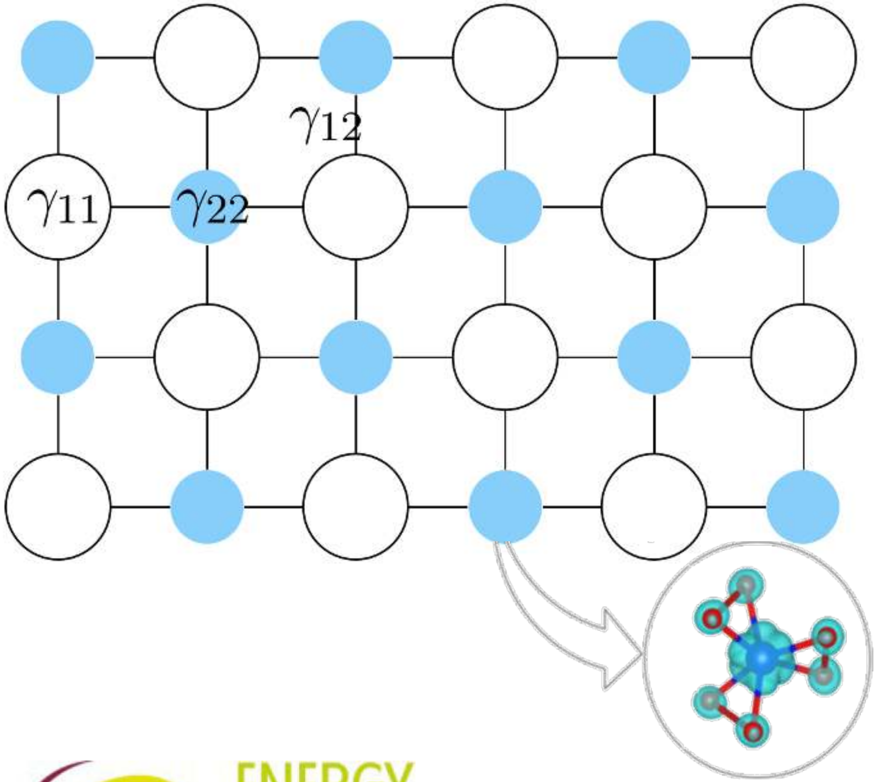
PLAYING WITH THE REDUCED DENSITY-MATRIX: *representability, functionals and embedding*

Matthieu Saubanère

Institut Charles Gerhardt
Montpellier, France



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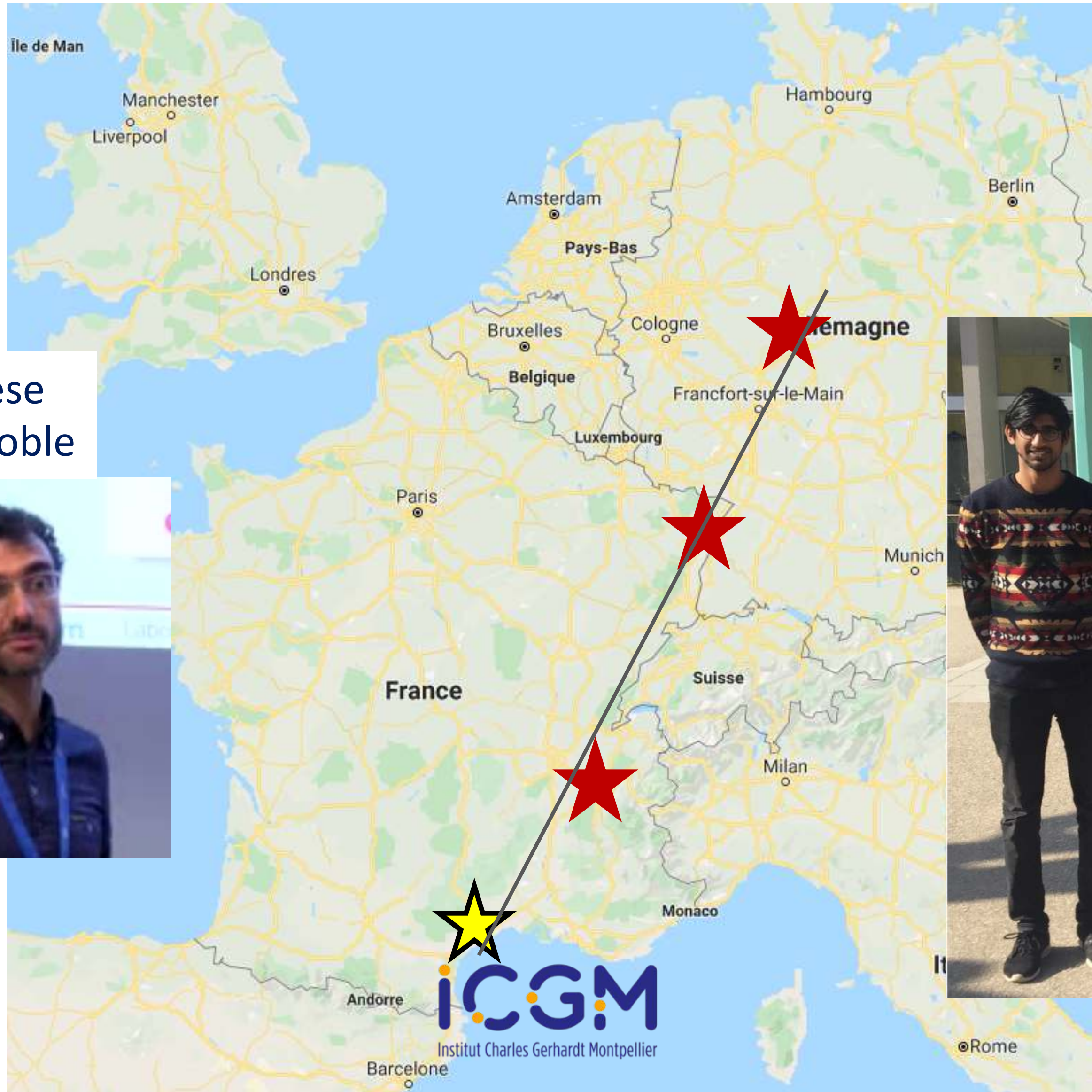
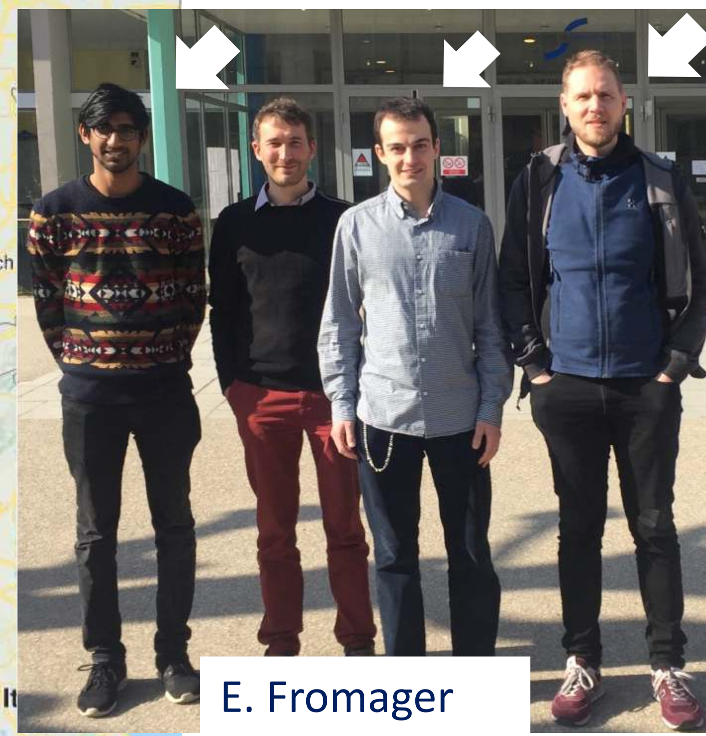
ENERGY RS2E

Collaborative Network



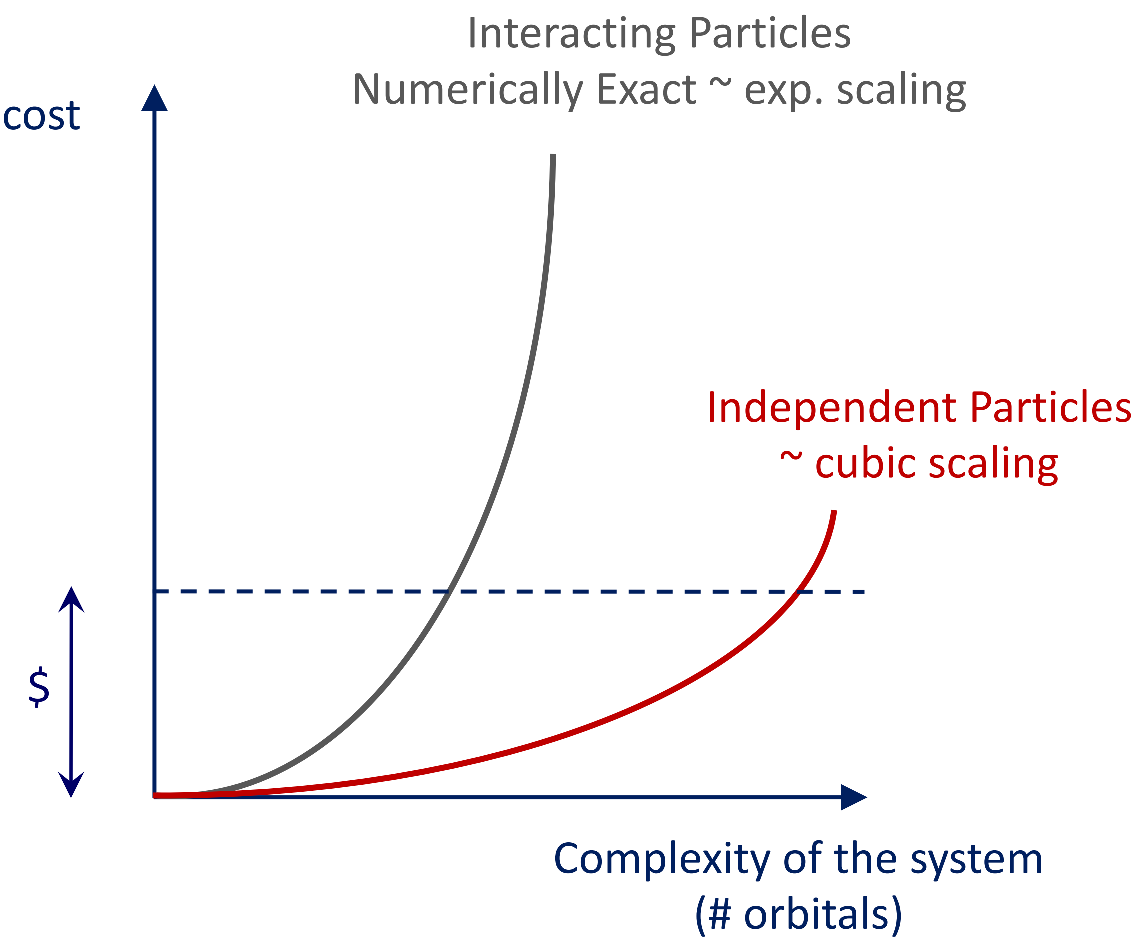
G.M. Pastor
Uni Kassel (DE)

