SIESTA webinar

MAX webinar series

Next one in the MAX Webinar series

Today's MAX Webinar on SIESTA

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MAX DRIVING THE EXASCALE TRANSITION

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SIESTA

Overview

ascale", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-
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The SIESTA code

SIESTA is DFT code, density-functional theory

(like many others in many ways)

Aim from inception: EFFICIENCY

Pioneer LINEAR-SCALING DFT code (or Order-N, O(N))

meaning: computational cost (CPU & memory) scaling linearly with number of atoms

The SIESTA code

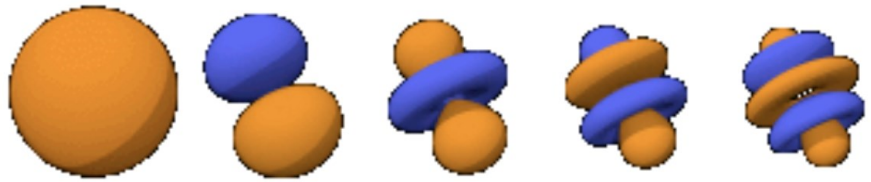
Based on ATOMIC-LIKE ORBITALS as basis sets, LCAO

(as in traditional quantum chemistry)

$$\phi_{Ilmn}(\mathbf{r_I}) = R_{Iln}(r)Y_{lm}(\hat{\mathbf{r}}_I)$$

Disadvantage: Convergence is more laborious

(no automatic way, responsibility on the user)



Advantage: Less basis functions needed => Efficiency

(rule of thumb, 3-5 functions per electron vs ~ 100 plane waves per electron)

Many other codes (DMOL, FHI-AIMS, CP2K, Gaussian, ADF, Qchem, NWChem, Turbomol, …)

The SIESTA *method*

Finite support basis functions

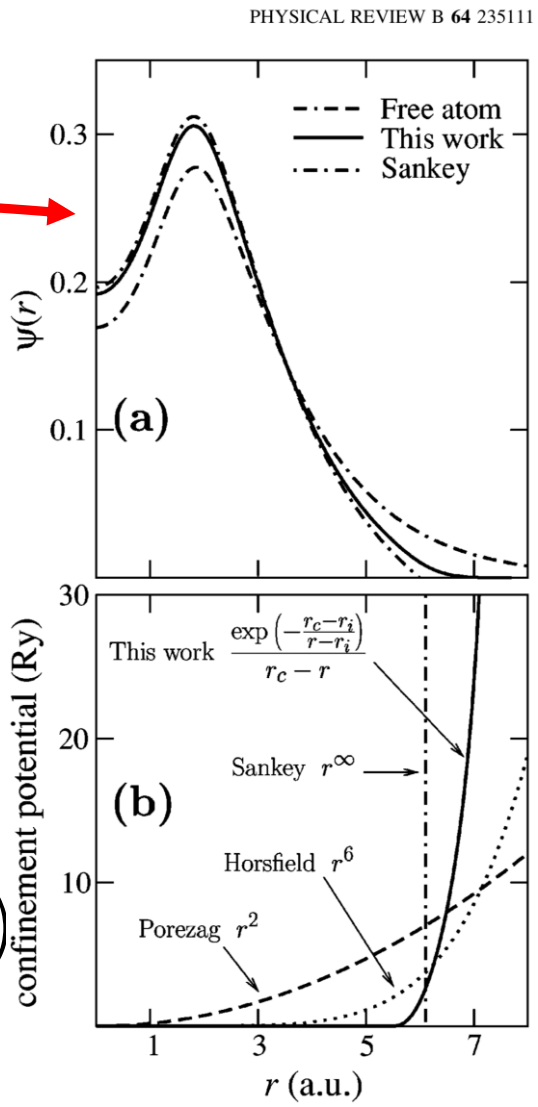
$$\phi_{Ilmn}(\mathbf{r_I}) = R_{Iln}(r) Y_{lm}(\hat{\mathbf{r}}_I)$$

=> Strictly sparse matrices (no matrix cutting)

Following Sankey and Niklewsky PRB 40, 3979 (1989)

As long as Finite-support and (Radial * Spherical Harmonic)

