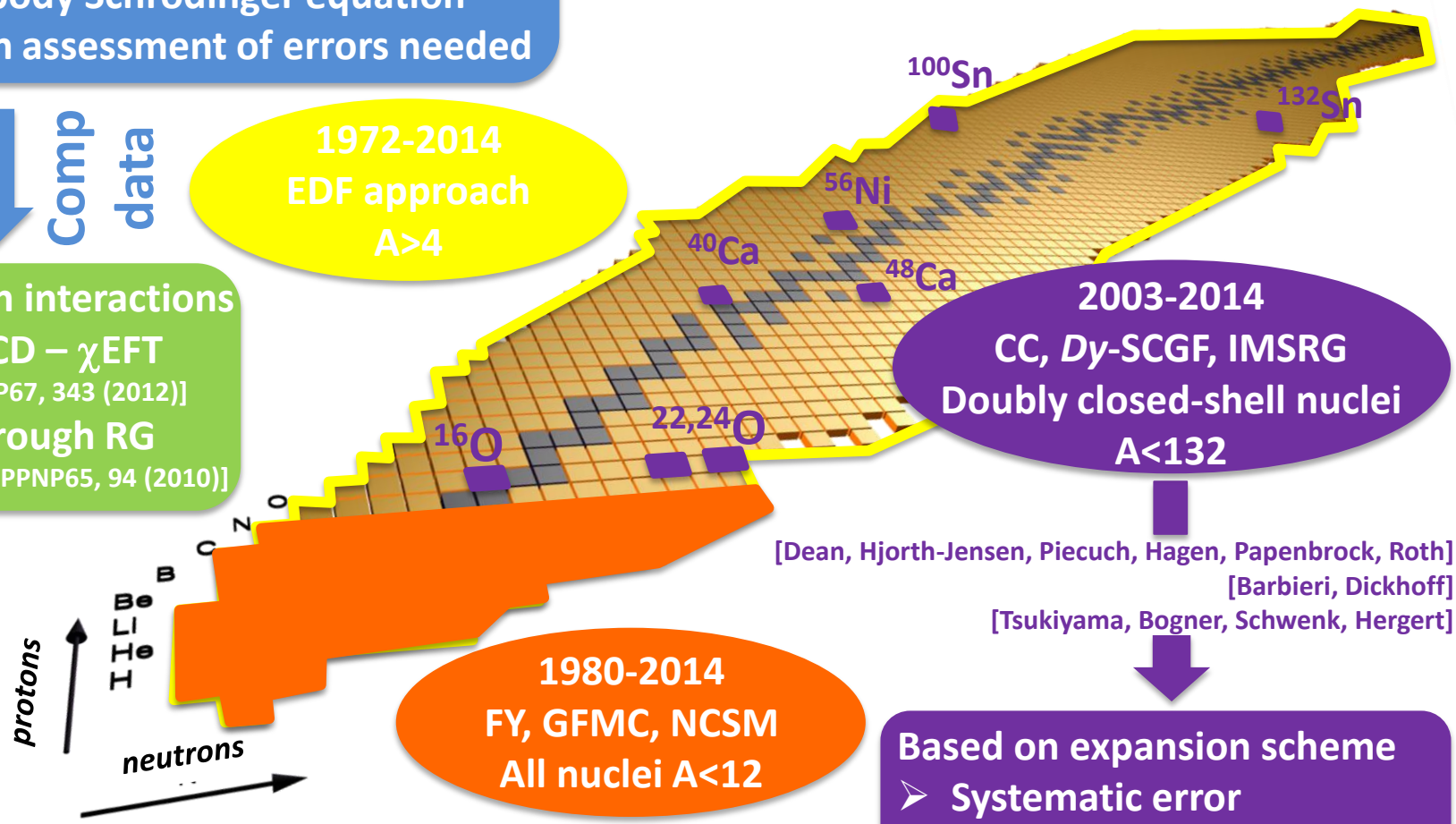

2003-2014
CC, *Dy*-SCGF, IMSRG
Doubly closed-shell nuclei
A<132

[Dean, Hjorth-Jensen, Piecuch, Hagen, Papenbrock, Roth]
[Barbieri, Dickhoff]
[Tsukiyama, Bogner, Schwenk, Hergert]

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Based on expansion scheme
- Systematic error
- Cross-benchmarks needed

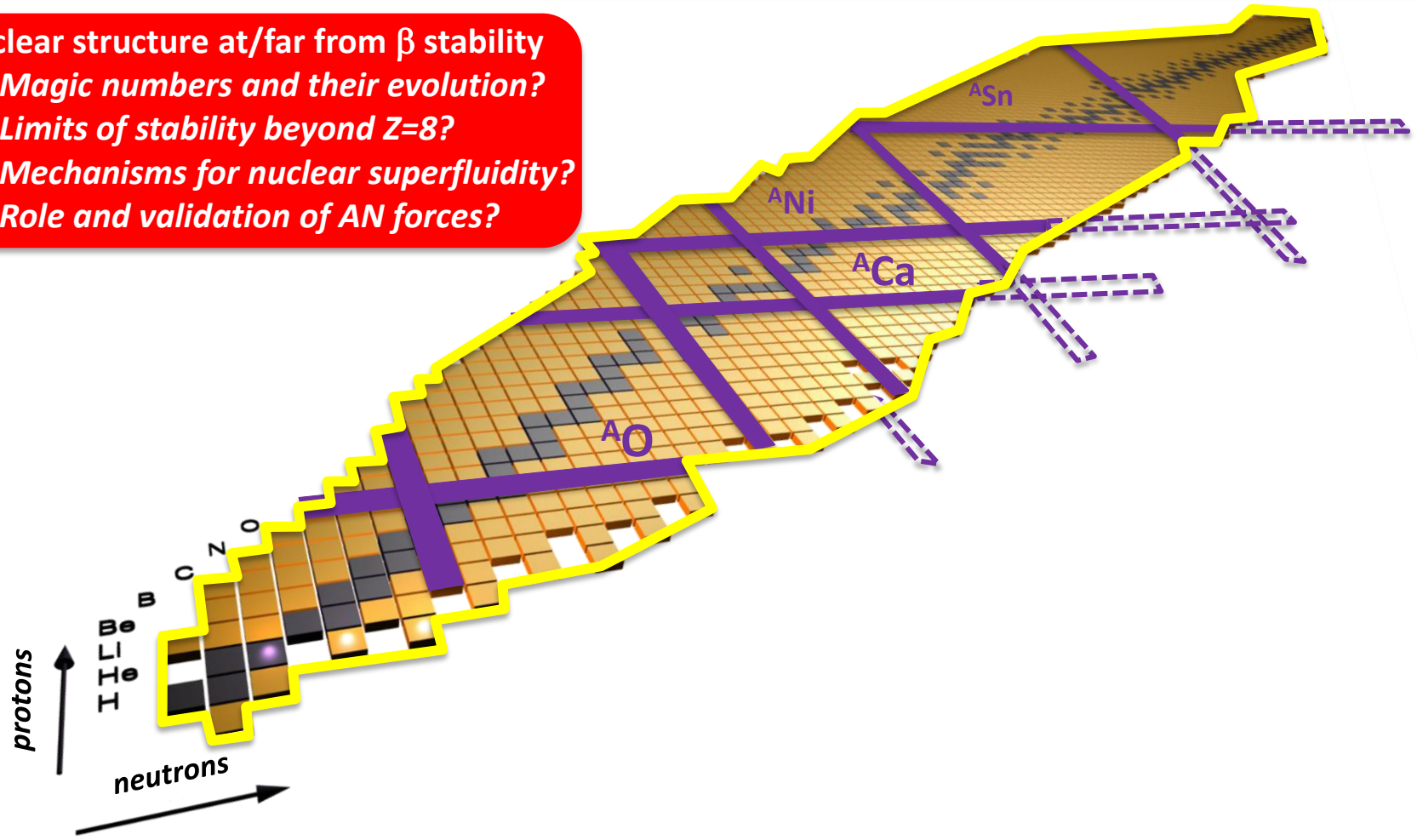
Ab-initio methods for singly open-shell nuclei