L. Genovese
CEA Grenoble



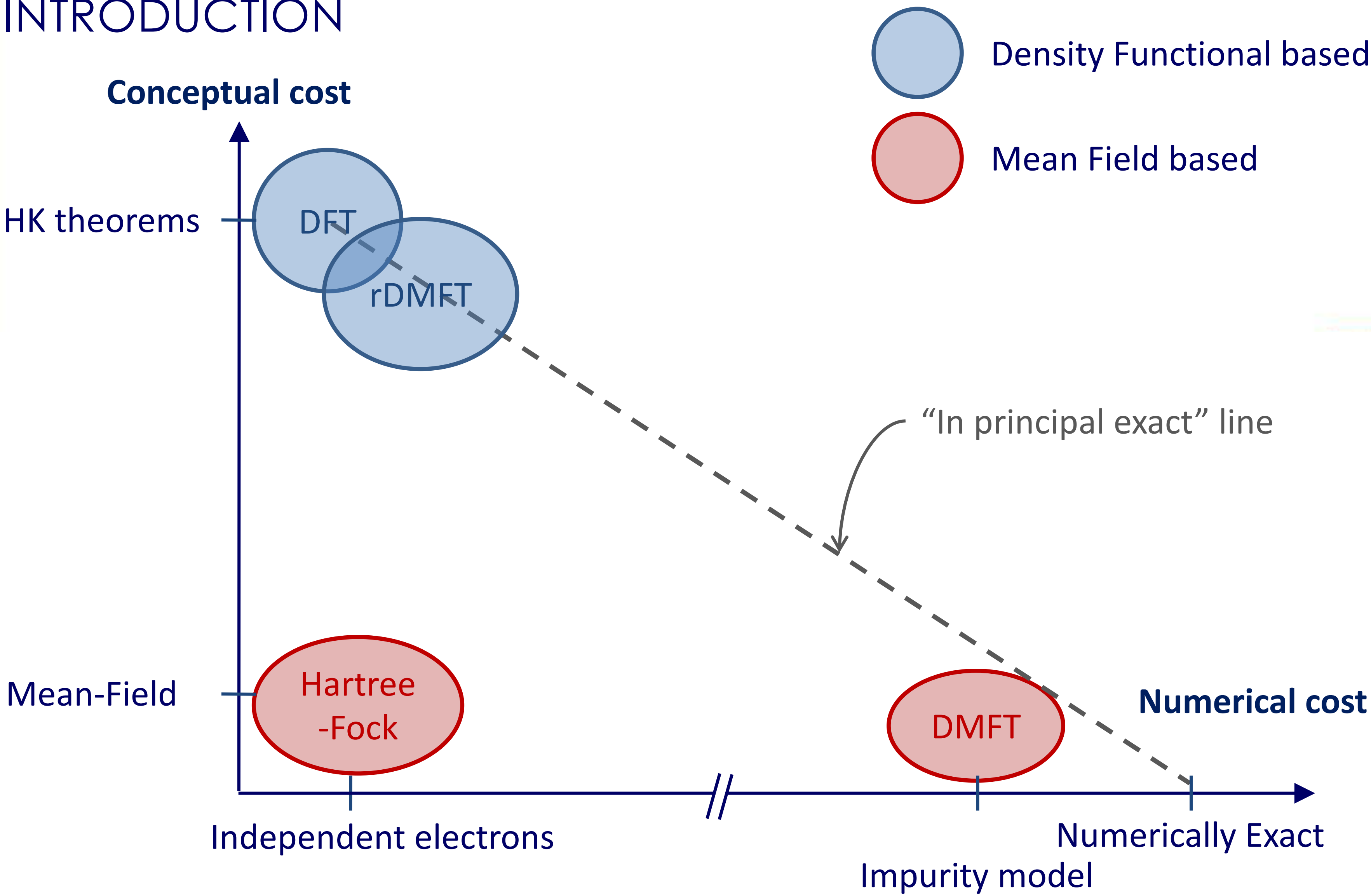
E. Fromager
L. Mazouin
S. Sekaran
Uni Strasbourg

INTRODUCTION



***<u>Challenge</u>*: Close the gap between what we want (accuracy) and what we can pay numerically !**

INTRODUCTION



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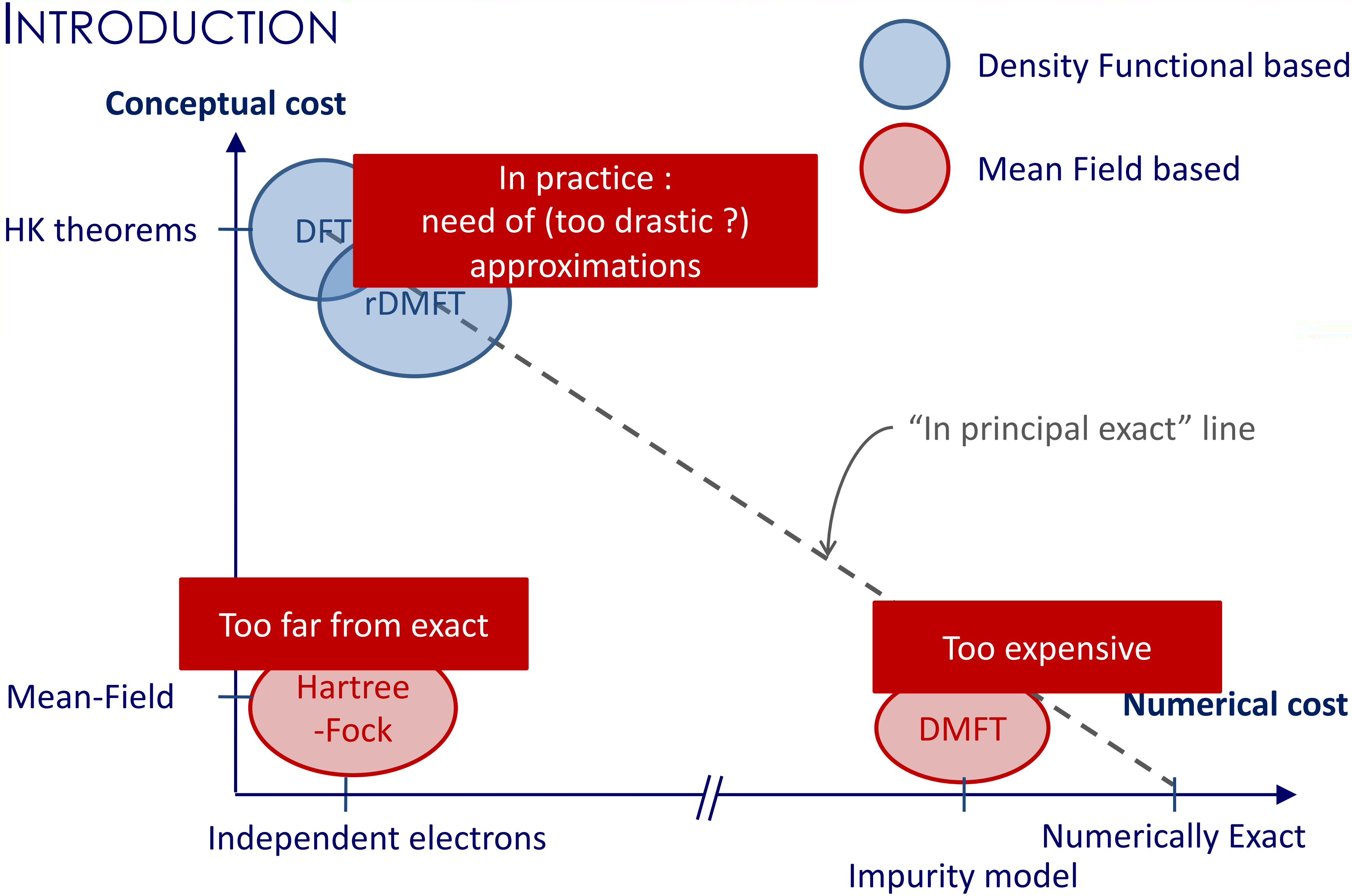

