Tutorial: WEST

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MICCoM School — July 16th, 2017

Computational Spectroscopy: Accuracy and Efficiency

Building **predictive** and **efficient** capabilities to compute spectroscopic properties requires **post-DFT accuracy**.

Qbox

QUANTUMESPRESSO

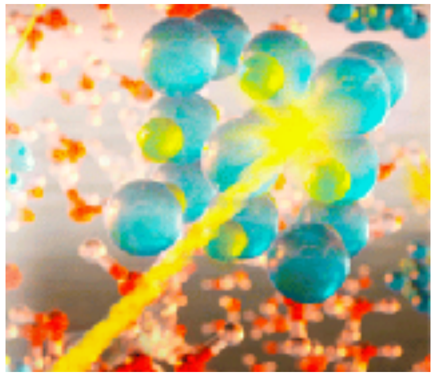
DFT → **MBPT**

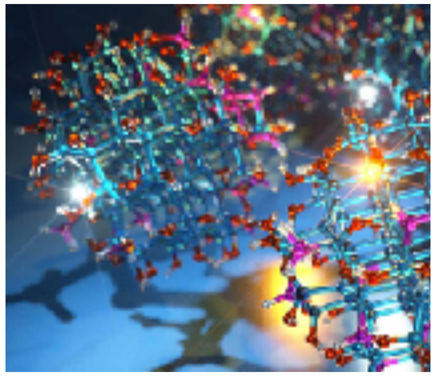
Density Functional Theory
Many-body Perturbation Theory

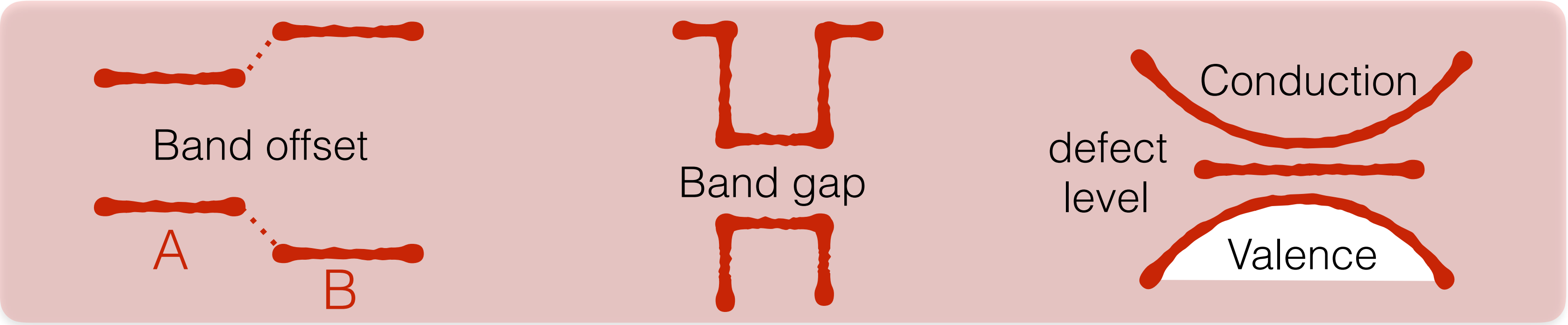
WEST!

F. Gygi: IBM J. Res. Dev. (2008)
P. Giannozzi et al, *J.Phys.:Condens.Matter* 21, 395502 (2009)

M. Govoni, G. Galli, J. Chem. Theory Comput. 11, 2680 (2015)







Many Body Perturbation Theory

- Self-energies yield better single particle single-particle electronic structures compared to DFT

$$E_n^{QP} = \varepsilon_n^{KS} + \langle \psi_n^{KS} | \hat{\Sigma}(E_n^{QP}) - \hat{V}_{xc} | \psi_n^{KS} \rangle$$

Single particle excitations, **Photoemission**

- Imaginary part of self-energies yields information on lifetimes

$$\tau^{-1} = Im\{\Sigma\}$$

Recombinations, **Mobilities**

- Propagation of two-particles (electron-hole), Bethe Saltpeter Equation

$$L = L_0 + L_0 \Xi L$$

(under development)

Neutral excitations, **Optical absorption**

G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. 74, 601 (2002)
Y. Ping, D. Rocca, and G. Galli, Chem. Soc. Rev. 42, 2437 (2013)