First objective: generalize many-body methods to study complete isotopic/isotonic chains

- **From a few 10s of nuclei to several 100s of nuclei = strong overlap with EDF methods**

Nuclear structure at/far from β stability

- ***Magic numbers and their evolution?***
- ***Limits of stability beyond Z=8?***
- ***Mechanisms for nuclear superfluidity?***
- ***Role and validation of AN forces?***



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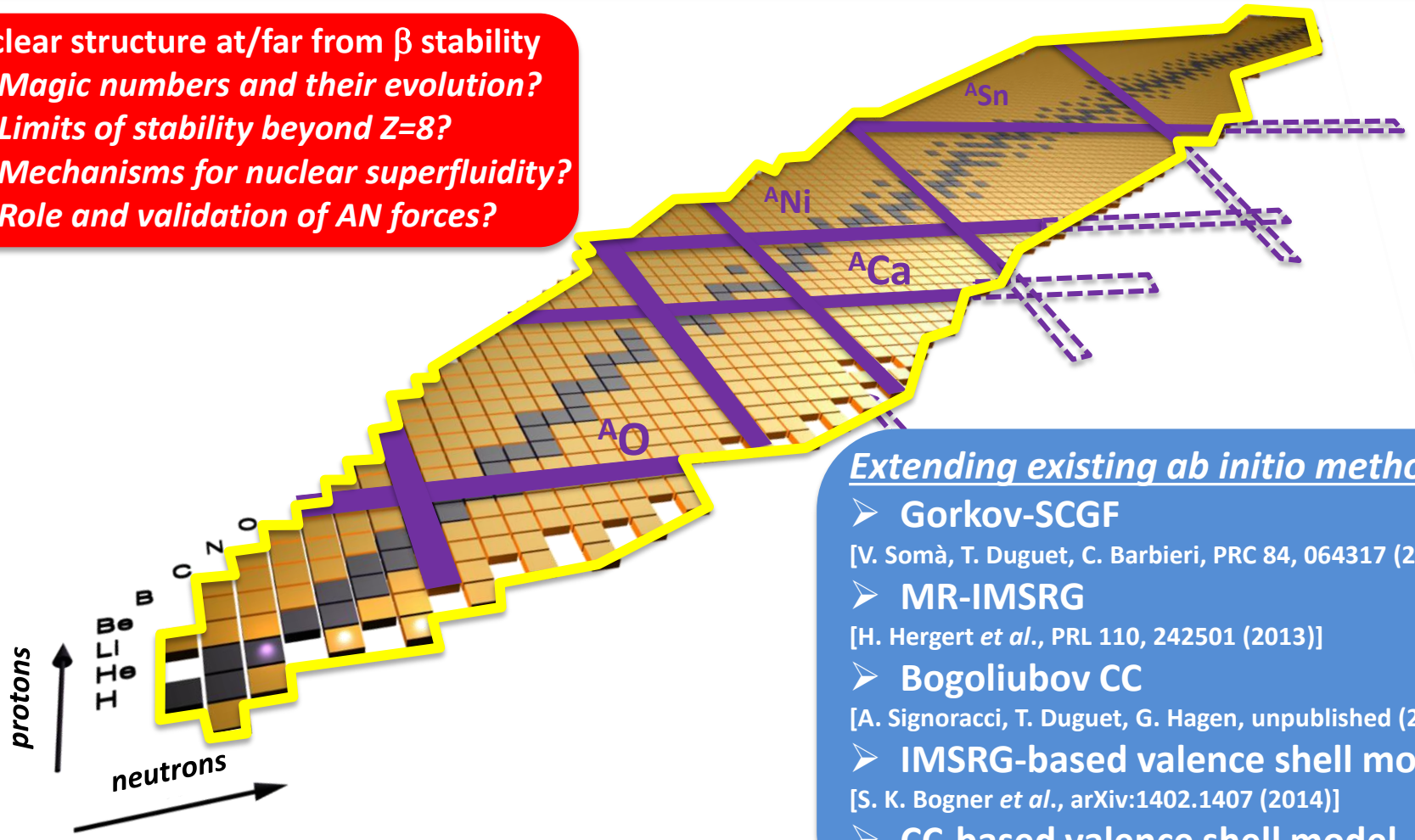

<u>Extending existing ab initio methods</u>

- **Gorkov-SCGF**

[V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]

- **MR-IMSRG**

[H. Hergert *et al.*, PRL 110, 242501 (2013)]

- **Bogoliubov CC**

[A. Signoracci, T. Duguet, G. Hagen, unpublished (2014)]

- **IMSRG-based valence shell model**

[S. K. Bogner *et al.*, arXiv:1402.1407 (2014)]

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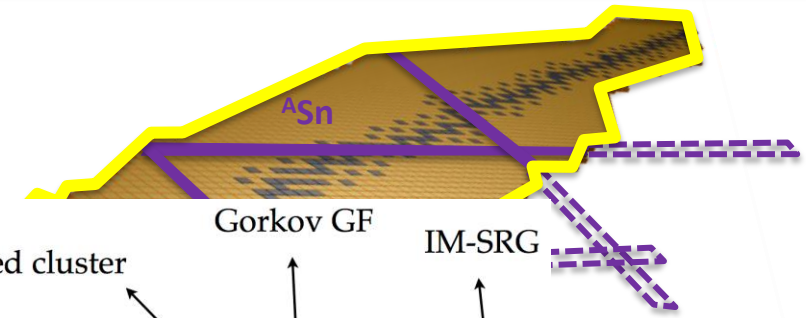