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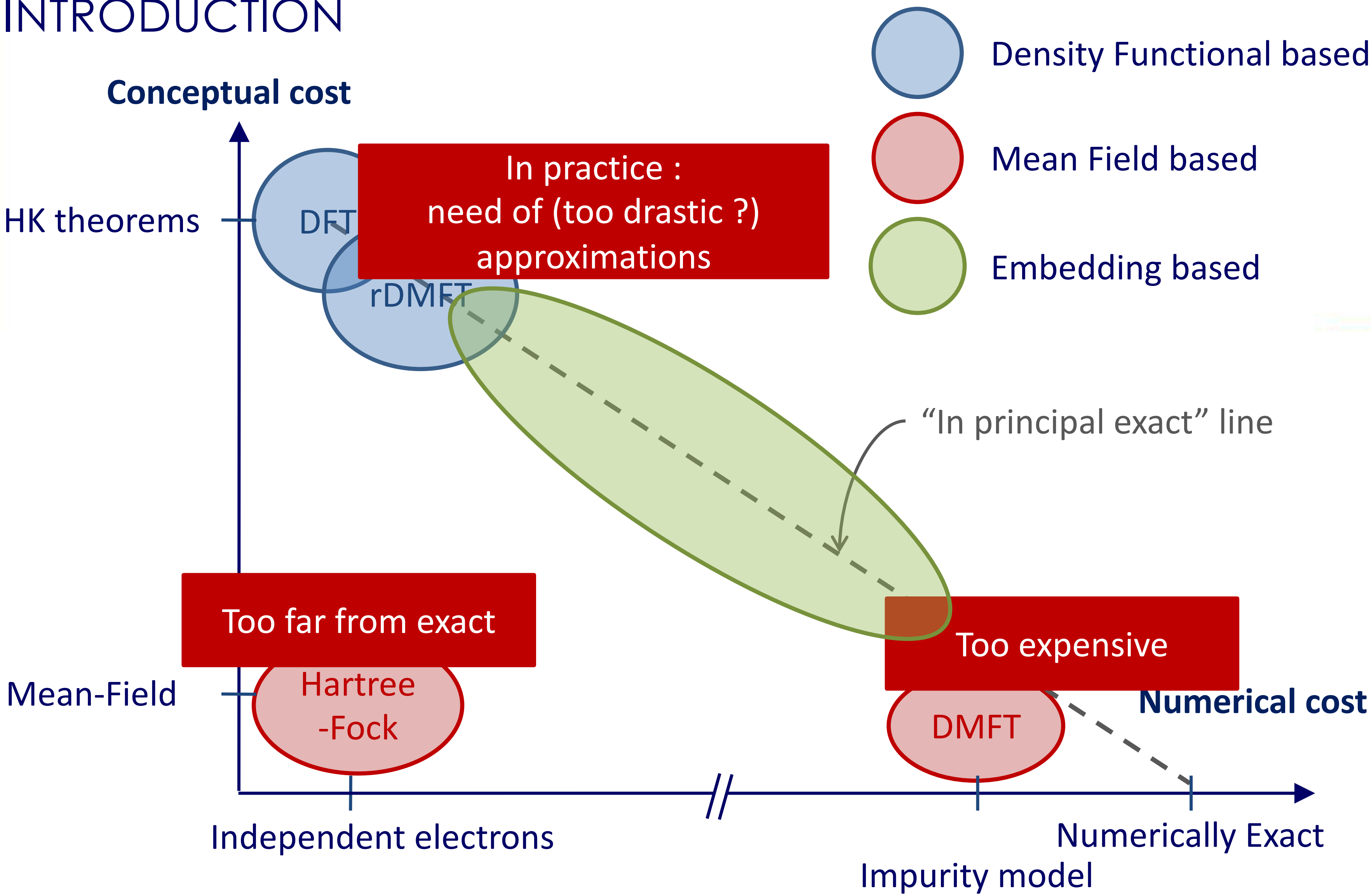

***Challenge*: An "In principle exact", versatile and controllable quality/cost method**

PHILOSOPHY OF EMBEDDING

«*Diviser chacune des difficultés que j'examinerais en autant de parcelles qu'il se pourrait, et qu'il serait requis pour les mieux résoudre*»*
R. Descartes, Discours de la méthode (1637)

*Divide each difficulty into as many parts as is feasible and necessary to resolve it.

Philosophy of embedding

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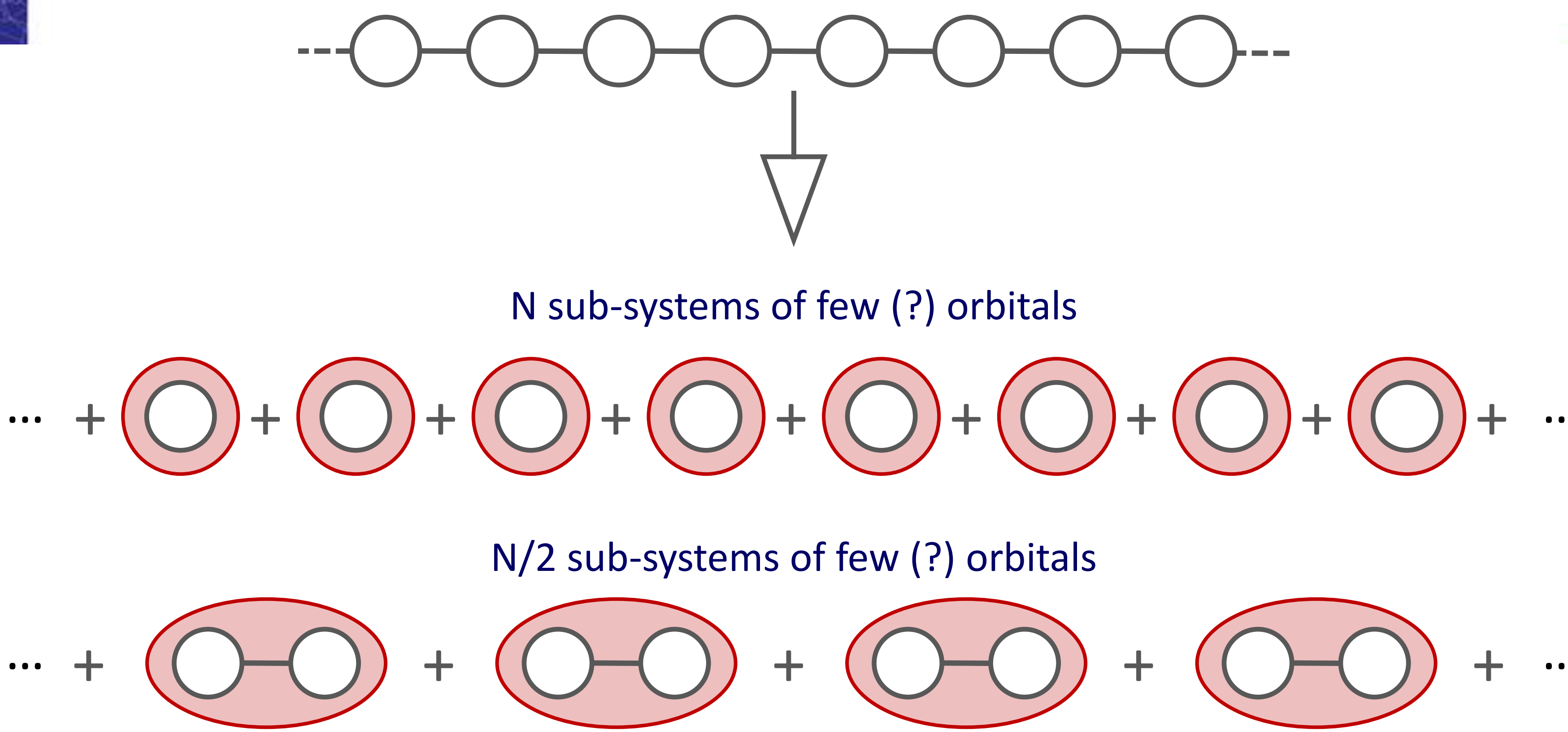
System with N orbitals