As many as wanted, wherever wanted, of any radial shape

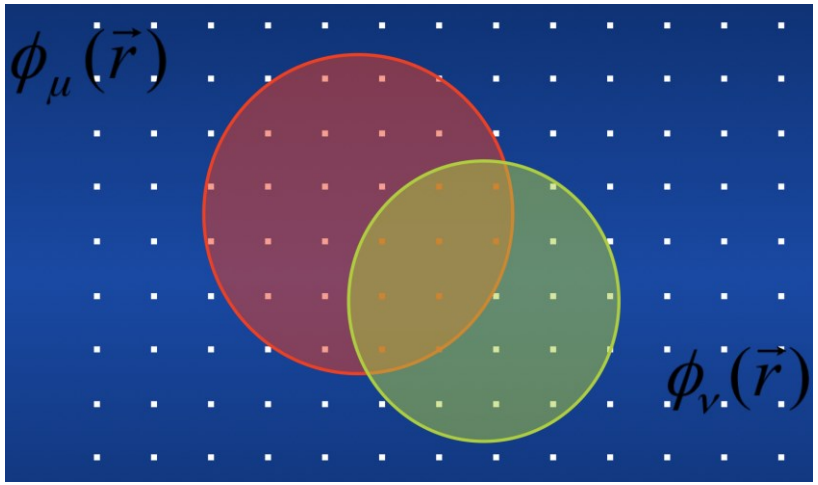


The SIESTA *method*

(1) ρ --> H : Computation of Hamiltonian and Overlap matrices:

FINITE SUPPORT + DISCRETISATION OF SPACE

(Pseudopotentials for core electrons)



$\Rightarrow$ Linear-scaling calculation of H and S matrices

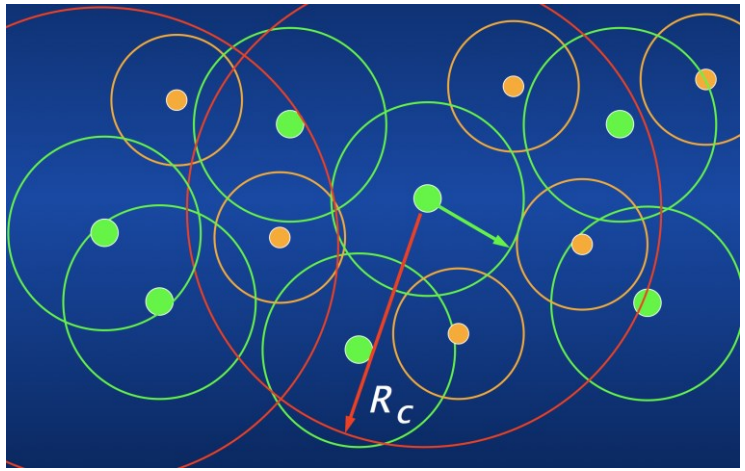
Ordejon, Artacho, Soler & PRB-RC 1996

Always linear scaling

Key efficiency

The SIESTA code

(2) *H* --> *E*, ρ : Solving the Kohn-Sham eigenproblem



- Originally: linear-scaling solvers
  based on localisation of solutions

- Now: Various solver options with various scalings, from *O(N)* to $O(N^3)$
  (diagonalisation, localised *O(N)* solvers, PEXSI, etc

(a talk on these later)

Evolution of the SIESTA code

From early on: Usual DFT offer (various GGAs, first-principles MD, etc)

(see J. M. Soler et al, JPCM 2001 for detailed description of method and early code).

It has evolved since then

(see A. Garcia et al, JCP 2020)

- TranSIESTA (ballistic electron transport)
- TDDFT in real time
- Full Spin-Orbit coupling, non-collinear magnetism
- Various eigensolvers with different scaling
- Density-functional perturbation theory
- Multiscale (QM/MM and second principles)
- TDDFT(ω) & *GW* post-processing
- Several analysis & postprocessing tools, etc.

