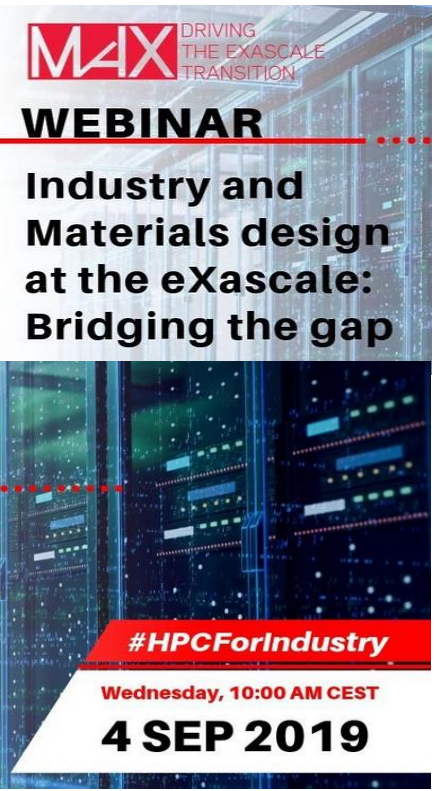
Boosting the impact of the SIESTA code in the industry through HPC and HTC



siesta

Pablo Ordejón
ICN2, Barcelona

M. Pruneda, A. Akhtar (ICN2)

A, García, V. Dikan (ICMAB)

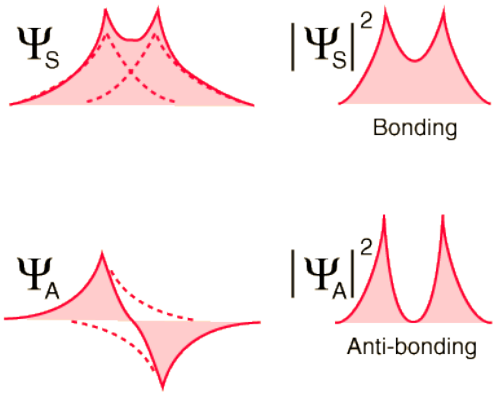
M. García, F. Martchesin, D. Simó (SIMUNE)

ICN2 Institut Català de Nanociència i Nanotecnologia
EXCELENCIA SEVERO OCHOA

ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA
EXCELENCIA SEVERO OCHOA

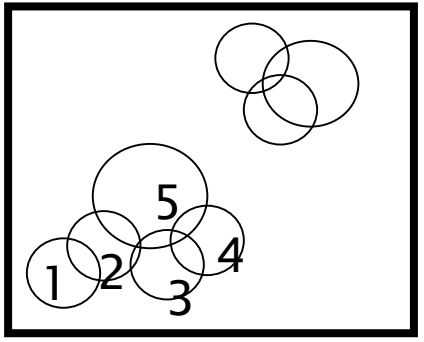
SIMUNE ATOMISTICS

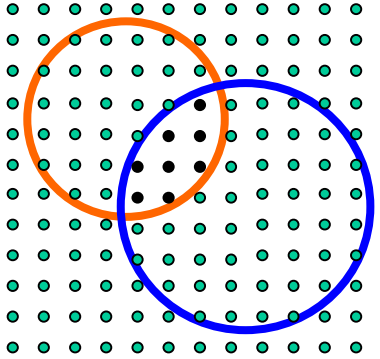
DFT with atomic orbitals

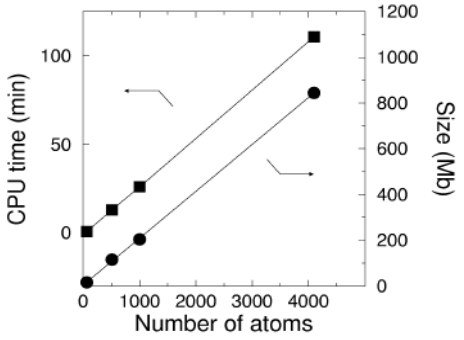


LCAO: $\psi_n(r) = \sum_\mu c_{n\mu} \phi_\mu(r)$

(pseudo)atomic orbitals
- Short ranged
- Arbitrarily complete



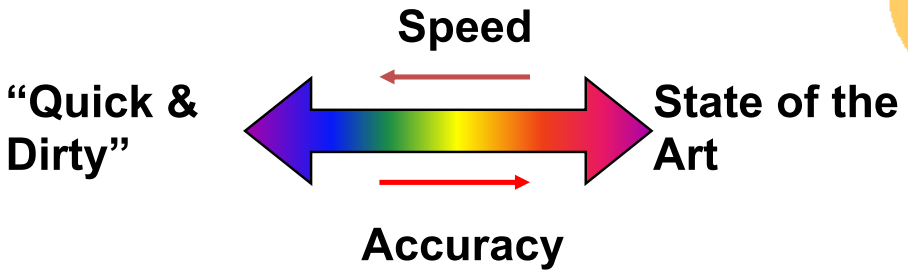




- Sparse representation (Hamiltonian, Density Matrix...)
- Calculation and storage of Hamiltonian scales linearly with system size
- Natural local language to exploit WF or DM localization: **linear scaling H solvers**