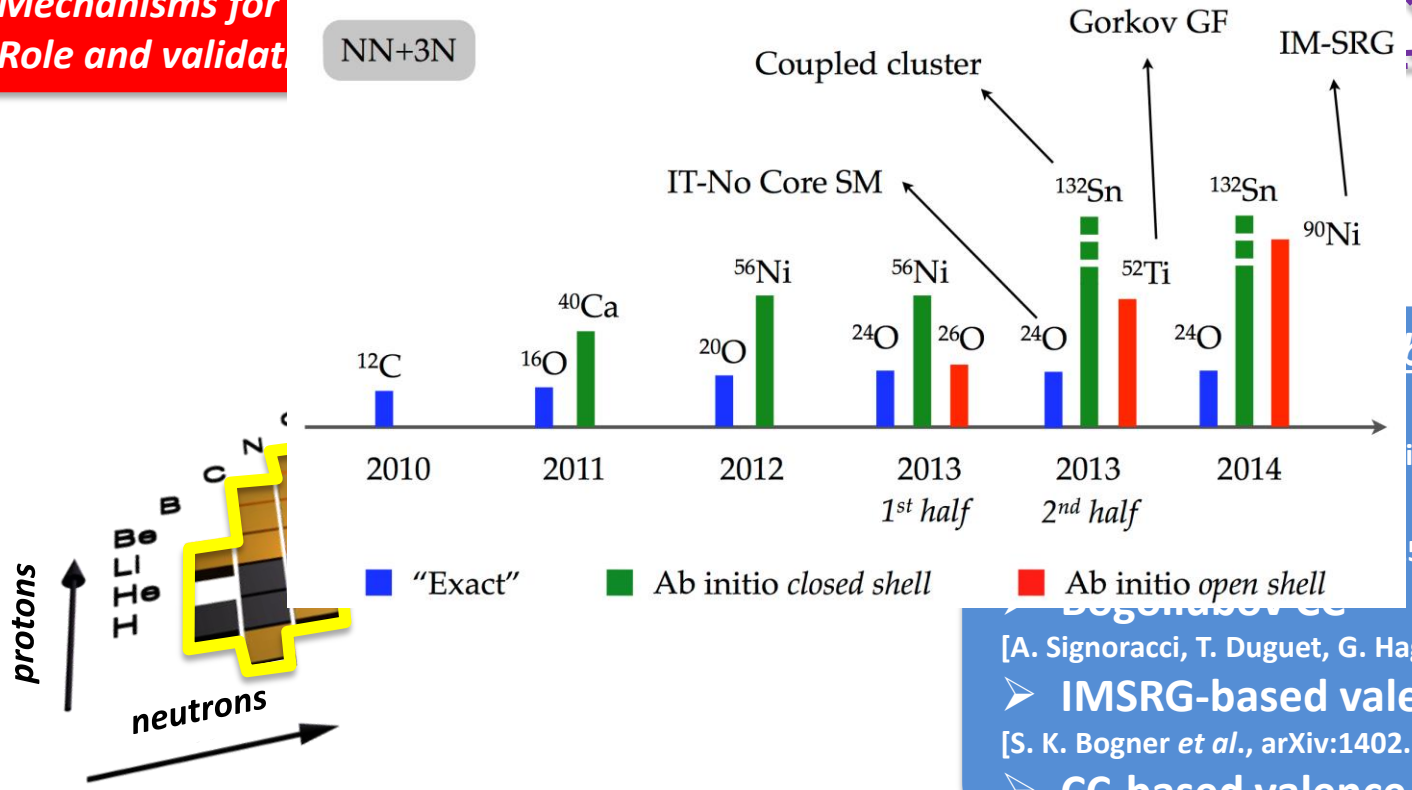

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Potential interplay

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2014 2015 2016 2017 2018 2019 2020

Ab-initio

Improve many-body scheme

Account for the continuum

Access doubly-open shell nuclei

Develop symmetry-restored theories

Bridge to *ab initio* reactions

long term

E.D.F.

Build EDF parameterizations with reduced systematic errors

Build well-defined EDF kernels for multi-reference calculations

Bridge structure and reactions

long term

FAIR Facility for Antiproton and Ion Research in Europe GmbH

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Prepared with J.P. Ebran

Energy density functional method (schematic)

Target state

Wave operator

Reference state

$$|\Psi_0\rangle = \Omega_0 |\Phi_0\rangle$$

A-body ground state

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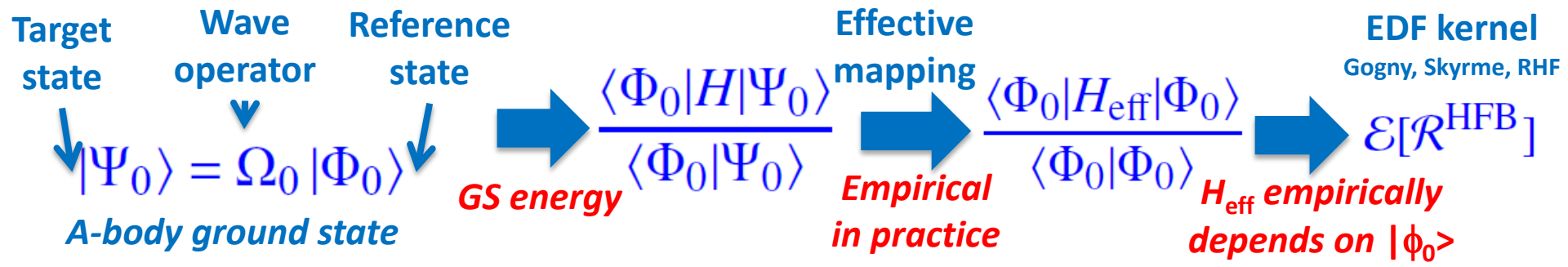

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EDF kernel

Gogny, Skyrme, RHF

$$\mathcal{E}[\mathcal{R}^{\rm HFB}]$$

$H_{\rm eff}$ empirically depends on $|\phi_0\rangle$

Closed shell

RHF reference

conserves A, (J^2,M)

Bulk correlations

Param. in $\mathcal{E}[\mathcal{R}^{\rm HFB}]$

Vary smoothly with A

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Breaking symetries

Vary smoothly with A_{sh}

ph degeneracy <-> Goldstone mode

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Vary quickly with A_{sh}

Multi-reference character

Finite inertia <-> *Resolve Goldstone mode*

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Empirical param based on T&E

**No link with microscopy*

**Uncontrolled extrapolations*

**No clear path for improvement*

MR EDF method ill defined

**SI and SP contaminations*

**Worse as we enrich it*

**Need microscopic guidance*

[M. Bender, T. Duguet, D. Lacroix, PRC (2009)]

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Many-body expansion

e.g. MBPT

Ab-initio energy kernel

$$\mathcal{E}[\mathcal{R}^{\mathrm{HFB}}; \{E_k^{\mathrm{HFB}}\}]$$

e.g. energy dependent

cf. orbital-dependent DFT

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Dy-SCGF & CC

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Closed shell

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- *conserves A, J², M*
- *Dy*-SCGF & CC

Breaks down for open-shell nuclei

Singly/doubly open shell

- UHF(B) reference
- *breaks A / J² and M*
- *Go*-SCGF & BCC

ph degeneracy
<->
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[T. Duguet, arXiv:1406.7183]

Multi-reference character

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Multi-reference character

Ab initio energy kernel
- *Same symmetry B&R principles
- *More general: energy dependent
- *Richer: explicit correlations

Can provide guidance for EDF kernel

Ab initio MR method
- *Analytically well defined
- *No SI and SP contaminations
- *Microscopic guidance

Looking into the next 10 years

2014 2015 2016 2017 2018 2019 2020

Ab-initio

Improve many-body scheme
Account for the continuum
Access doubly-open shell nuclei
Develop symmetry-restored theories
Bridge to *ab initio* reactions
long term

E.D.F.