Open source for academics since 1999

Fully Open source (GPL) since 2014. http://gitlab.com/siesta-project

Usage of the SIESTA code

Extremely varied contexts (phys, chem, materials, bio, geo, nano, engin)

(hard to follow the SIESTA user community, around 14k papers citing SIESTA core papers, ~1k/year)

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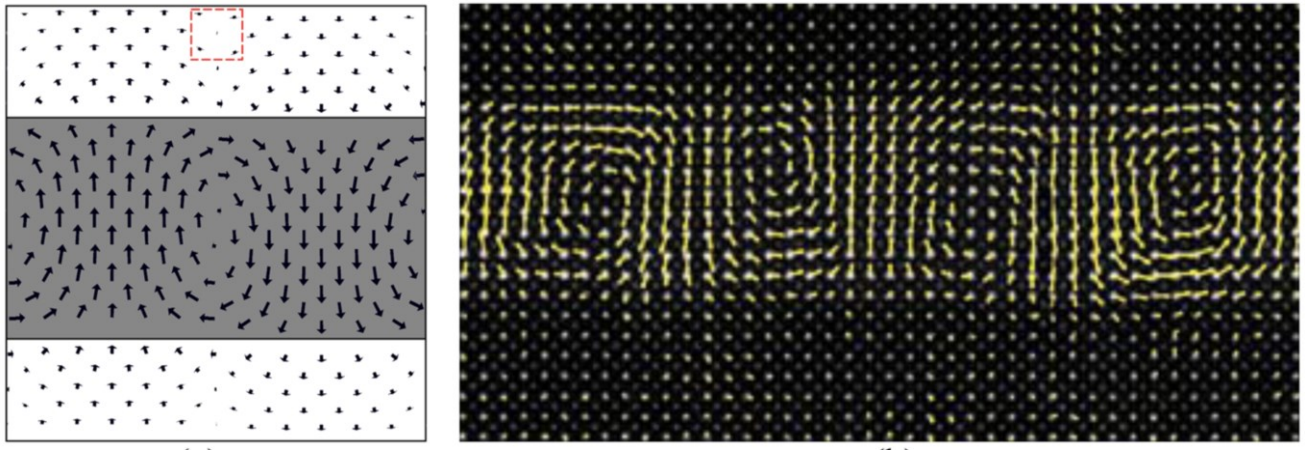
Materials:

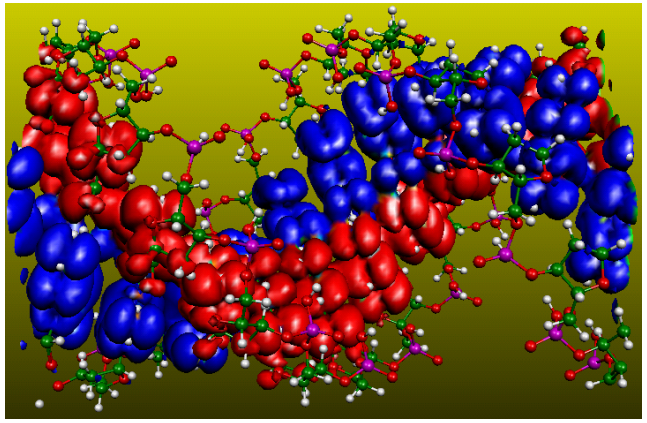


Vortices of local polarisation in ferroelectric/paraelectric superlattices

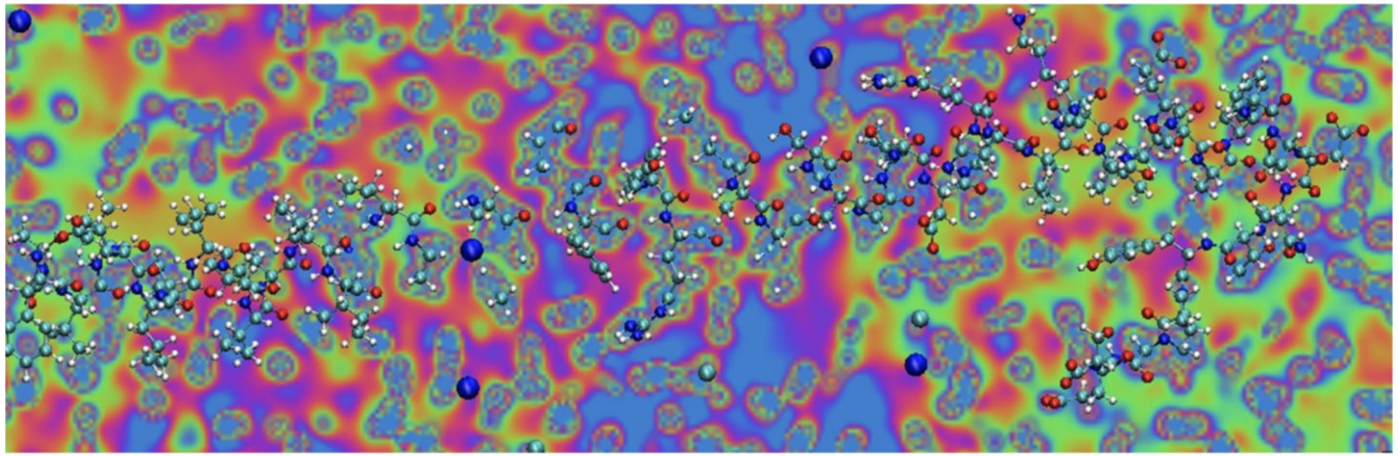
P. Aguado-Puente & J. Junquera PRB 2012

Usage of the SIESTA code

Bio:



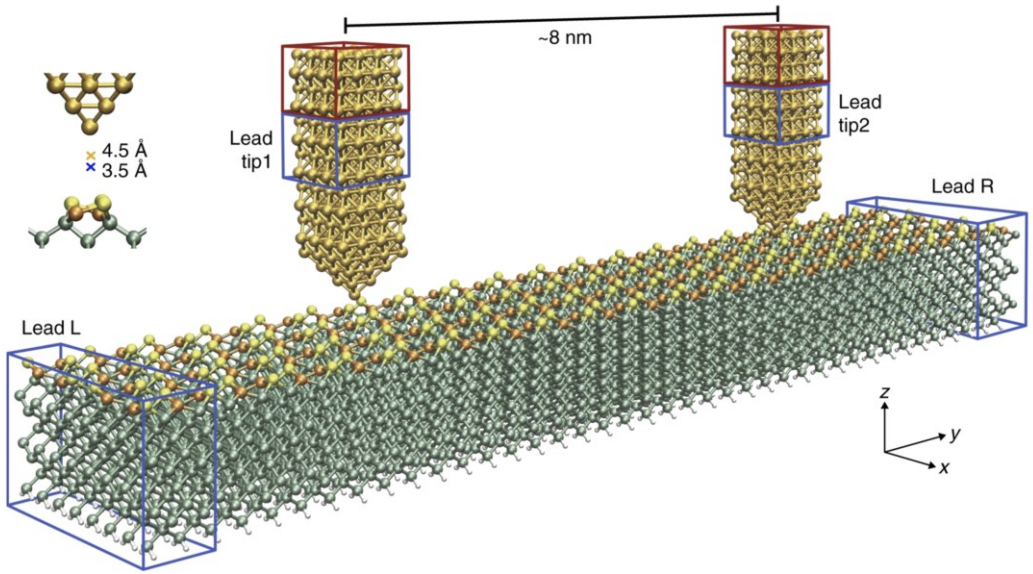
From quite early on:
DNA structure and electronic structure
P. J. de Pablo et al PRL 2000



Electrostatics around pilin protein of Geobacter Sulfurreducens in wet conditions
(a natural nano-electric wire) G. T. Feliciano et al JPCA 2012

Usage of the SIESTA code

Nano transport



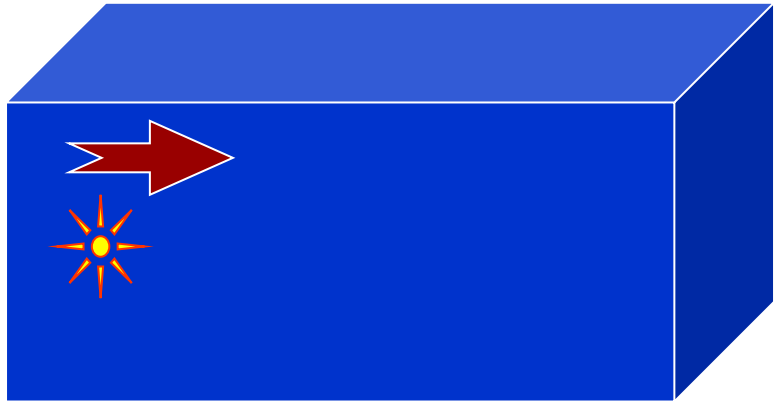
Four-terminal electron transport on Ge surface and gold tips