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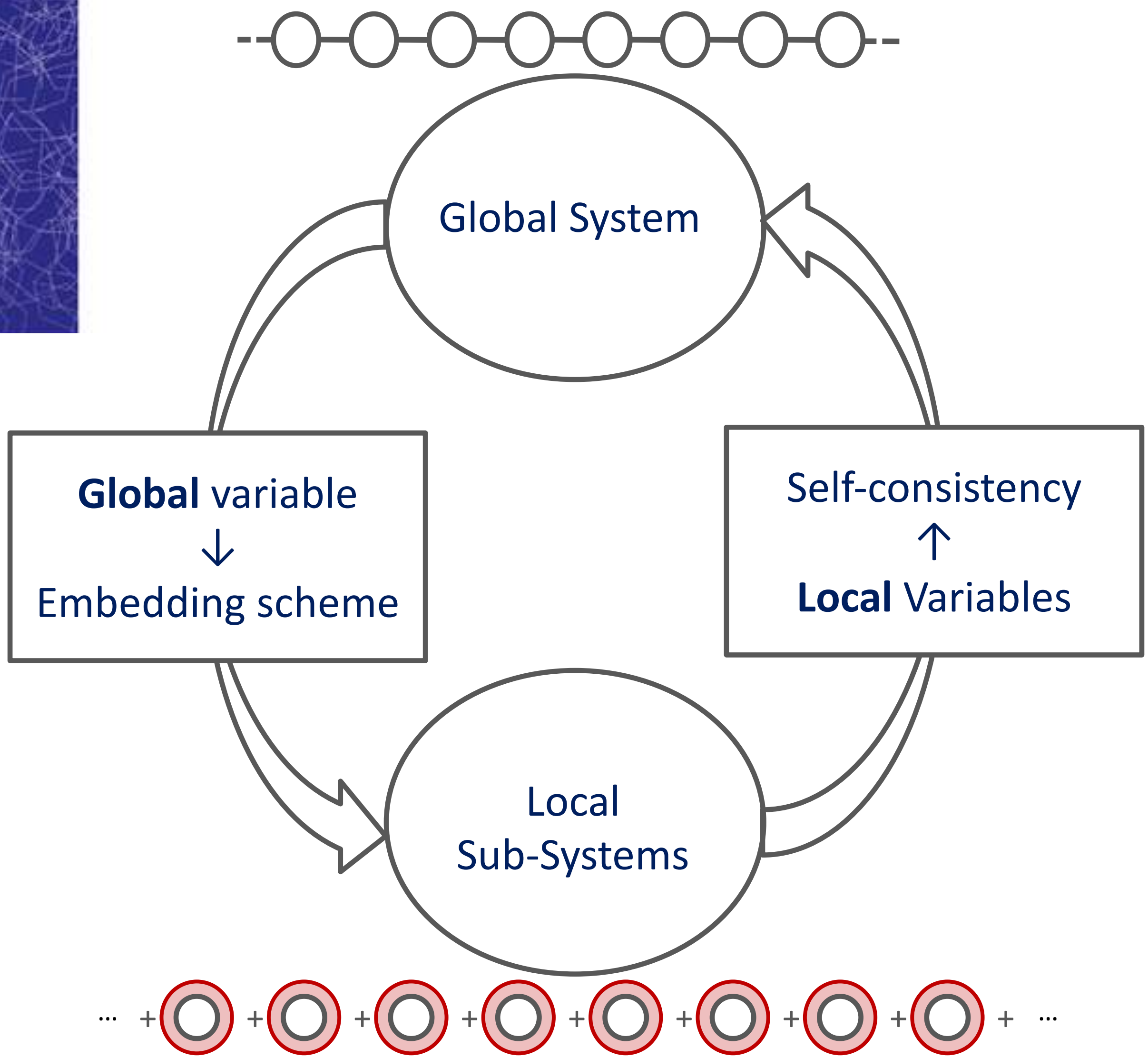
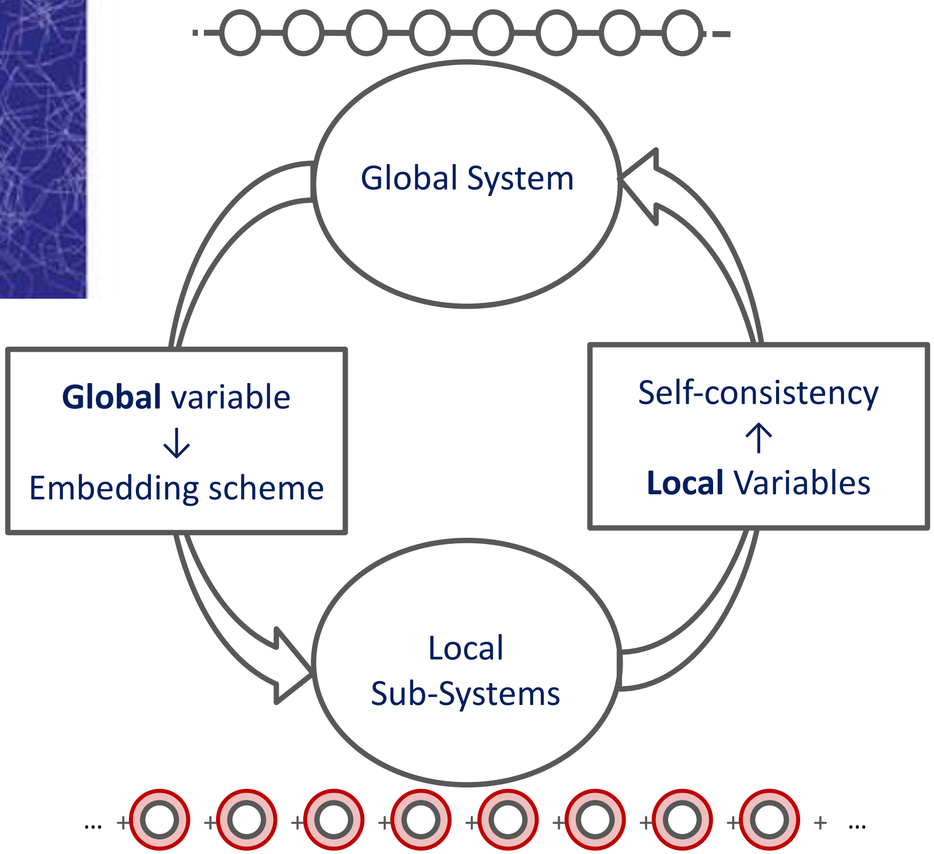
EMBEDDING SELF CONSISTENT APPROACH



EMBEDDING SELF-CONSISTENT APPROACH



Embedding scheme (Global variable):

Wave-Function → Schmidt transformation

DMET[1] with Slater-determinant only

PSOET[3] with KS wave-function

Density → ?

Density-matrix → ?

Green's function → Luttinger-Ward func.

SEET[2]

[1] G. Knizia, G.K.L. Chan, PRL 109, 186404 (2012)

[2] T. Nhuyen Lan, A. Kananeka, D. Zdig, JCP 143, 241102 (2015)

[3] B. Senjean, PRB 100, 035136 (2019)

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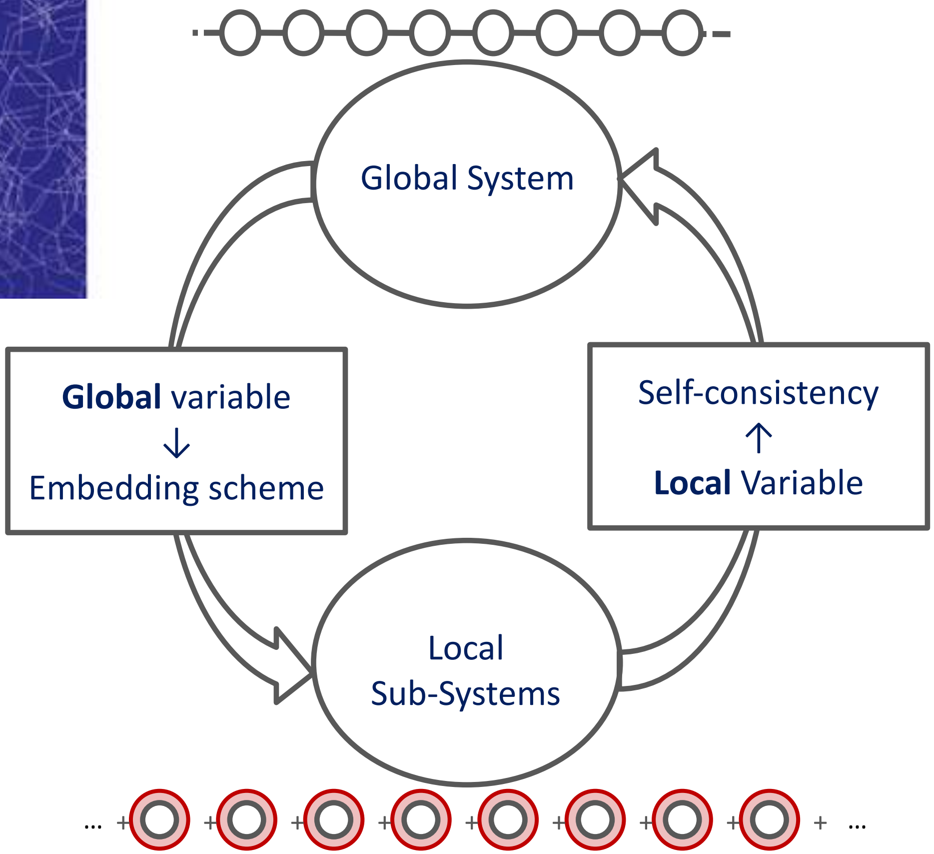

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Self-consistency (Local variable):

Density → Kohn-Sham v_{xc}
PSOET
Density-matrix → Matching local and global
DMET
Self-Energy → Dyson Eq.
SEET

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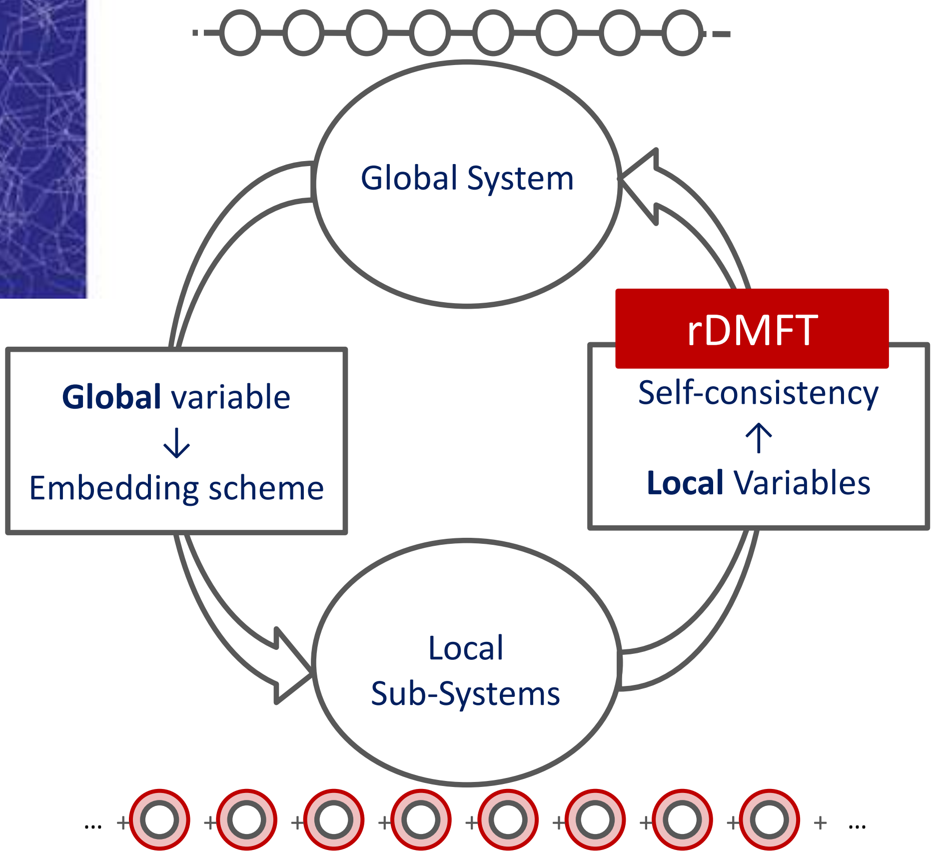
Embedding self-consistent approach



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Full density-matrix self-consistent scheme

THE REPRESENTABILITY PROBLEM

Reduced Density Matrix Functional Theory (rDMFT)

- Non-idempotent matrices not representable by a non-interacting system !
- No one-to-one relation between non-local potential and density matrix !