Build EDF parameterizations with reduced systematic errors
Build well-defined EDF kernels for multi-reference calculations
Bridge structure and reactions
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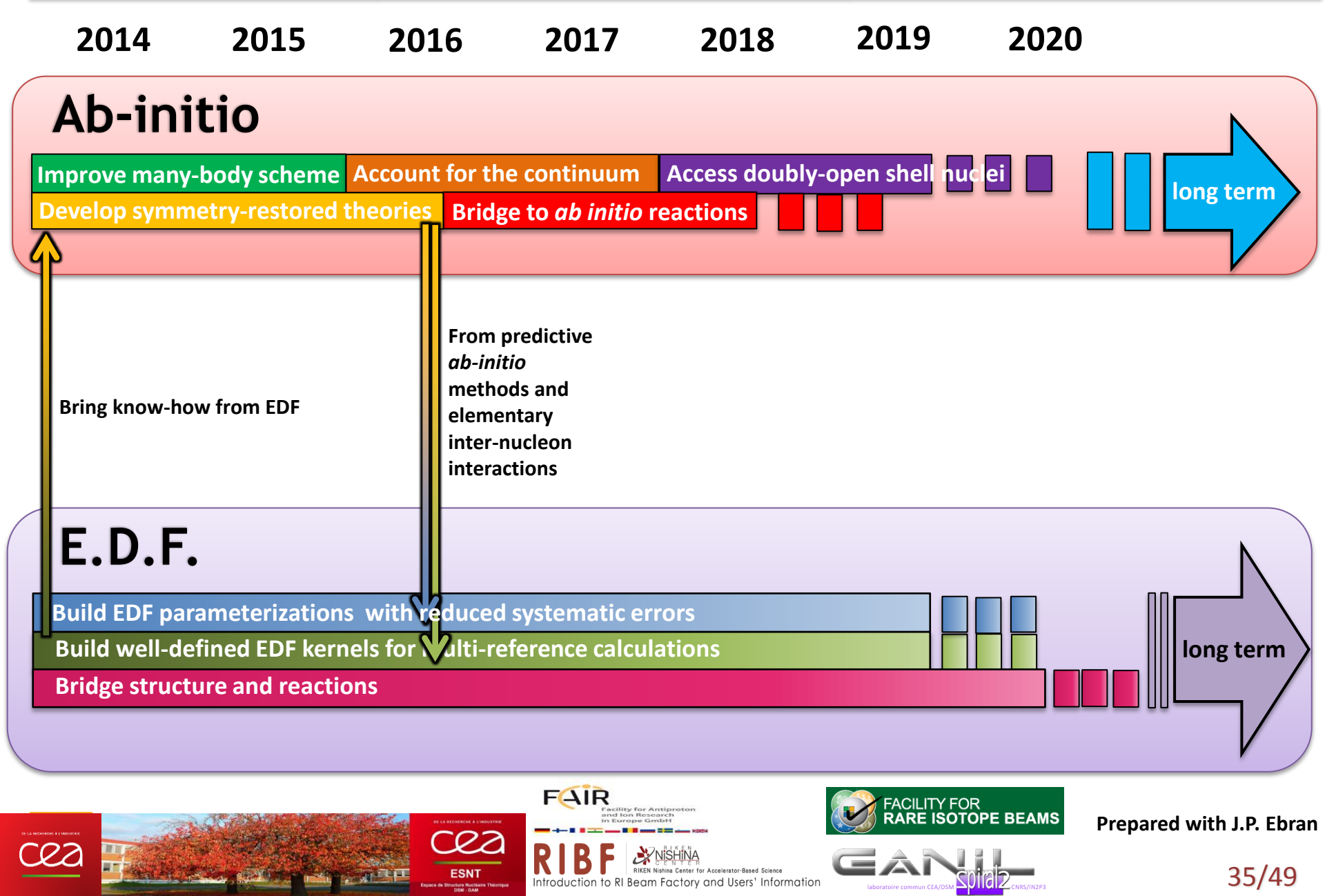

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Towards *ab-initio* optical potentials

[V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]

Ab-initio Gorkov self-consistent Green's function theory

Dressed 1-body Gorkov Green's function

Gorkov's equation of motion

$$G_{ab}(\omega) = G^{(0)}_{ab}(\omega) + \sum_{cd} G^{(0)}_{ac}(\omega)\Sigma_{cd}(\omega)G_{db}(\omega)$$

$$\Sigma_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & \Sigma^{22}_{ab}(\omega) \end{pmatrix}$$

Irreducible self energy

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$$\Sigma_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & \Sigma^{22}_{ab}(\omega) \end{pmatrix}$$

Irreducible self energy

$\omega < 0$

Bound 1-nucleon +/- energies

$$E^{\pm}_k \equiv \pm\left(E^{A\pm1}_k - E^{A}_0\right)$$

Towards *ab-initio* optical potentials

[V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]

Ab-initio Gorkov self-consistent Green's function theory

Dressed 1-body Gorkov Green's function

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$$\Sigma^{11}(\vec{r},\vec{r}';\omega) = \sum_{ab} \varphi^*_a(\vec{r})\Sigma^{11}_{ab}(\omega)\varphi_b(\vec{r}')$$

[C. Mahaux, R. Sartor, ANP 20, 1 (1991)]

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Consistent structure and reaction *ab-initio* information

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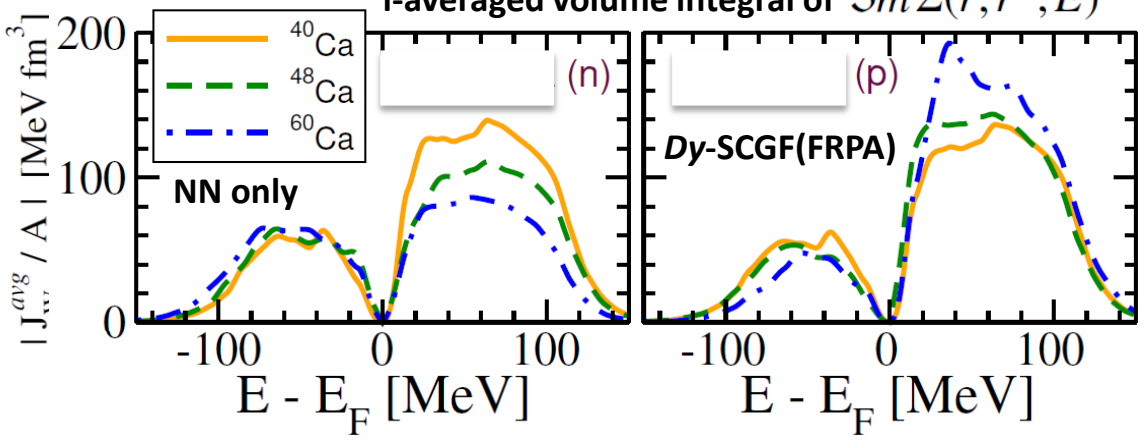
Closed shell

l-averaged volume integral of $\Im m\,\Sigma(\vec{r},\vec{r}';E)$



[S. J. Waldecker, C. Barbieri, W. H. Dickhoff, PRC 84, 034616 (2011)]