(see more later) M. Kolmer et al Nature Commun. 2019

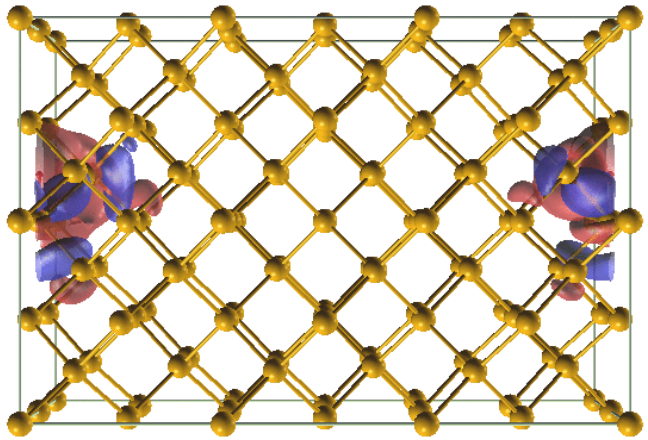
TD-DFT(t): Far from equilibrium processes

$$H^{KS}\psi_n(\mathbf{r},t) = i\hbar\,\partial_t\psi_n(\mathbf{r},t)$$

Ion projectiles shooting through matter



Deformation electron density
Proton through bulk Ge (in straight trajectory)



Electronic stopping processes

(Pruneda et al PRL 2007, Zeb et al PRL 2012, Correa et al PRL 2012, Ullah et al PRL 2018)

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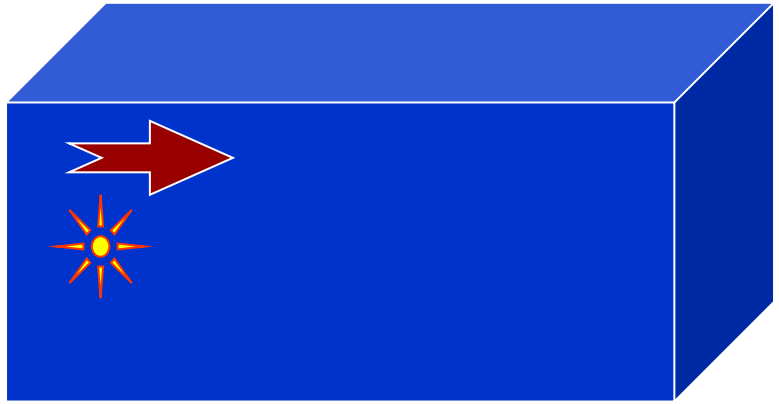
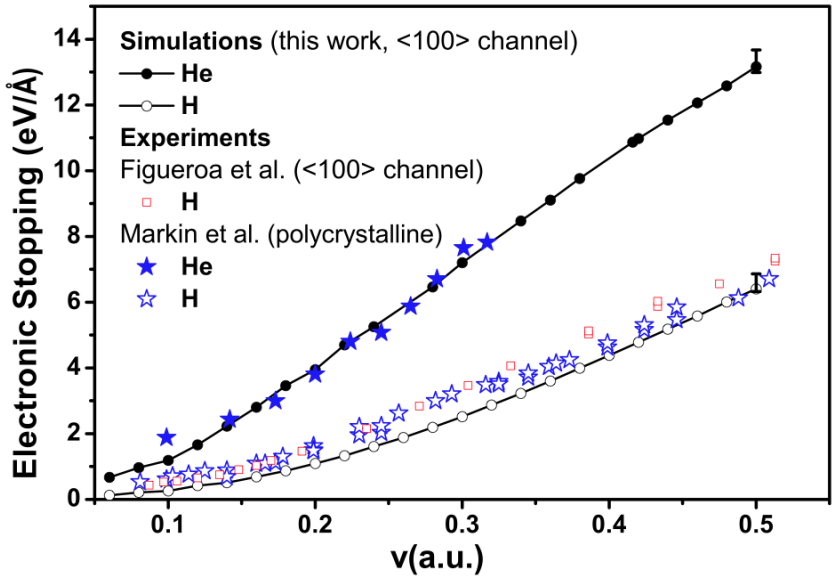