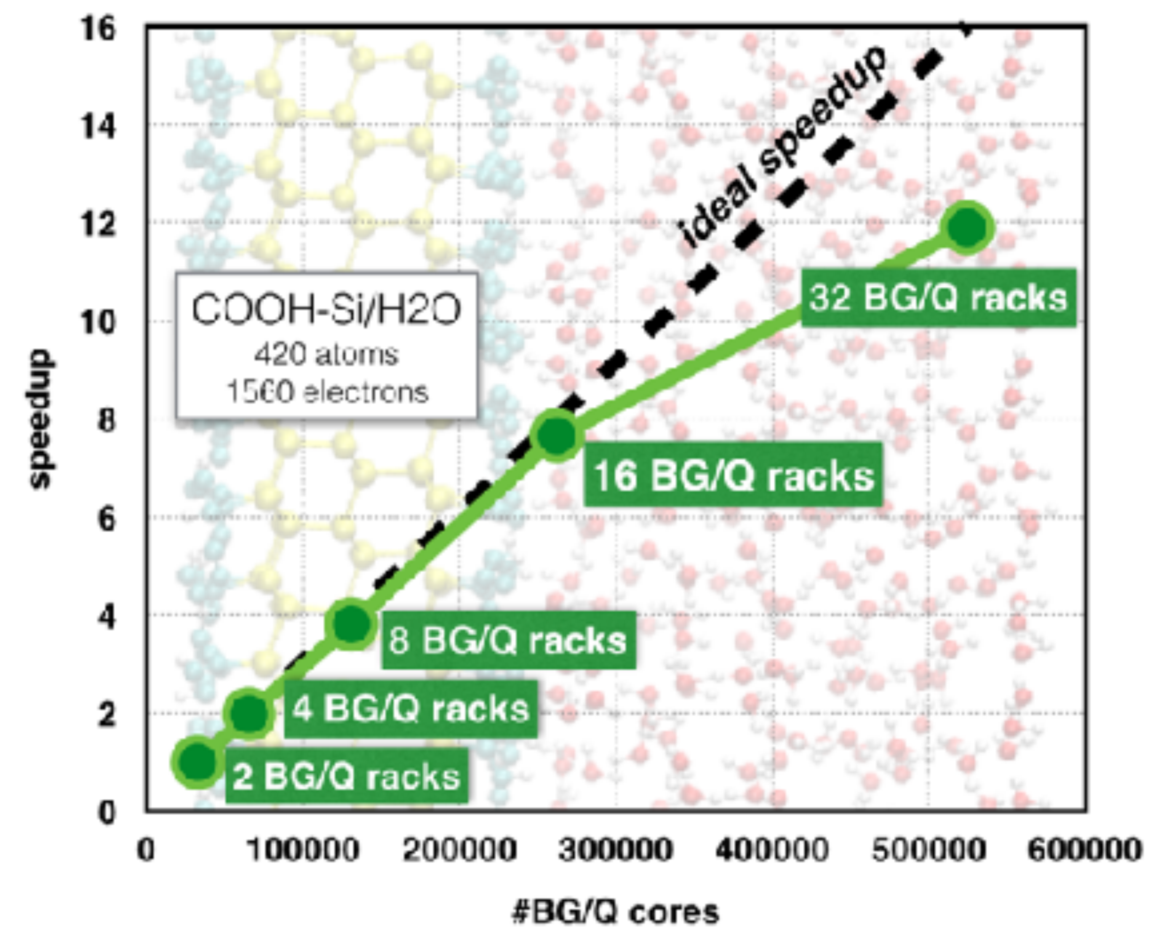
Large scale GW calculations

WEST! is a parallel code for Many-Body Perturbation Theory calculations

Benefits of the implementation

- eliminated summations over empty states
- low-rank decomposition achieved with PDEP
- parallel iterative solvers
- scalable to ~500k cores
- reduced pre-factors of $O(N^4)$ scaling