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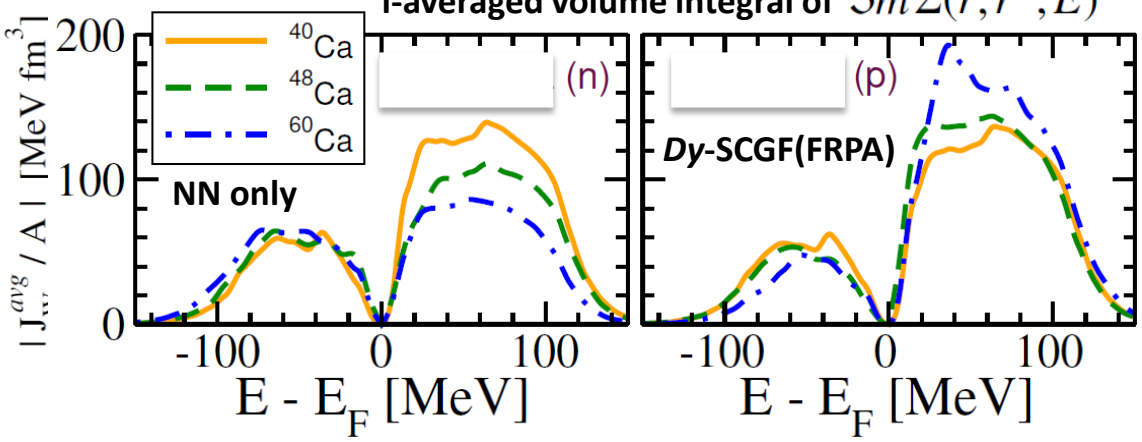
***Ab-initio* optical potential**

- *In closed and open shell nuclei
- *Nucleus by nucleus access
- *Constrain effective parametrization
  - *Non locality (i.e. l dependence)*
  - *Isospin dependence*

Closed shell

l-averaged volume integral of $\Im m\,\Sigma(\vec{r},\vec{r}';E)$



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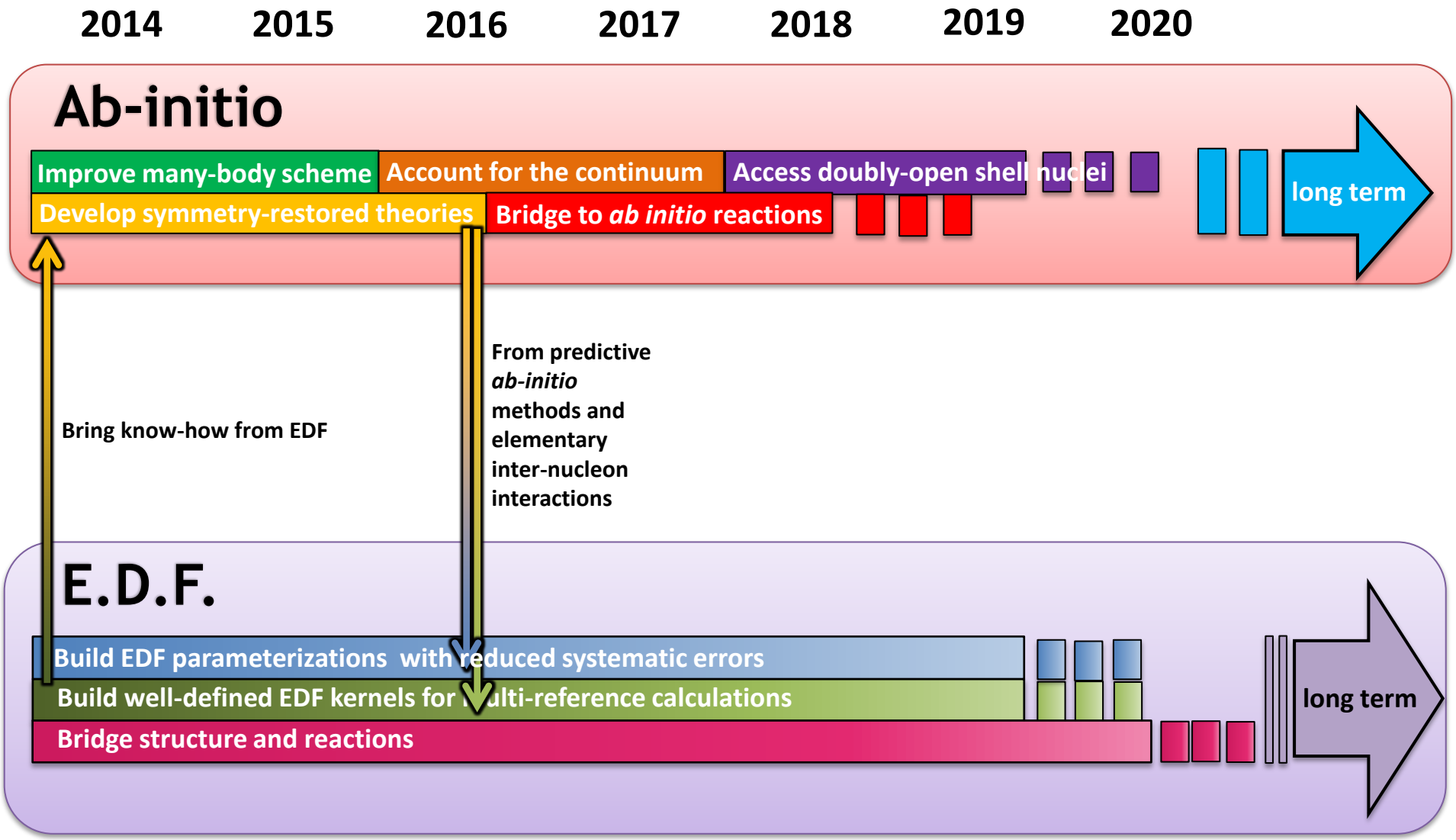
Looking into the next 10 years