Electronic stopping power

H and He projectiles through bulk gold



Electronic stopping processes

(Pruneda et al PRL 2007, Zeb et al PRL 2012, Correa et al PRL 2012, Ullah et al PRL 2018)

SIESTA development for HPC and scalability

SIESTA (diagonalisation & PEXSI)

DNA (1D)

Graphene – BN stack (2D)

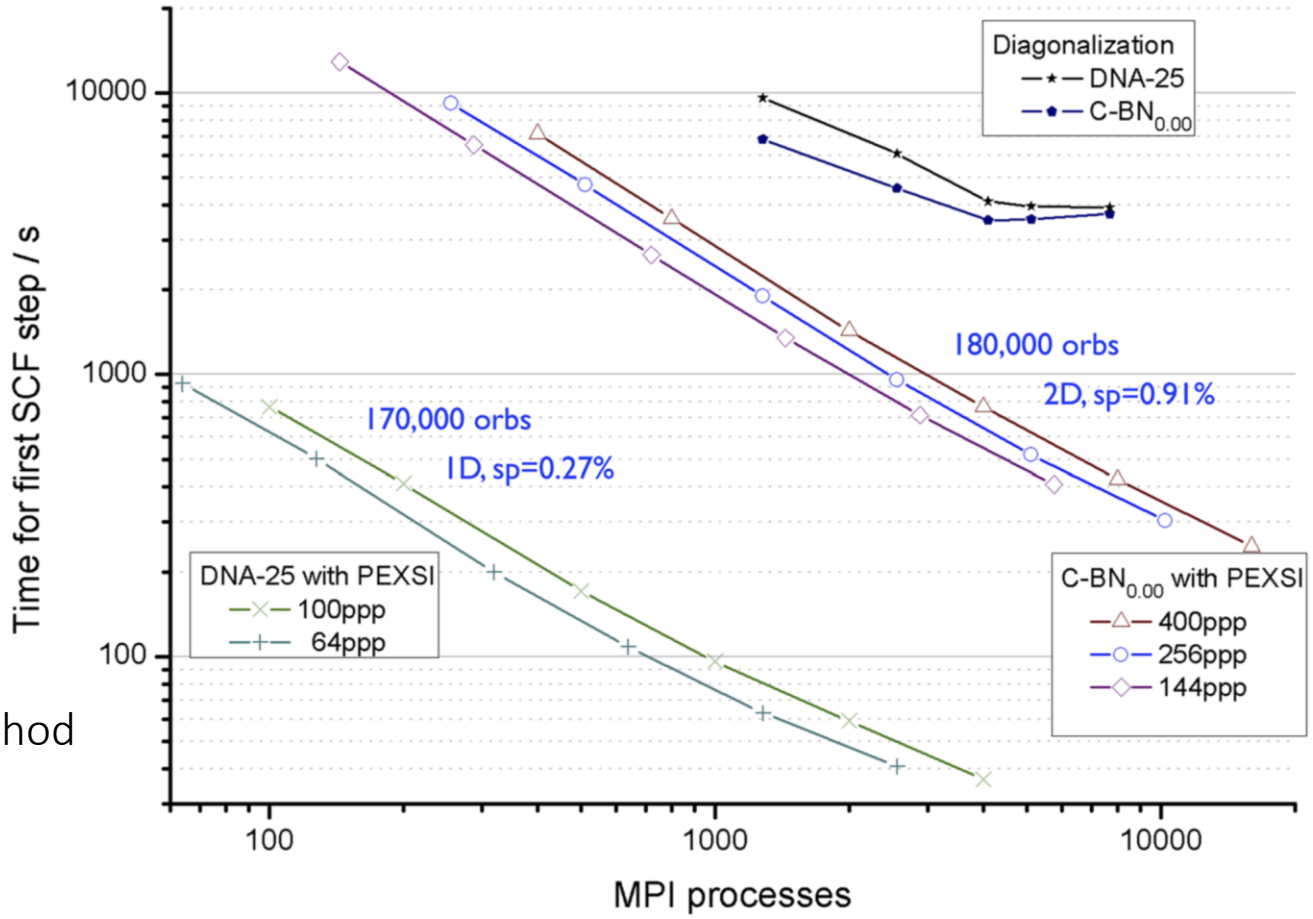
sp: sparsity of Hamiltonian

ppp: Processes per pole

PEXSI: Pole EXpansion and Selected Inversion method

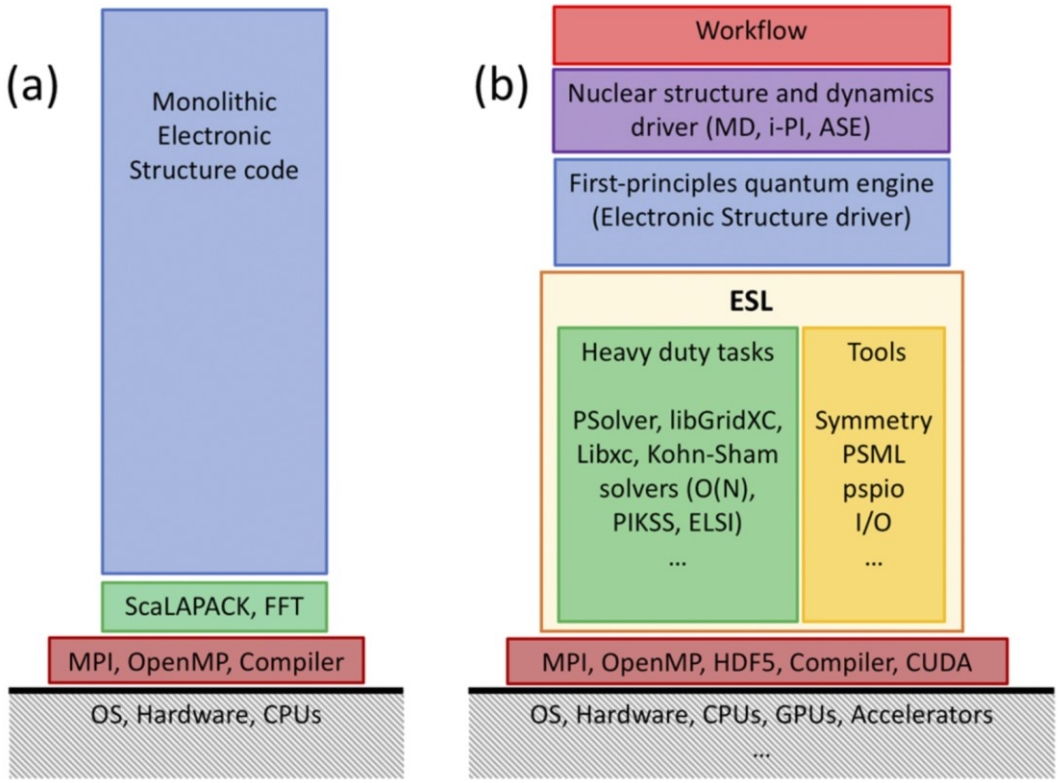
(Green's functions' based)