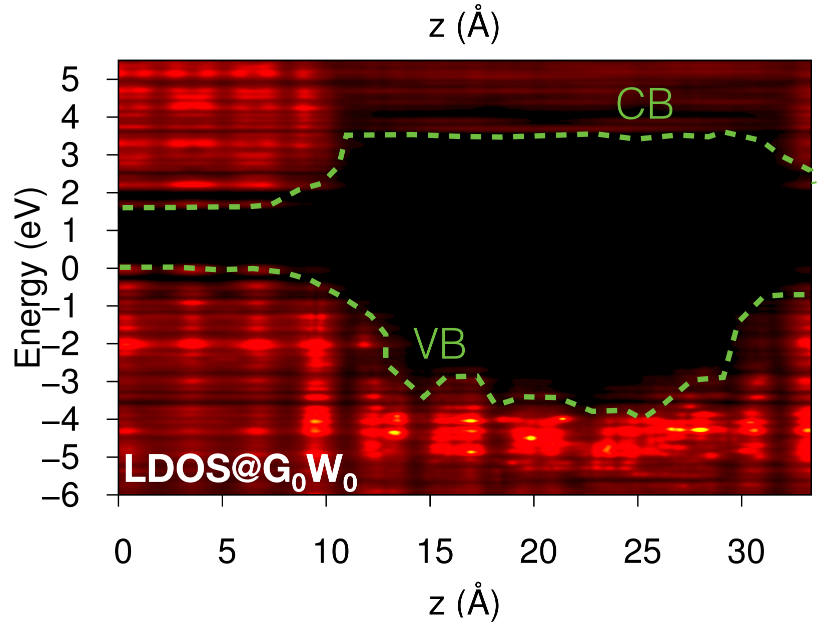
Scalability



WEST: use cases

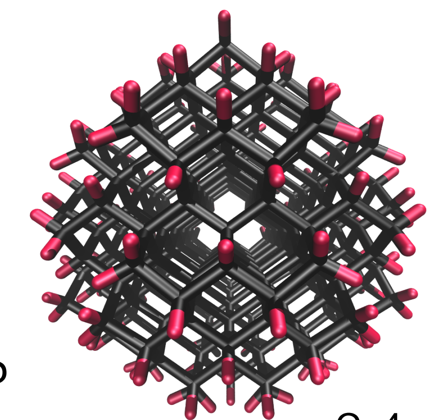
- Interfaces
- Liquids/Solutions
- Nanoparticles
- Defects
- Solids
- Molecules
- Perovskites

- **Coupling w/ Ab intio Molecular Dynamics (AIMD)**
- **Inclusion of spin-orbit coupling**



COOH-Si/H_2O

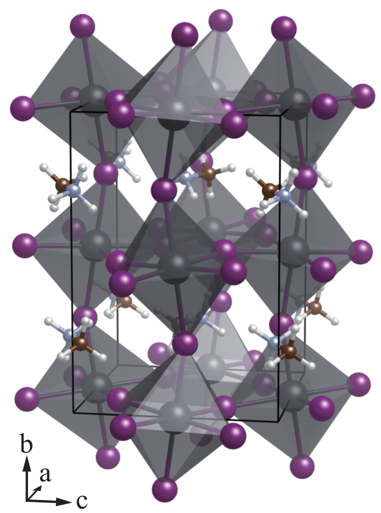
1560 electrons

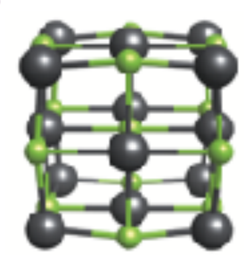


Si-NP

1344 electrons

2.4 nm





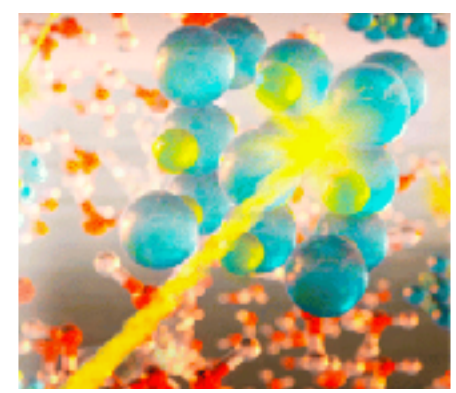
$MAPbI_3$

320 electrons

PbSe NP

274 electrons

CdTe, ZnTe **1152 electrons**

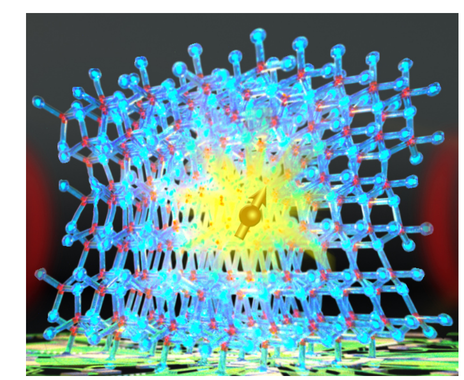


$(NaCl)_{aq}$

432 electrons

Multiple configurations

(128 / AIMD trajectory)