• Arbitrarily complete bases

- s, p, d, ...
- Single-ζ, multiple -ζ
- Off-site orbitals
- Diffuse functions



• Atomic forces and stress

- Relaxations
  - Atomic coordinates
  - Cell shape & size
- Phonons, elastic constants, ...
- Thermal transport

- Molecular Dynamics:
  - E, V
  - T, V (Nose Thermostat)
  - P (Parrinello-Rahman)
  - T, P

• Electronic structure information

- Band structures (k-point sampling)
- Population analysis
- Charge distributions
- Electrostatic Potentials

- Density of States
- Spin distributions
- Non-collinear spin states
- STM image simulation....

Current capabilities & developments:

- **Hybrid QM/MM simulations**
  (with D. Estrin, UBA)
  Theor. Chem. Acc **128**, 825 (2011)

- **Beyond DFT: GW for electronic excitations**
  (with F. Giustino, Oxford)
  Phys. Rev. B **85**, 245125 (2012)

- **Linear Response (Phonons)**
  Phys. Rev. **65**, 075210 (2002)
  (massive revamping ongoing)

- **Non-equilibrium transport - TranSIESTA**
  (with M. Brandbyge and K. Stokbro, DTU)
  Phys. Rev. B **65**, 165401 (2002)

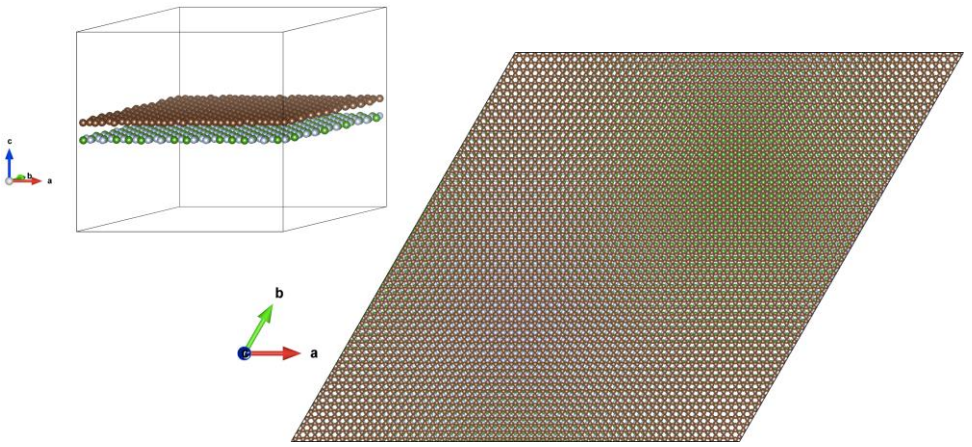
- **TD-DFT in real time**
  (D. Sanchez-Portal, San Sebastian)
  Phys. Rev. B **66**, 235416 (2002)

- **Spin-Orbit coupling**
  (Sanvito –Dublin - and Ferrer –Oviedo)
  J. Phys. Cond Matt. **19** 489001 (2007)
  (J. Cerdá, CSIC)
  J. Phys.: Cond. Mat. **24** 086005 (2012)

- **ıssively parallel efficiency in Supercomputers**
  (with J.M.Cela, BSC)