→ **No Kohn-Sham type scheme available**

[1] M. Saubanère, M.B. Lepetit, G.M Pastor, PRB 94, 045102 (2016)

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1) Non-interacting electrons systems at (fictive) finite temperature ![1]

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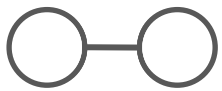
Density-matrix (linear) Interpolation Ansatz (DIVA)

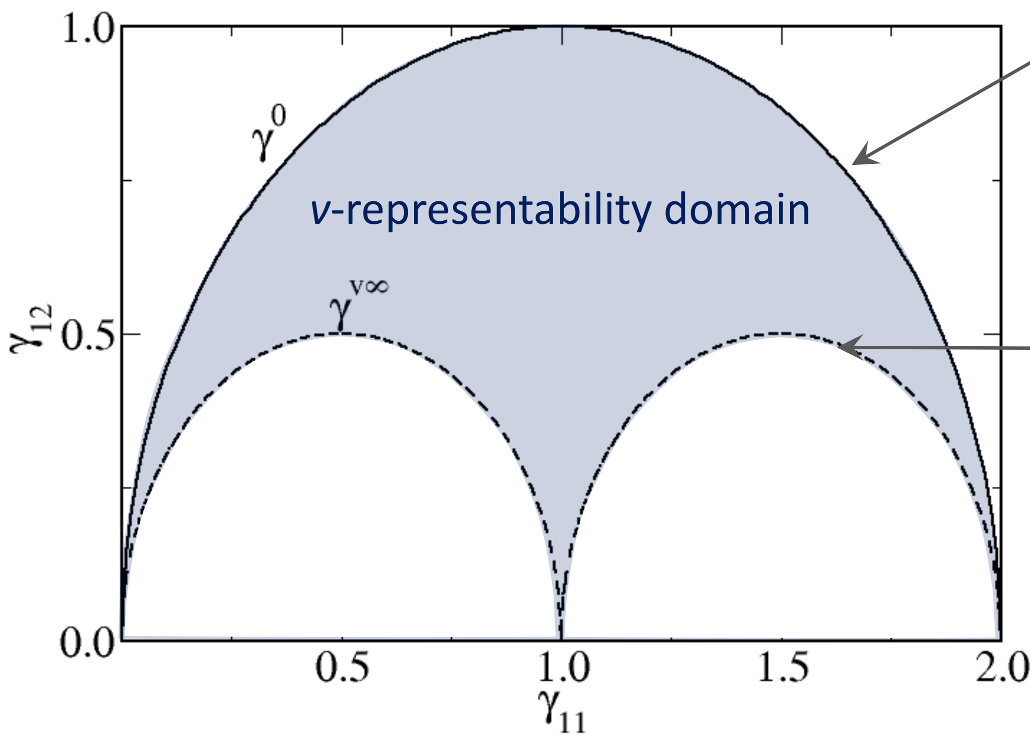
Collaboration : S. Sekaran, L. Mazouin & E. Fromager (Univ. Strasbourg)

Example : the half-band filled Hubbard Dimmer



Site 1 v_1

Site 2 v_2



Non-interacting upper bond
Trivial !

Strongly-interacting lower bond
Non-trivial

DENSITY-MATRIX (LINEAR) INTERPOLATION ANSATZ (DIVA)

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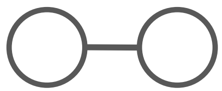

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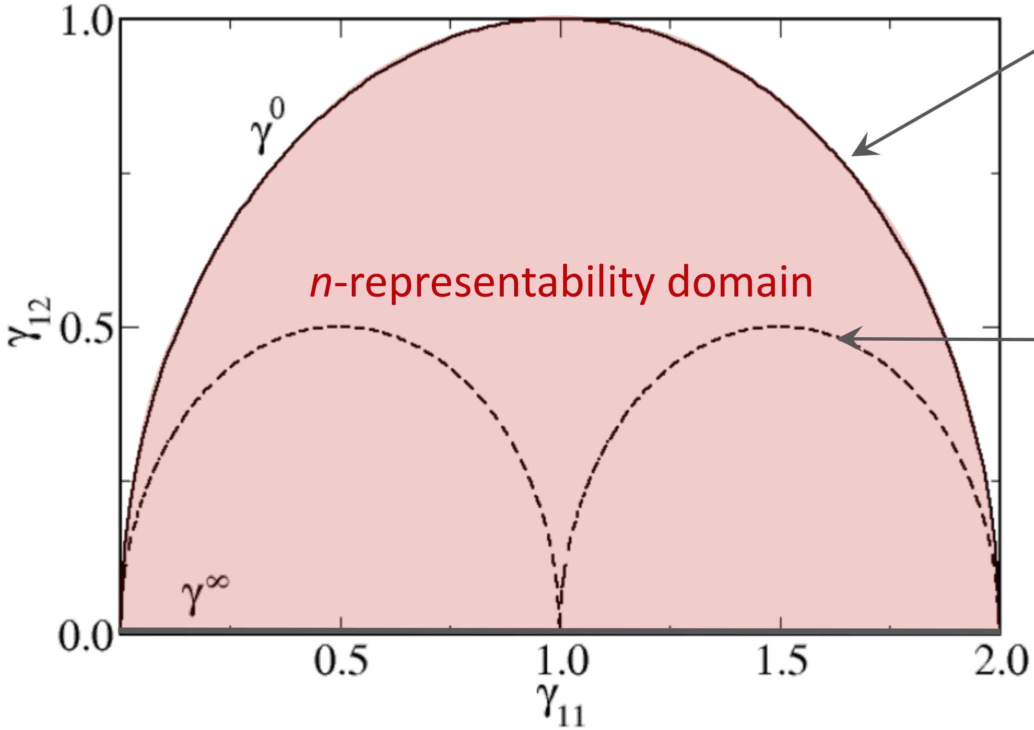

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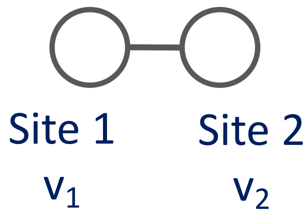

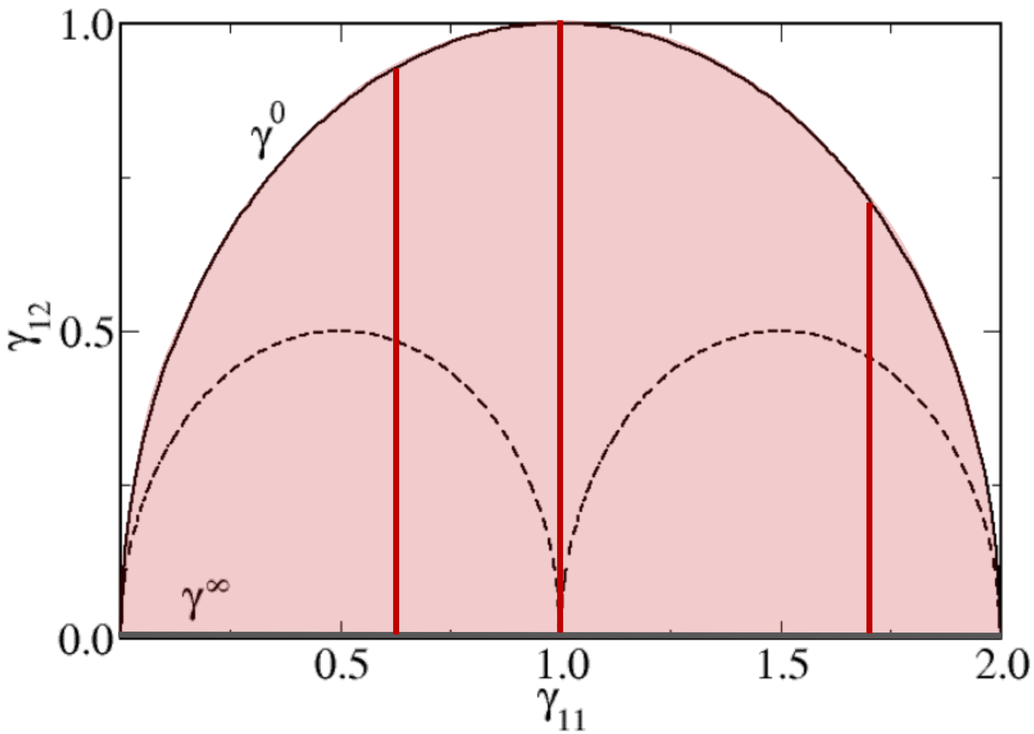

Idea :
Span the *n*-representability domain following the density-constant lines.