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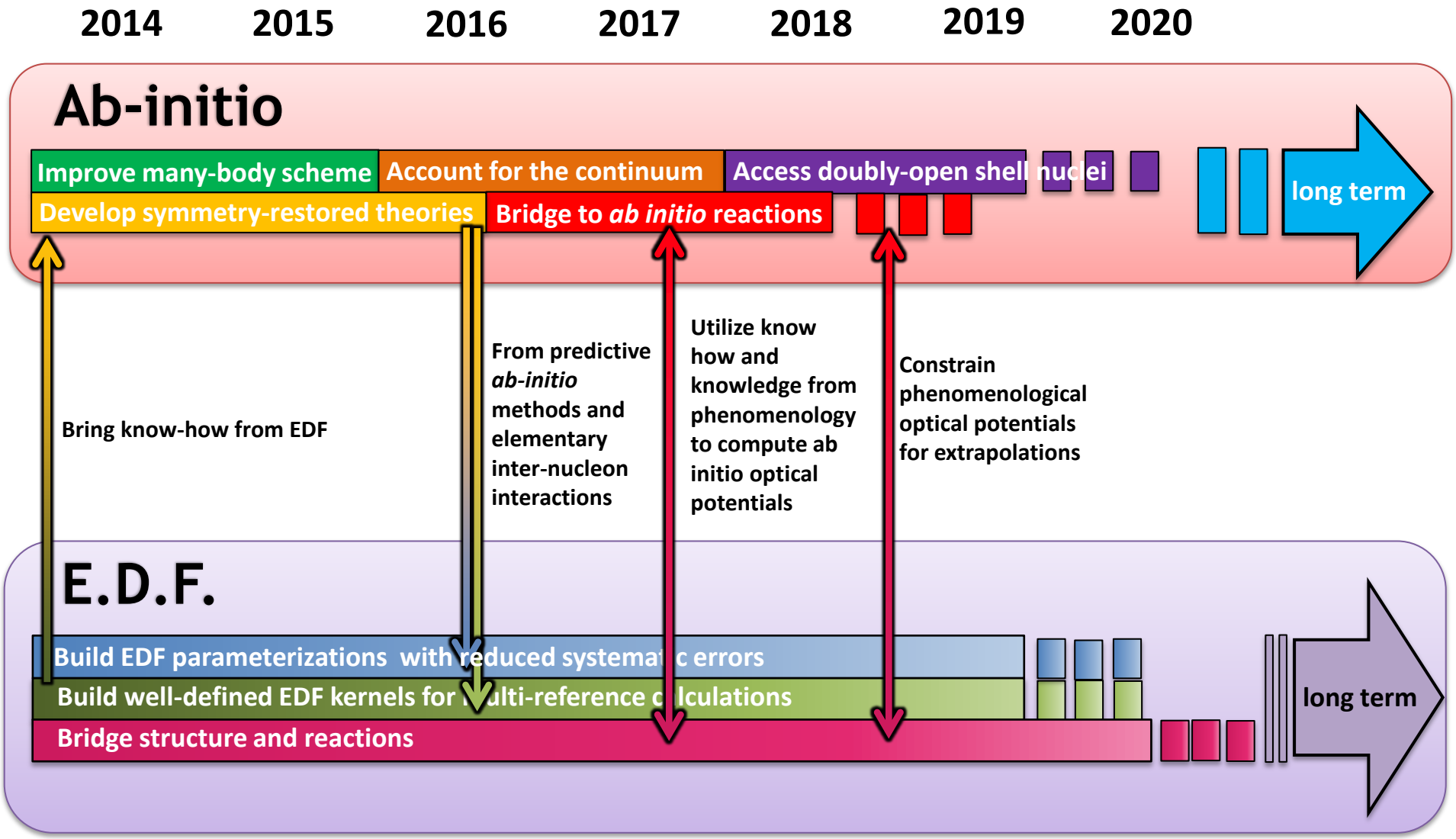

Introduction to RI Beam Factory and Users' Information

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

Binding energy of ^{A}O

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

Input

Inter-nucleon interactions

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

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

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

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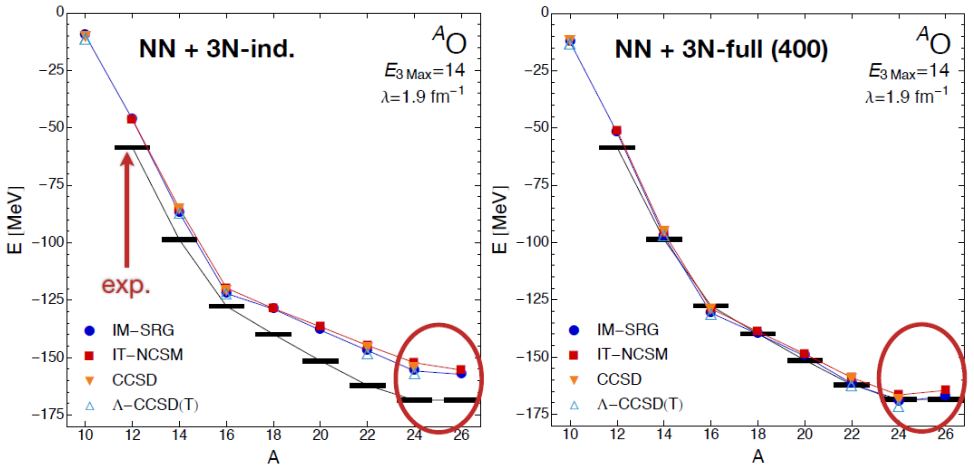
- SRG evolved down to λ = 1.9 fm^{-1}

[H. Hergert *et al.*, PRL 110, 242501 (2013)]



Similarly for *Dy*-SCGF-ADC(3)

[A. Cipollone, C. Barbieri, P. Navratil., PRL 111, 062501 (2013)]

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- Correct location of drip-line

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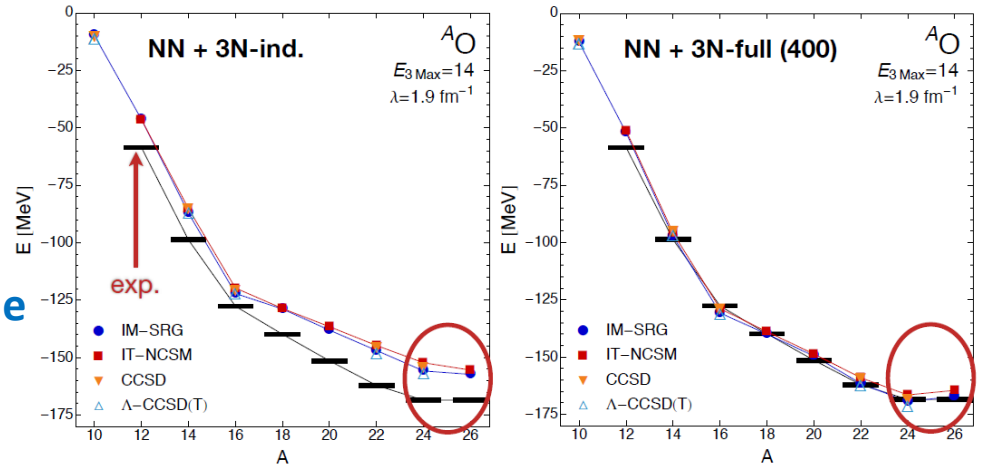