V_N-AlN

1920 electrons

M. Govoni, G. Galli, J. Chem. Theory Comput. 11, 2680 (2015)
P. Scherpelz, I. Hamada, M. Govoni, G. Galli, J. Chem. Theory Comput. 12, 3523 (2016)
A. Gaiduk, M. Govoni, R. Seidel, J. Skone, B. Winter, G. Galli, JACS Comm. 138, 6912 (2016)
H. Seo, M. Govoni, G. Galli, Sci. Rep. 6, 20803 (2016)

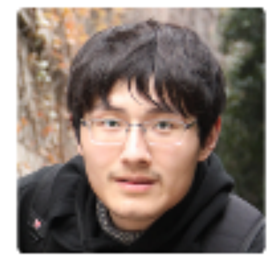
WEST: team, performance

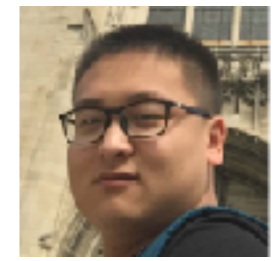
Team


G. Galli

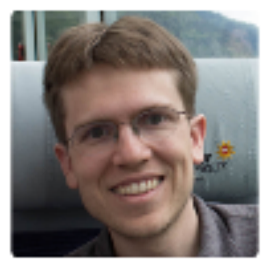

M. Govoni

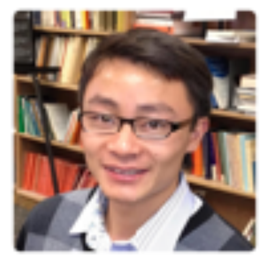

N. Brawand

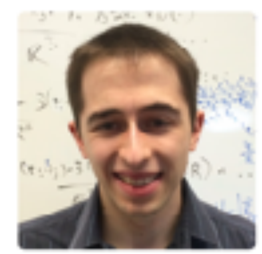

H. Ma


H. Yang


I. Hamada


P. Scherpelz


H. Zheng


R. McAvoy


N.L. Nguyen

Towards **exascale** computing

Early Science programs at ANL and NERSC

next architectures: Intel Xeon Phi

Materials by design in the mid-WEST

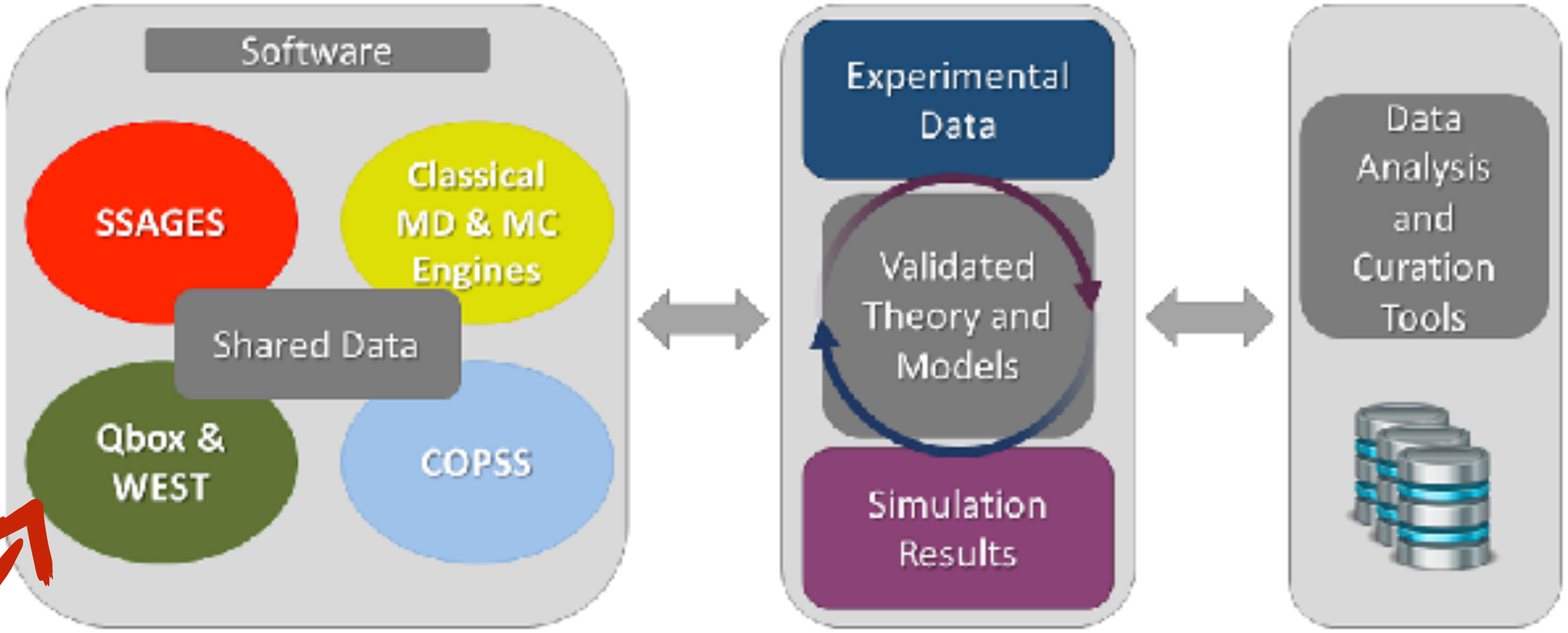
Midwest Integrated Center for Computational Materials