$$\gamma[\underline{\rho},\{z_{ij}\}] = \sum_{i<j,\sigma} \underline{\gamma}^0[\underline{\rho}] - z_{ij}\,\mathbb{1}_{ij}\left(\underline{\gamma}^0[\underline{\rho}] - \gamma^\infty[\underline{\rho}]\right)\mathbb{1}_{ij}$$

$$= \begin{pmatrix} \rho_1 & (1-z_{12})\gamma^0_{12} & (1-z_{13})\gamma^0_{13} & \cdots \\ (1-z_{12})\gamma^0_{21} & \rho_2 & (1-z_{23})\gamma^0_{23} & \cdots \\ (1-z_{13})\gamma^0_{31} & (1-z_{23})\gamma^0_{32} & \rho_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

DIVA Variational scheme

Collaboration : S. Sekaran, L. Mazouin & E. Fromager (Univ. Strasbourg)

$$E^{\text{DIVA}}[\underline{\rho}, \underline{z}] = T^0[\underline{\rho}] + (\underline{V}_{\text{ext}} + \underline{V}_H) \cdot \underline{\rho} + F[\underline{\rho}, \underline{z}]$$

$$F[\underline{\rho}, \underline{z}] = T[\underline{\rho}, \underline{z}] - T^0[\underline{\rho}] + W[\underline{\rho}, \underline{z}] = -\underline{z}T^0[\underline{\rho}] + W[\underline{\rho}, \underline{z}]$$

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Minimization process :

1

$$\delta\underline{\rho}\left\{\underline{V}_{\mathrm{ext}} + \underline{V}_{\mathrm{H}} + \frac{T^0[\underline{\rho}]}{\delta\underline{\rho}} + \left.\frac{\delta F[\underline{\rho}, \underline{z}]}{\delta\underline{\rho}}\right|_{z}\right\} = 0$$

$$\left\{\underline{V}_{\mathrm{ext}} + \underline{V}_{\mathrm{H}} + \underline{T}^0 + \underline{V}_{xc}|_{\underline{z}}\right\}|\Psi^{\mathrm{KS}}\rangle = \varepsilon|\Psi^{\mathrm{KS}}\rangle \qquad \underline{V}_{xc}|_{\underline{z}} = \left.\frac{\delta F[\underline{\rho}, \underline{z}]}{\delta\underline{\rho}}\right|_{\underline{z}}$$

$\rightarrow$ Kohn-Sham like equation !

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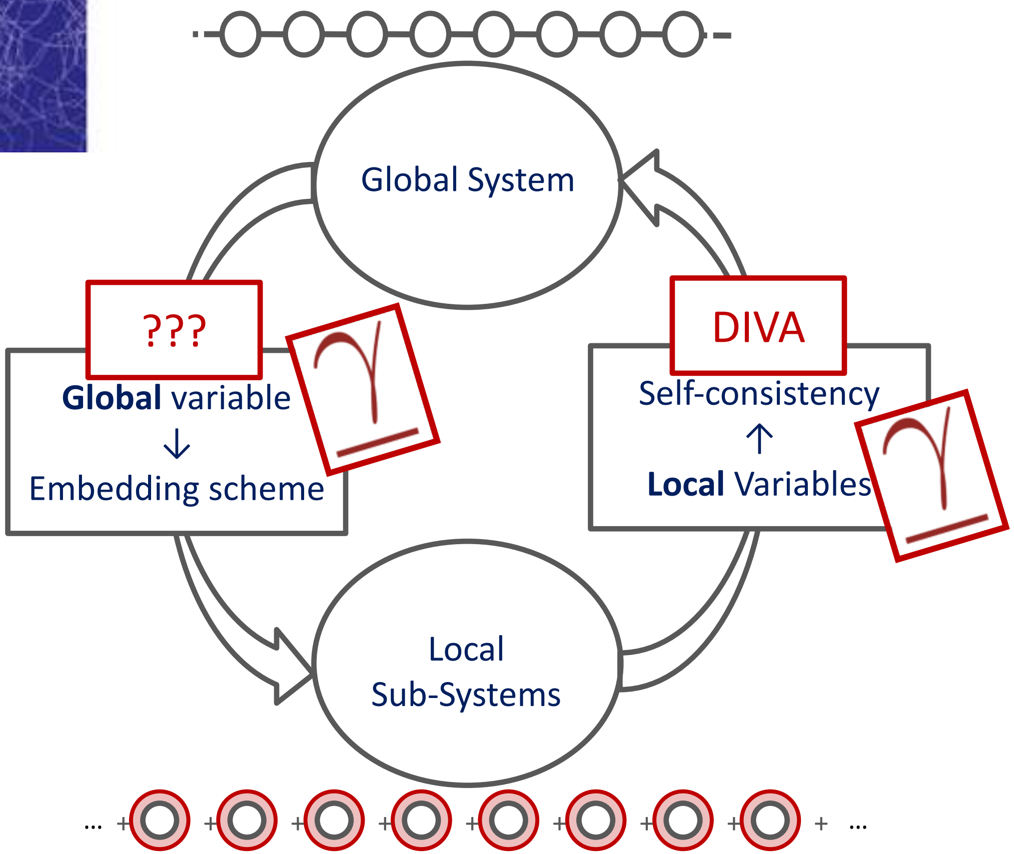
2

$$\delta\underline{z}\left\{-T^0[\underline{\rho}] + \left.\frac{\delta W[\underline{\rho}, \underline{z}]}{\delta\underline{z}}\right|_{\underline{\rho}}\right\} = 0 \qquad 0 \leq z \leq 1$$

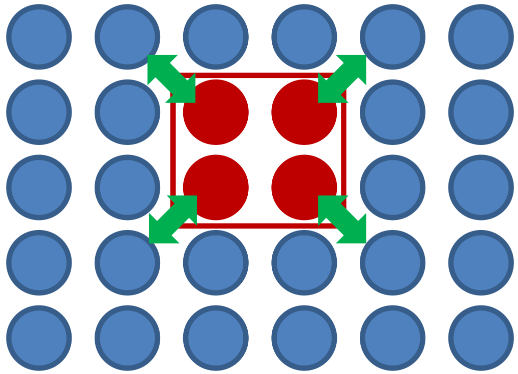
Back to embedding



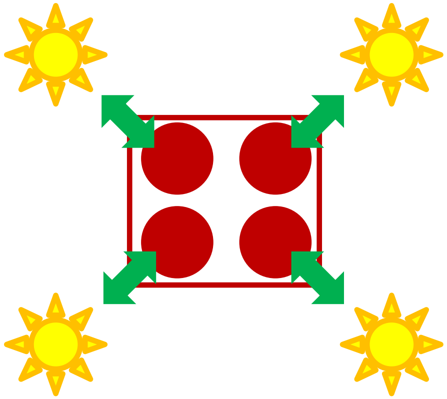
How to proceed the embedding with The density-matrix ?

Open or Closed sub-systems ?

E.g. : The Hubbard model:



1 Open system/Exact factorization:



Collaboration : G.M. Pastor (Univ. Kassel, DE)

- Use an effective bosonic field
- Schrieffer-Wolf transformation

Thesis (2011) https://kobra.uni-kassel.de/handle/123456789/2012012540416

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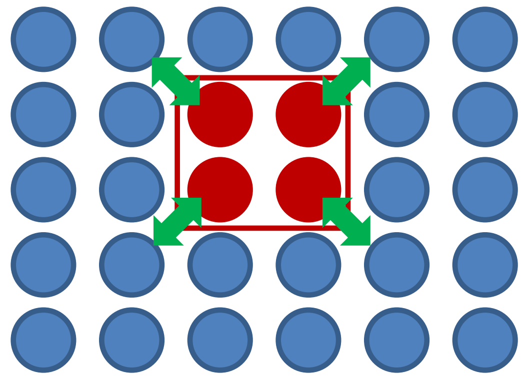

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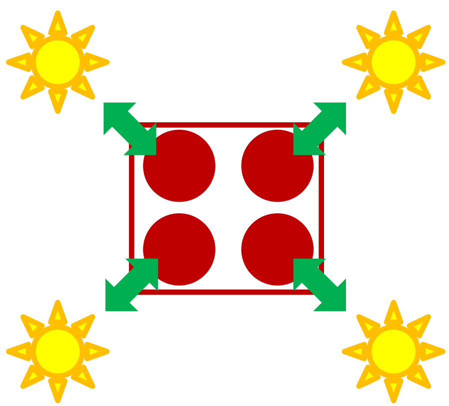
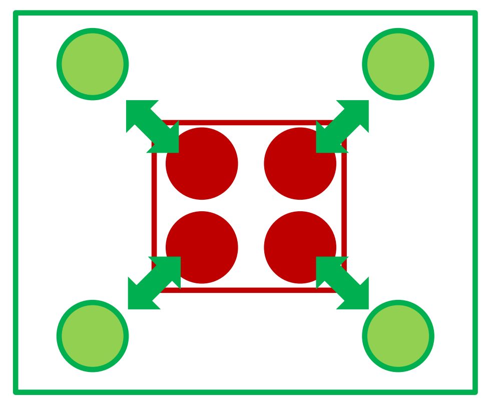


2 Closed system Adding effective orbitals:



E.g. DMET

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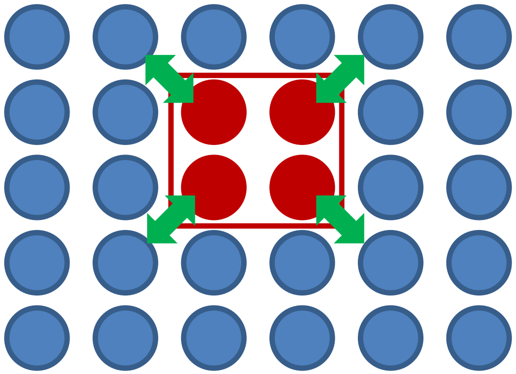