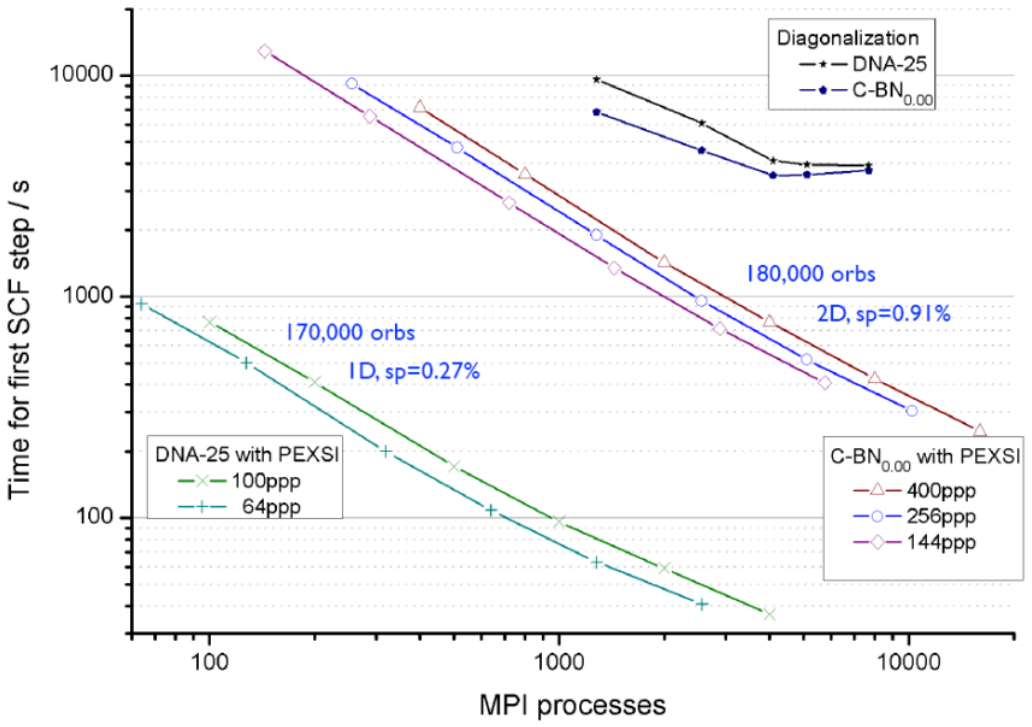
Massive Parallelization

DNA strand 17,875 atoms



Graphene / BN (Moire pattern) 12,770 atoms

Strong scaling



MOTOROLA

Phenix Corporate Labs (US)
Dielectric thin films

SUMITOMO CHEMICAL

Tsukuba (Japan)

AIR PRODUCTS

CARBUROS METALICOS
Grupo Air Products

Allentown (US) - Barcelona (Spain)
Deposition of metallic thin films for interconnects
Hydrogen storage materials

MAX ABENGOA RESEARCH

Seville (Spain)
Nanofluids for thermal storage

MAX FAE

Barcelona (Spain)
Oxygen-sensing devices

Material Design Consultancy, Services & Products

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PROVIDES: COMPUTER SIMULATION SERVICES – ATOMISTIC SIMULATIONS

CLIENTS: COMPANIES DEVELOPING INNOVATIVE AND CUTTING-EDGE TECHNOLOGY BASED ON ADVANCED MATERIALS PROPERTIES

VALUE PROP.: TRANSLATION
REDUCED BARRIER FOR ADOPTION
FACILITATE USAGE

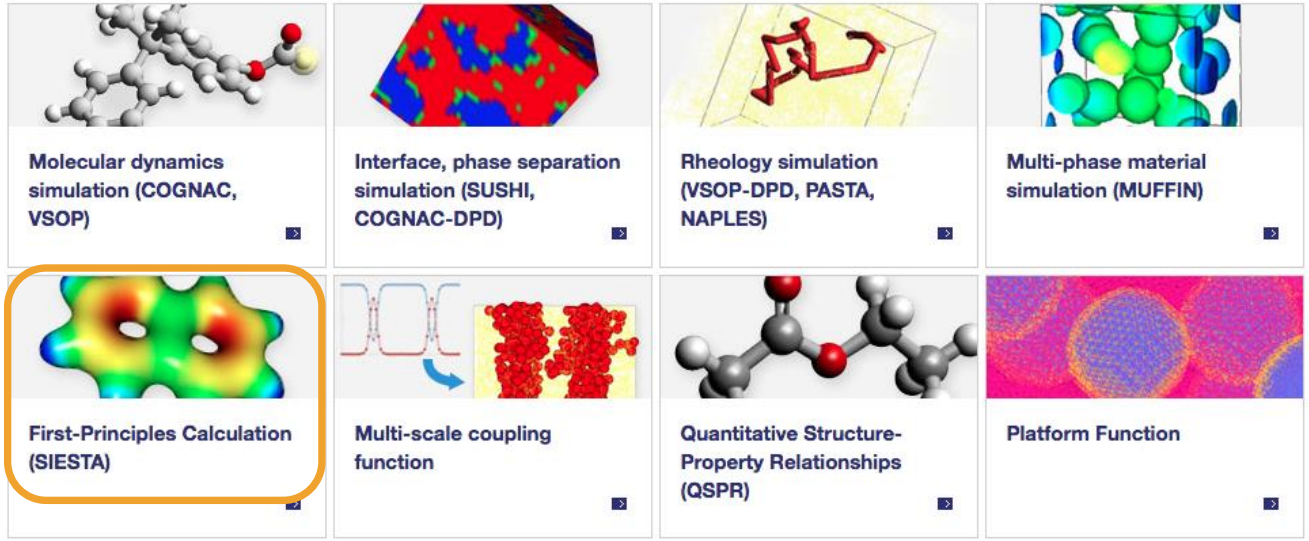
SIMUNE's Collaboration Projects

J-OCTA
Integrated Simulation System for SoftMaterials

株式会社JSOL

An integrated simulation software for polymeric material

J-OCTA predicts material properties with multi-scale simulation technology (from atomic to micrometer scale). It can be used to simulate...



https://www.j-octa.com

Lessons from MaX Industrial Observatory Activities and from SIMUNE

- Software: Ready to Go - Easy to Use - Serviced
- On-Demand Services (Software as a Service)
- User Interfaces
- Workflows for Complex Properties (Industrial Problems)
- Automation (handling the simulations, runs, results, storage, ...)
- HTC rather than HPC... So far....
- Time to Solution is Critical (HTC/HPC may become essential even for "small" problems)
- Multiscale - Multiphysics
- Integration of Ab-Initio in Industrial Workflows will become a reality (JSOL; INTERSECT EU project)

pablo.ordejon@icn2.cat