MICCoM develops and disseminates interoperable **open source software, data, and validation procedures**, enabling the community to simulate and predict properties of functional materials for energy conversion processes.

Funded by:

U.S. DEPARTMENT OF ENERGY

MICCoM



http://miccom-center.org

WEST: structure of the code

Without **E**mpty **ST**ates

DFT

$\hat{H}_{KS}|\psi_i\rangle = \varepsilon_i|\psi_i\rangle$

PDEP

$\hat{\epsilon}^{-1}_{\omega=0}|\phi_n\rangle = \lambda_n|\phi_n\rangle$

Lanczos W

$\omega \neq 0$

Lanczos G

$\omega \neq 0$

Contour Deformation

$\Sigma(\omega) = \int d\omega' G(\omega+\omega')W(\omega')$

QP-energies

$E_i^{QP} = \varepsilon_i + \langle\psi_i|\hat{\Sigma}(E_i^{QP}) - \hat{V}_{xc}|\psi_i\rangle$

WEST builds on QuantumEspresso **pw.x**

wstat.x

Calculation of the dielectric screening (Iterative diagonalization)

wfreq.x

GW calculation

westpp.x

Post-processing

westpy.py

Python plotting suite

M. Govoni, G. Galli, J. Chem. Theory Comput. 11, 2680 (2015)

We are currently coupling WEST & Qbox

`wstat.x`: iterative diagonalization of the dielectric matrix w/o empty states

Iterative diagonalization techniques for ground- and excited-states calculations

DFT

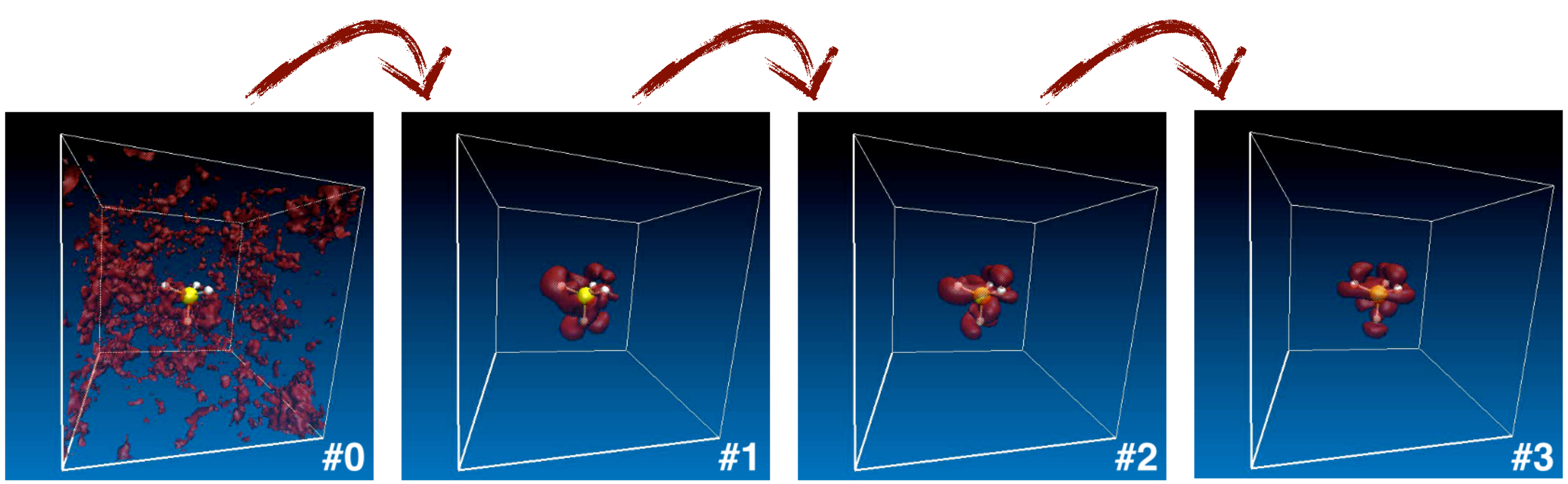
$$H\,|\psi_n\rangle = \varepsilon_n\,|\psi_n\rangle$$

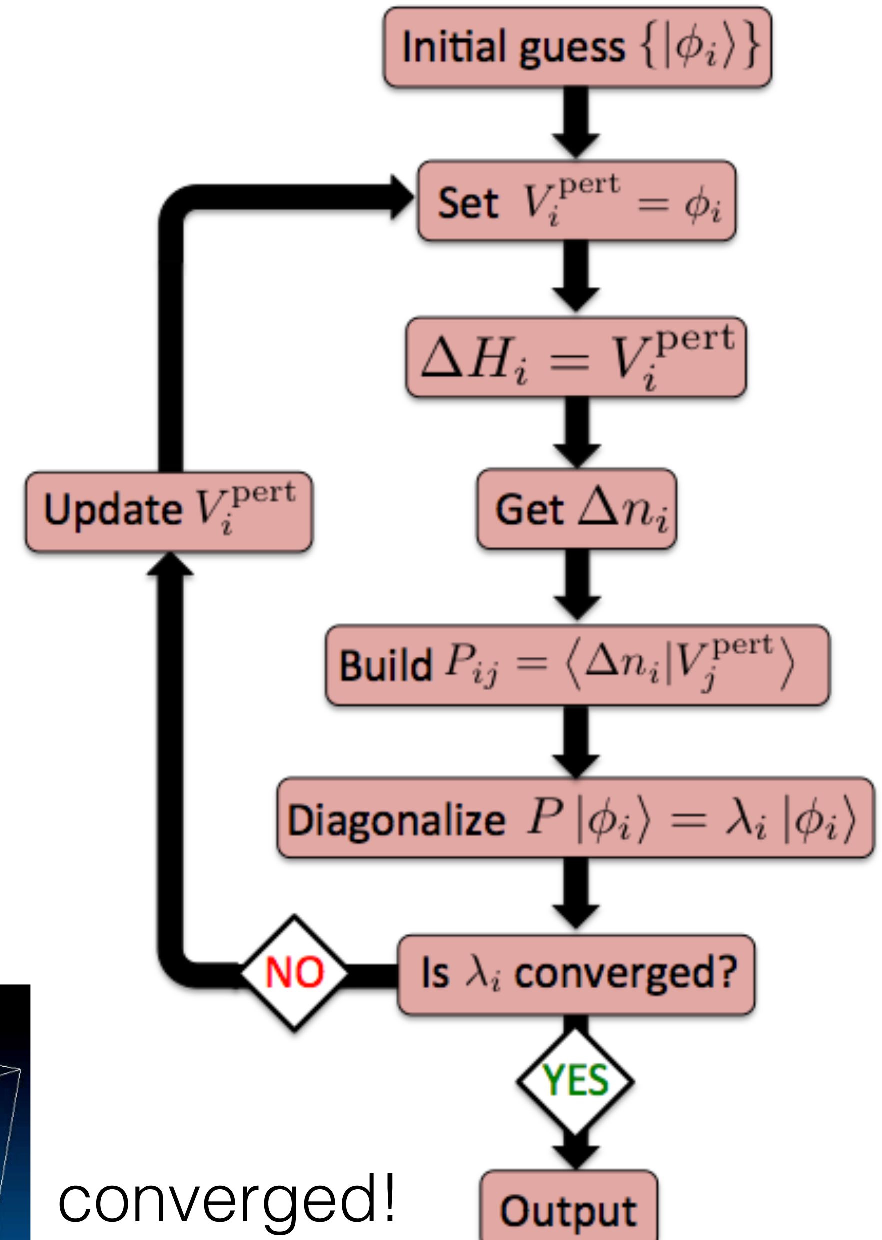
Schrödinger Eq.
Recursively apply the Hamiltonian