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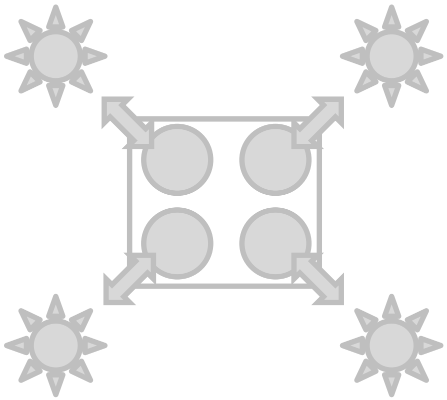

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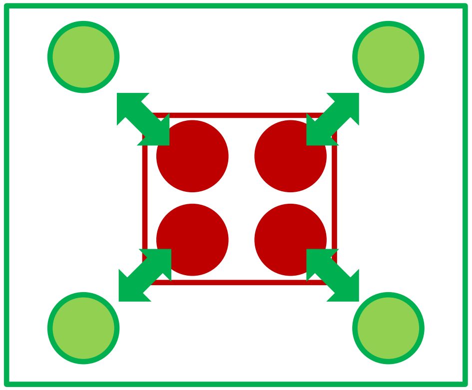
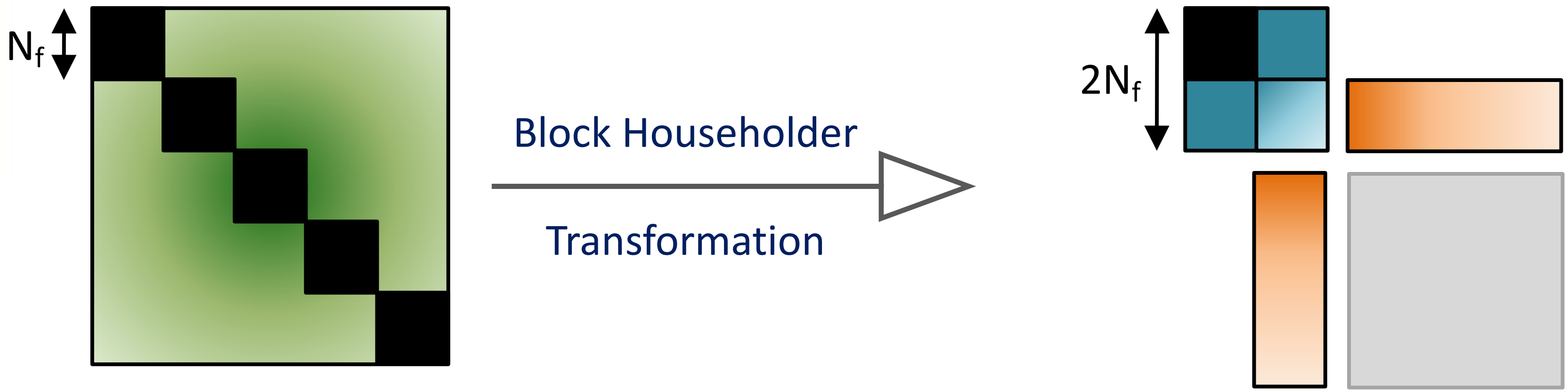


Collaboration : S. Sekaran, L. Mazouin & E. Fromager (Univ. Strasbourg)

Householder Transformation

Global density matrix

For each fragment : a reduced System



■ Fragments

■ Effective zone

■ Effective zone with charge leaks

■ Energy leaks

■ Frozen inactive bath

✓ Equivalent to a Schmidt transformation for non-interacting systems

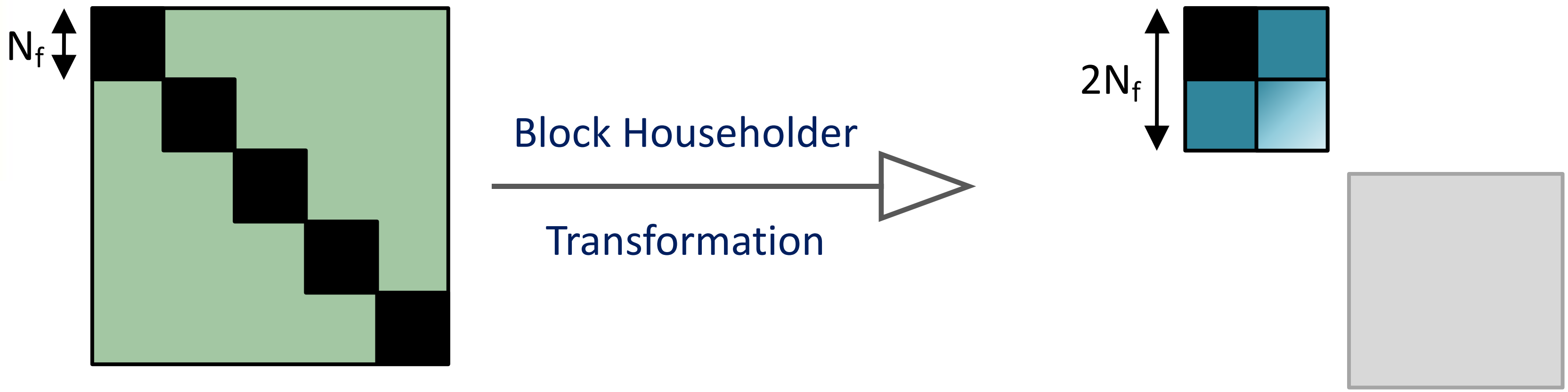
✓ Leads to quasi-unconnected sub-systems

Collaboration : S. Sekaran, L. Mazouin & E. Fromager (Univ. Strasbourg)

DIVA + HOUSEHOLDER TRANSFORMATION

DIVA Global density matrix

For each fragment : a reduced System



- Fragments
- $(1 - z)$ renormalized zone
- Effective zone
- Effective zone with charge leaks
- Frozen inactive bath

✓ **Leads to a fully unconnected open sub-system of size $2N_f$**

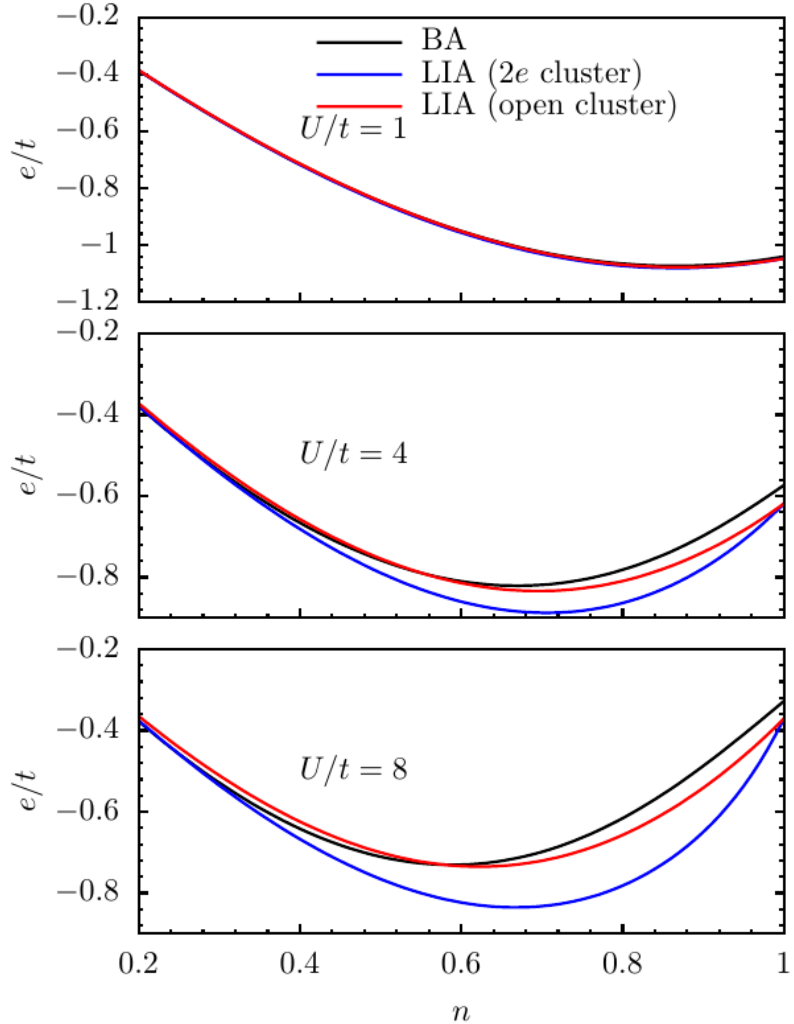
✓ **For each sub-systems : compute** $W[\underline{\rho}, \underline{z}]$

✓ **Exact for $N_f = N/2$**

<u>Collaboration :</u> S. Sekaran, L. Mazouin & E. Fromager (Univ. Strasbourg)