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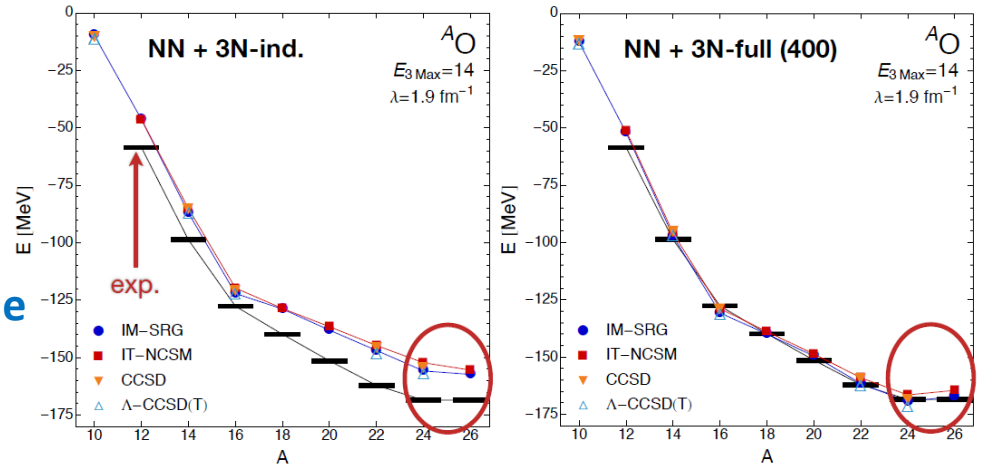
Many-body methods
- Excellent cross-benchmarks!
- Converging expansions to ~1%
- Various systematic errors ~1-2%
  - *Omitted induced AN forces*
  - *Basis truncations (SRG, 3NF, NO2B)*

[H. Hergert *et al.*, PRL 110, 242501 (2013)]



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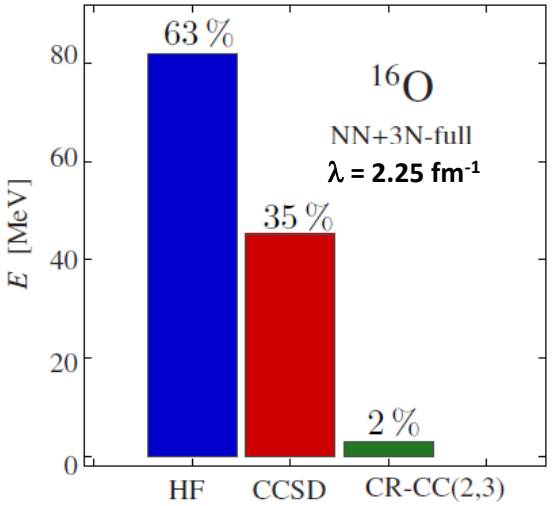
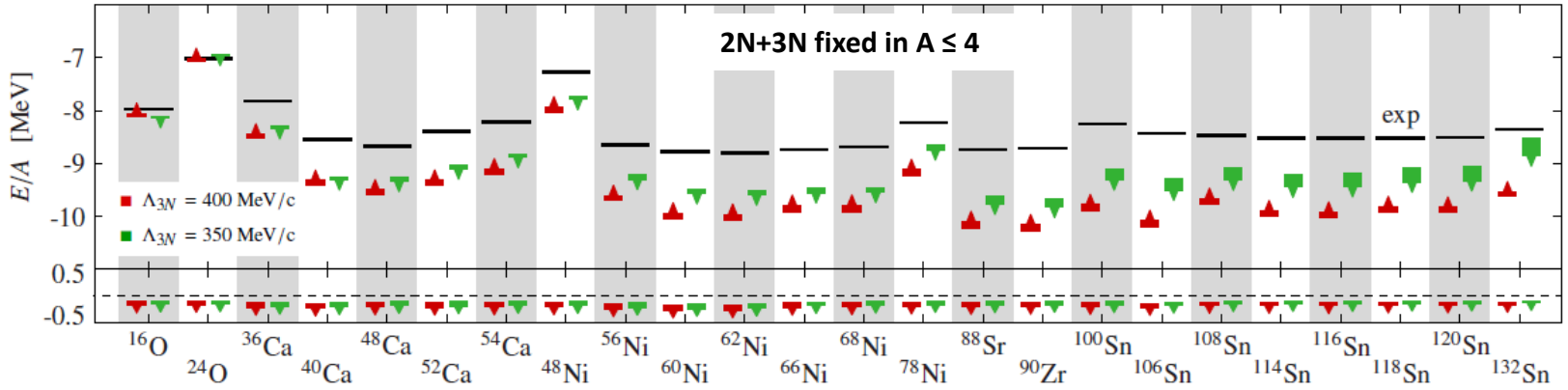


[S. Binder et al., PLB 736 (2014) 119]

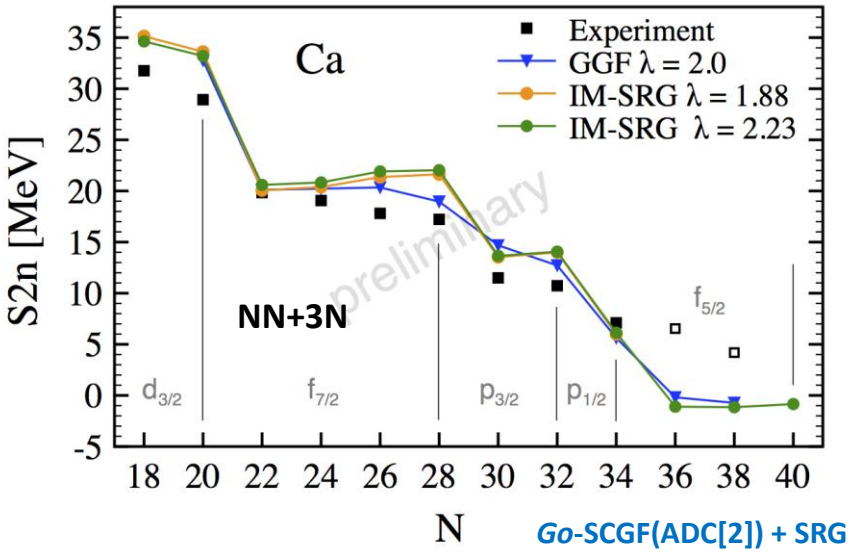
Towards heavier and open-shell nuclei

Binding energy per particle in closed (sub)shell nuclei up to ^{132}Sn [S. Binder *et al.*, PLB 736 (2014) 119]



CR-CC(2,3) + SRG
E_{max} = 12 HO shells
E_{3max} = 18

Two-neutron separation energy along Z=20



[Somà et al., PRC 89, 061301 (2014)]