GW

$$P\,|\phi_i\rangle = \lambda_i\,|\phi_i\rangle$$

Sternheimer's eq.
Recursively apply the irreducible polarizability





converged!

S. Baroni *et al.* Rev. Mod. Phys. 73, 515 (2001)
H. Wilson *et al.* Phys. Rev. B 79, 245106 (2009)

`wfreq.x`: GW calculation

Quasiparticle (QP) states and energies may be obtained replacing Vxc with the **electron self-energy**

$$\left(\hat{T} + \hat{V}_{ion} + \hat{V}_H + \hat{\Sigma}(E_n^{QP})\right)|\psi_n^{QP}\rangle = E_n^{QP}|\psi_n^{QP}\rangle \quad \text{MBPT}$$

$$\left(\hat{T} + \hat{V}_{ion} + \hat{V}_H + \hat{V}_{xc}\right)|\psi_n\rangle = \varepsilon_n|\psi_n\rangle \quad \text{DFT}$$

First order perturbation theory

One-shot GW (G_0W_0)

$$E_n^{QP} = \varepsilon_n^{KS} + \underbrace{\langle\psi_n^{KS}|\hat{\Sigma}(E_n^{QP}) - \hat{V}_{xc}|\psi_n^{KS}\rangle}_{\text{Perturbation}}$$

Based on DFT Hamiltonian

Based on DFT Density

$$\rho = \sum_n |\psi_n^{KS}|^2$$

L. Hedin, Phys. Rev. 139, A796 (1965)
G. Strinati, H.J. Mattausch, W. Hanke Phys. Rev. Lett. 45, 290 (1980)
M. Heibertsen, S. Louie, Phys. Rev. Lett. 55, 1418 (1985)
F. Aryasetiawan, O. Gunnarsson, Rep. Prog. Phys. 61, 237 (1998)
G. Onida, L. Reining, A. Rubio, Rev. Mod. Phys. 74, 601 (2002)

WEST: input

Input in JSON format

DFT → PDEP

$$\hat{H}_{KS}|\psi_i\rangle = \varepsilon_i|\psi_i\rangle \qquad \hat{\epsilon}^{-1}_{\omega=0}|\phi_n\rangle = \lambda_n|\phi_n\rangle$$

```
{
    "input_west": {
        "qe_prefix": "silane",
        "west_prefix": "silane",
        "outdir": "./"
    },
    "wstat_control": {
        "wstat_calculation": "S",
        "n_pdep_eigen": 50
    }
}
```

wstat.in

Keyword that identifies the directory where the output of DFT calculation resides

Keyword that identifies the directory where the calculation is saved

Output directory

Start from scratch

Number of eigenpotentials

WEST: output

Output in JSON format

DFT → PDEP

$$\hat{H}_{KS}|\psi_i\rangle = \varepsilon_i|\psi_i\rangle \qquad \hat{\epsilon}^{-1}_{\omega=0}|\phi_n\rangle = \lambda_n|\phi_n\rangle$$

```
{
    "runjob": { … },
    "software": { … },
    "config": { … },
    "parallel": { … },
    "input": { … },
    "system": { … },
    "exec": { … },
    "output": { … },
    “timing": { … }
}
```

- Status of execution
- Version of software
- Configuration of the platform where the code ran
- Details about parallelization
- Input variables (for future reference)
- Details about the system under study
- Log of execution
- Output
- Timings

wstat.json

WEST: extract information from the output

```
{
     "runjob": { … },
     "software": { … },
     "config": { … },
     "parallel": { … },
     "input": { … },
     "system": { … },
     "exec": { … },
     "output": { … },
     “timing": { … }
}
```

wstat.json

```
import json

# read data from JSON file
with open(‘west.wstat.save/wstat.json’) as file:
    data = json.load(file)

# show values
print(data[“input”][“wstat_control”][“n_pdep_eigen”])
print(data[“runjob”][“completed”])
print(data[“output”][“eigenval”])
```

Import JSON library

Read the output file

Recall an input variable

Is the simulation done?