PRELIMINARY RESULTS: SINGLE SITE FRAGMENT

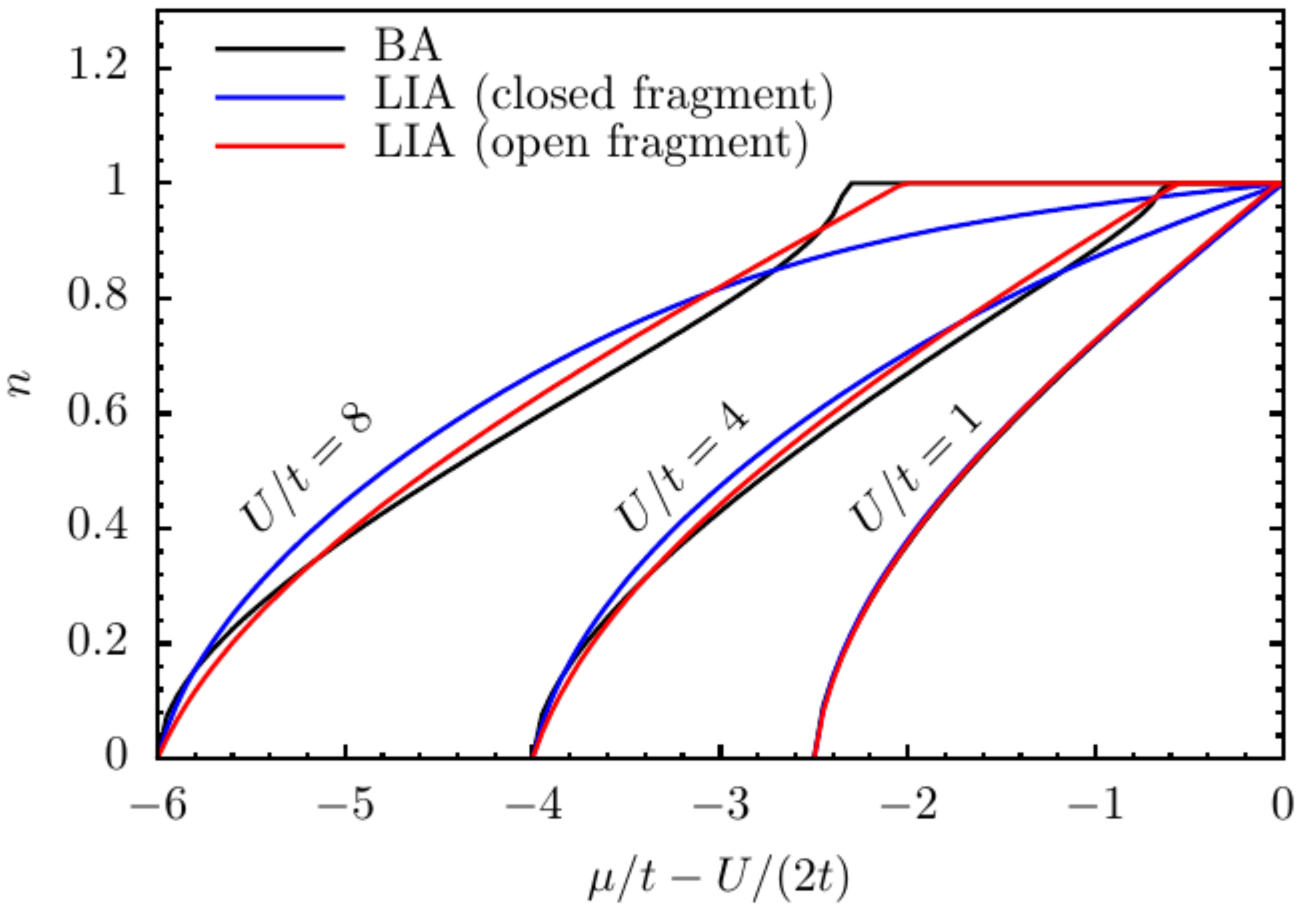
1D periodic Hubbard chain : per site energy



Collaboration : S. Sekaran, L. Mazouin & E. Fromager (Univ. Strasbourg)

PRELIMINARY RESULTS: SINGLE SITE FRAGMENT

1D periodic Hubbard chain : chemical potential



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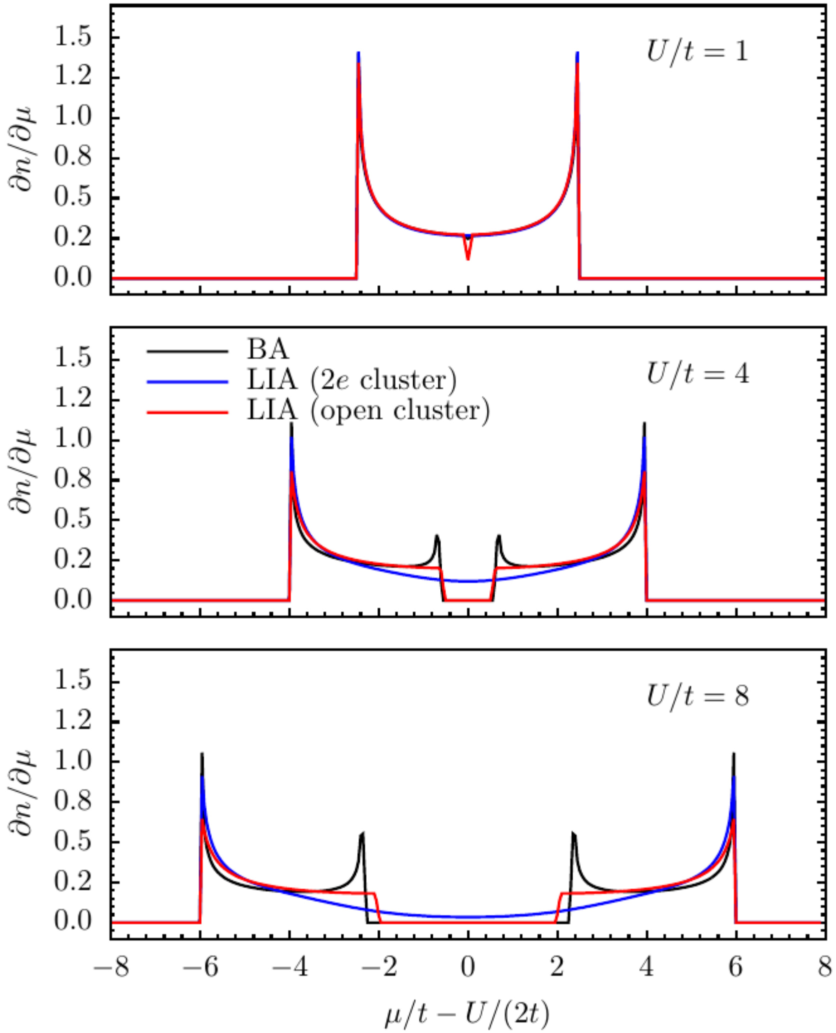
PRELIMINARY RESULTS: SINGLE SITE FRAGMENT

1D periodic Hubbard chain : charge susceptibility



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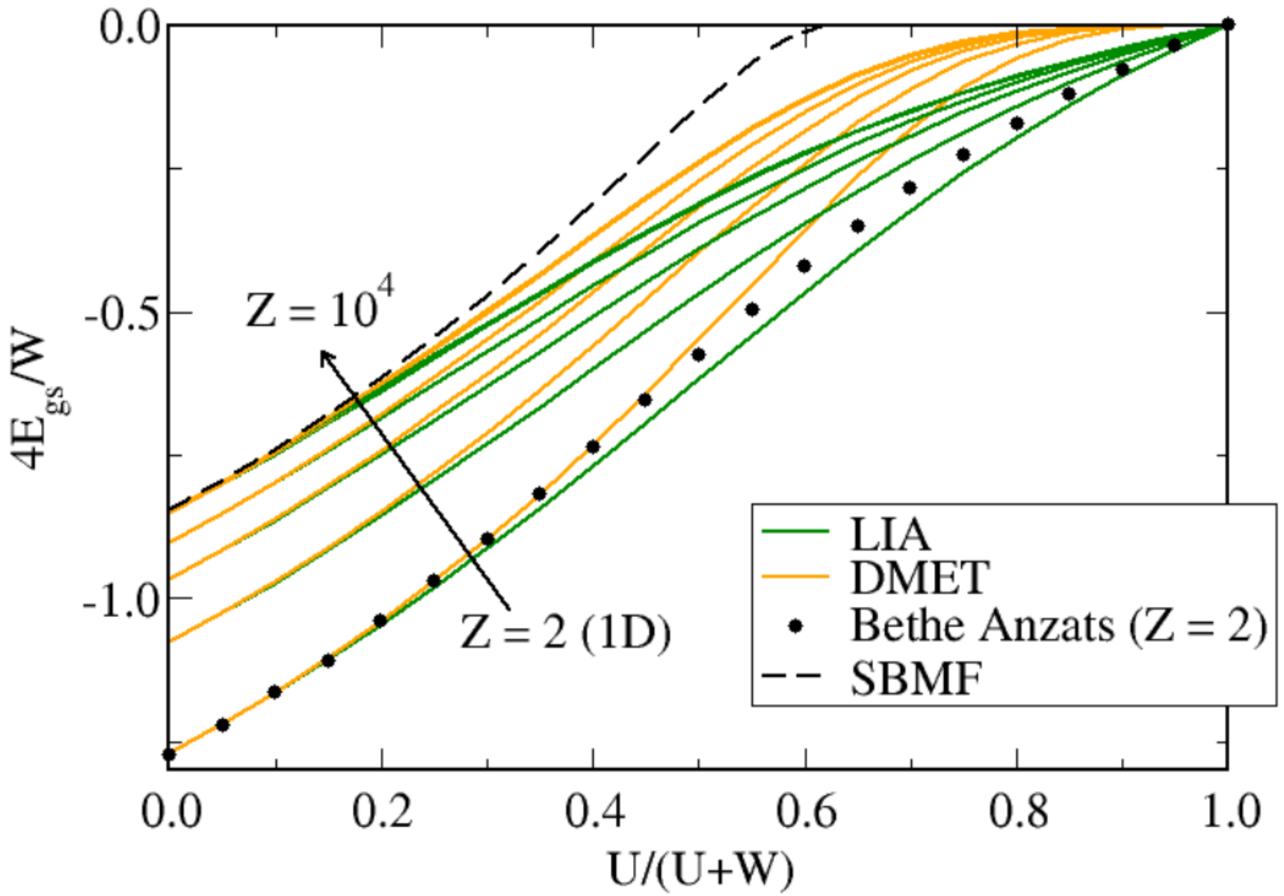
PRELIMINARY RESULTS: SINGLE SITE FRAGMENT

Toward higher dimensions : Bethe Lattices



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PERSPECTIVES

ACKNOWLEDGMENTS

JCJC-DESCARTES project

Partners : E. Fromager (Uni. Strasbourg)
B. Lasorne (ICGM)

MACMA project
Aàp science de base pour l'énergie

Partner: L. Genovese (CEA, Grenoble)