Diagonalisation: ScaLAPACK



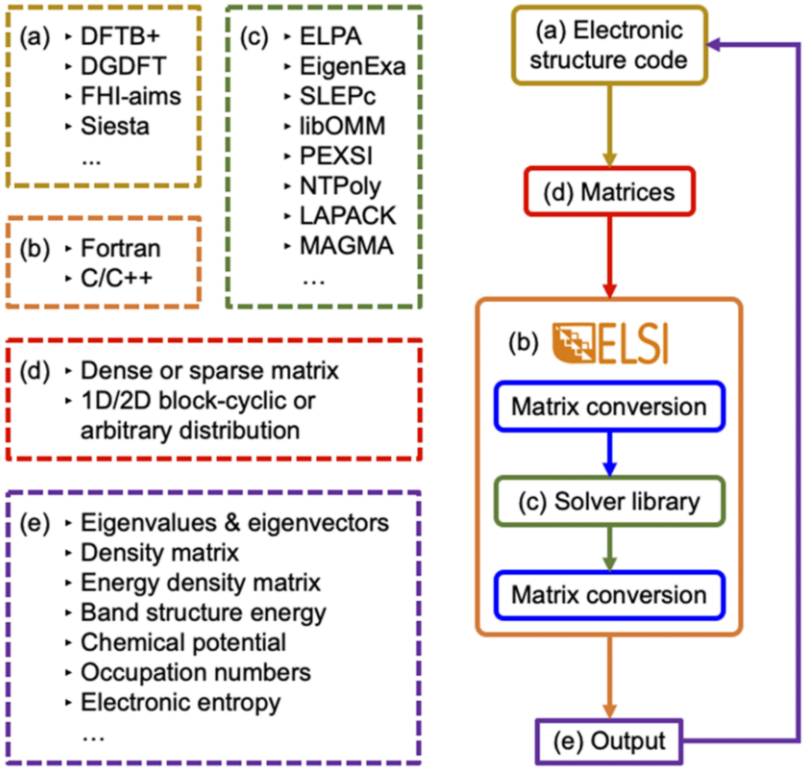
A. Garcia et al, JCP 2020

Changing paradigm

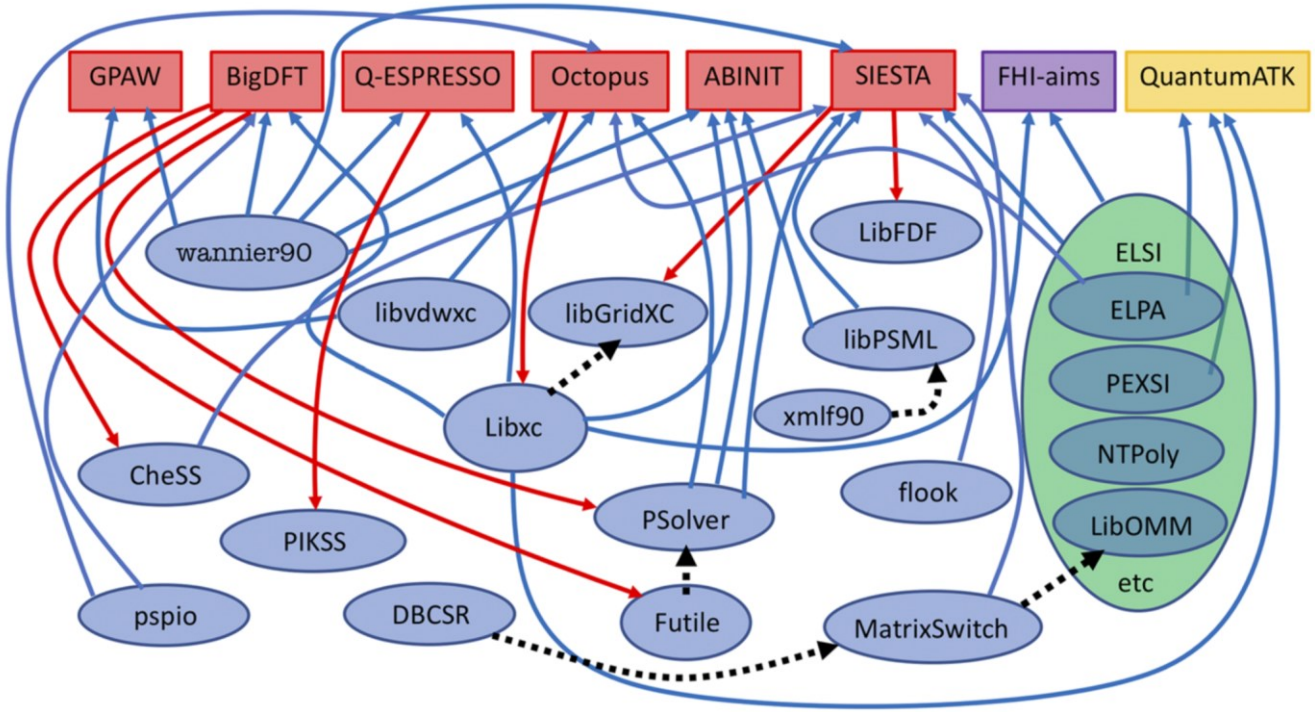


SIESTA development for HPC and scalability

ELSI (NSF-USA)



Electronic Structure Library (ESL) - CECAM



MJT Oliveira et al, JCP 2020

DRIVING THE EXASCALE TRANSITION

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THANKS