Go-SCGF(ADC[2]) + SRG
E_{max} = 14 HO shells
E_{3max} = 16

From first generation of calculations

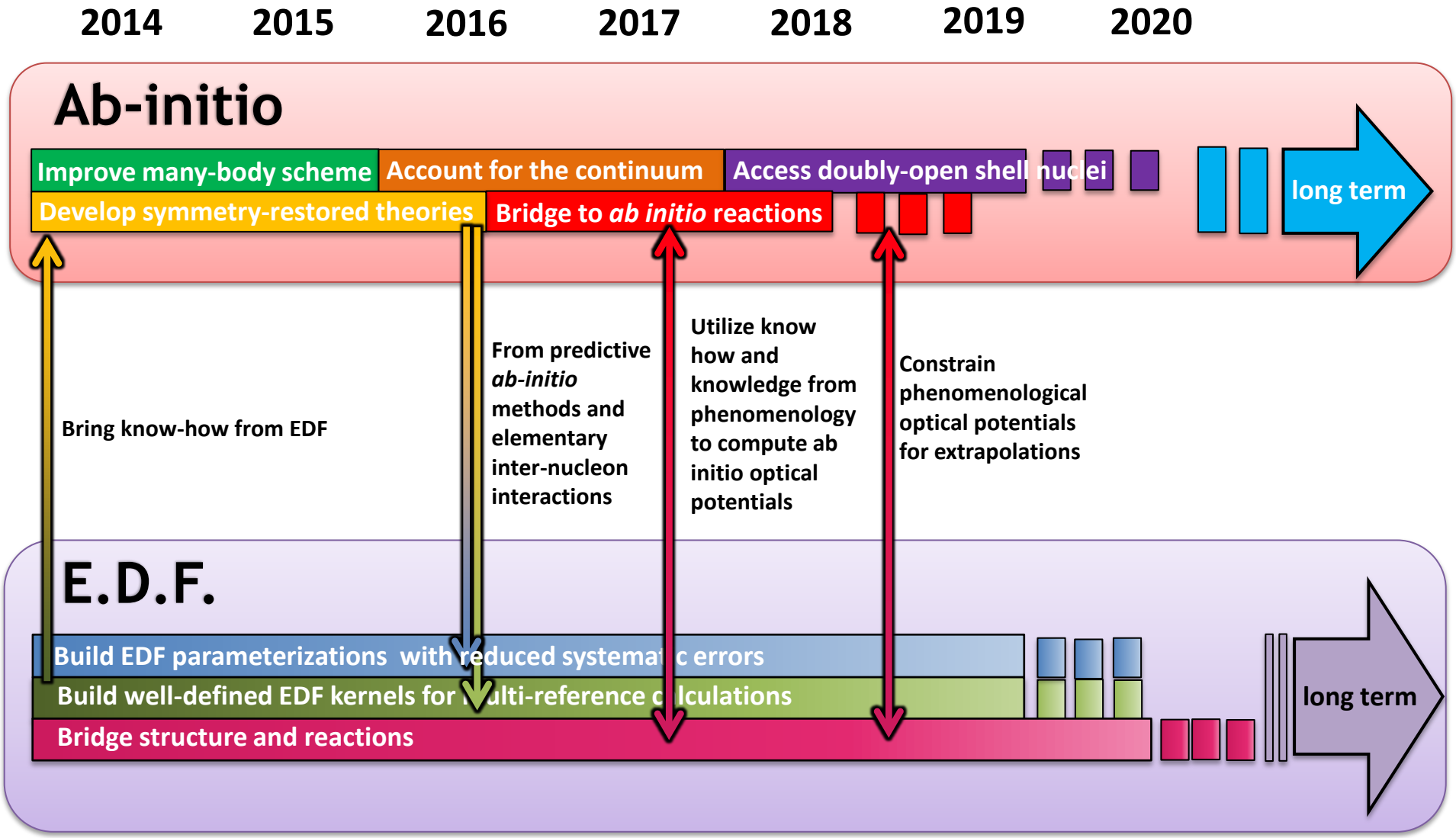
- E/A trend correct from 3NF
- Systematic over binding by ~1MeV
- Charge radii consistently too small by ~20%
- Relative energies satisfactory
- Magic N=20,28 arise from 3NF but exaggerated

Current Chiral 2NF+3NF put to critical test

Saturation? High partial waves? Chiral order? Δ-full?

Improvements needed on many-body/interactions to provide *precise enough pseudo-data*

Looking into the next 10 years



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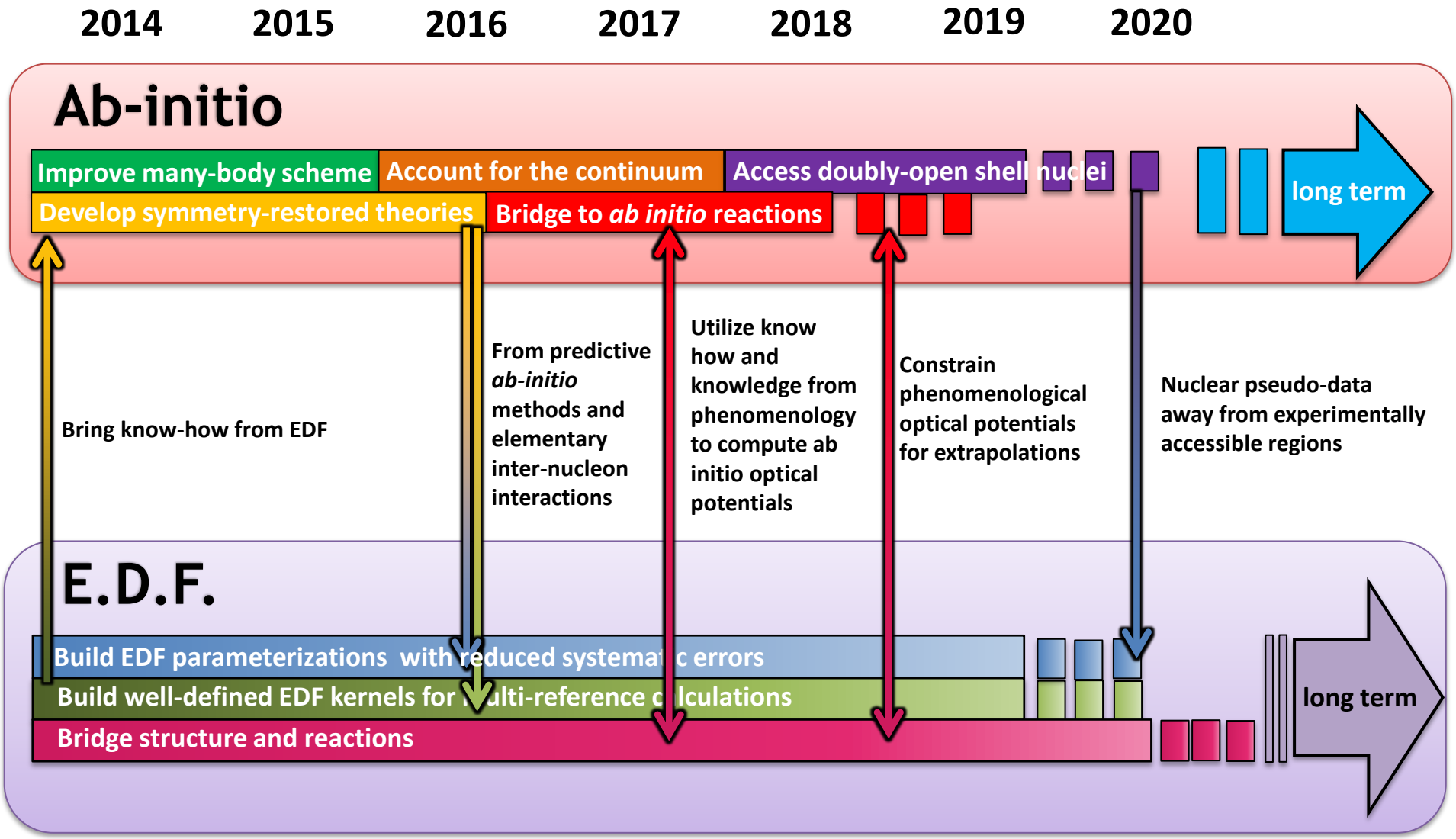

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