Manipulate output

Run WEST

```
mpirun -n 4 wstat.x -i wstat.in
```

Number of cores

Input file

MPI launcher/manager

Name of the program

```
mpirun -n 4 wfreq.x -i wfreq.in
```

```
mpirun -n 4 westpp.x -i westpp.in
```

```
import westpy
westpy.command()
```

Python plotting suite

WEST: parallelization schemes

Message Passage Interface (MPI) 6 **cores** running in parallel

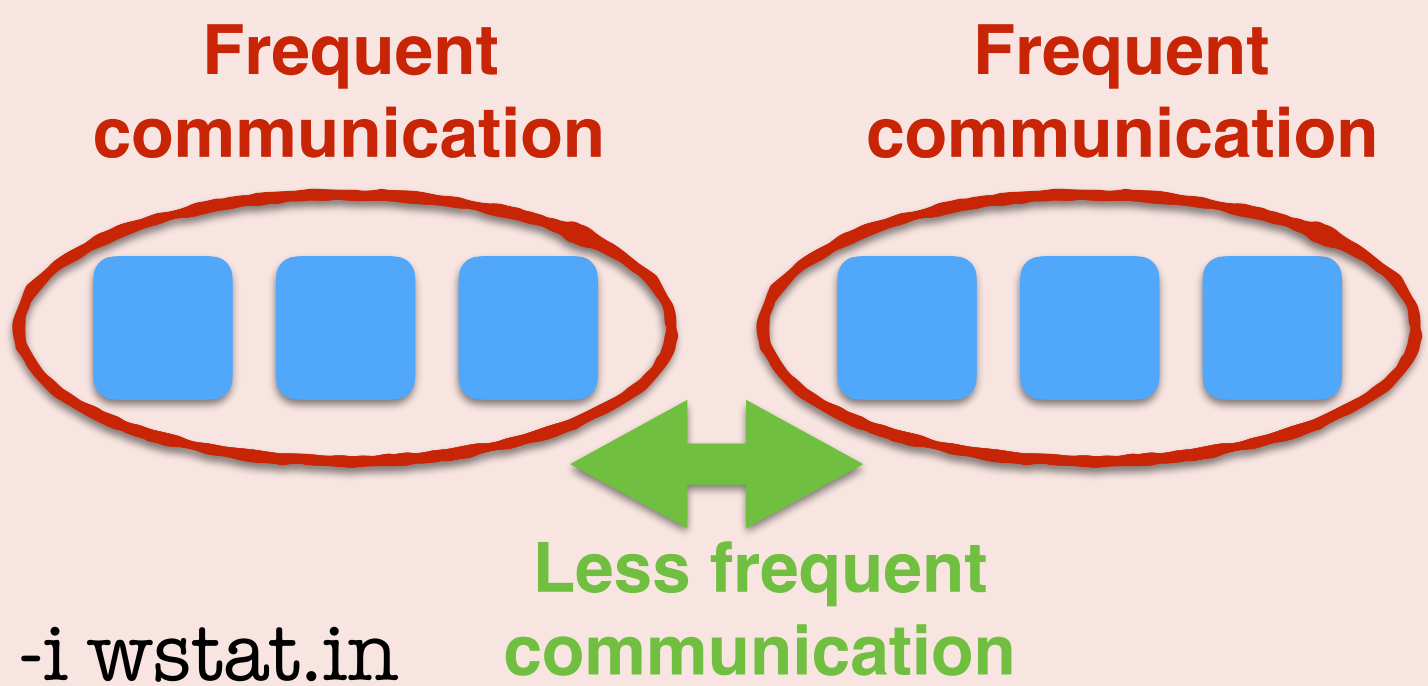
The computation is distributed evenly across all cores

mpirun -n 6 wstat.x -i wstat.in

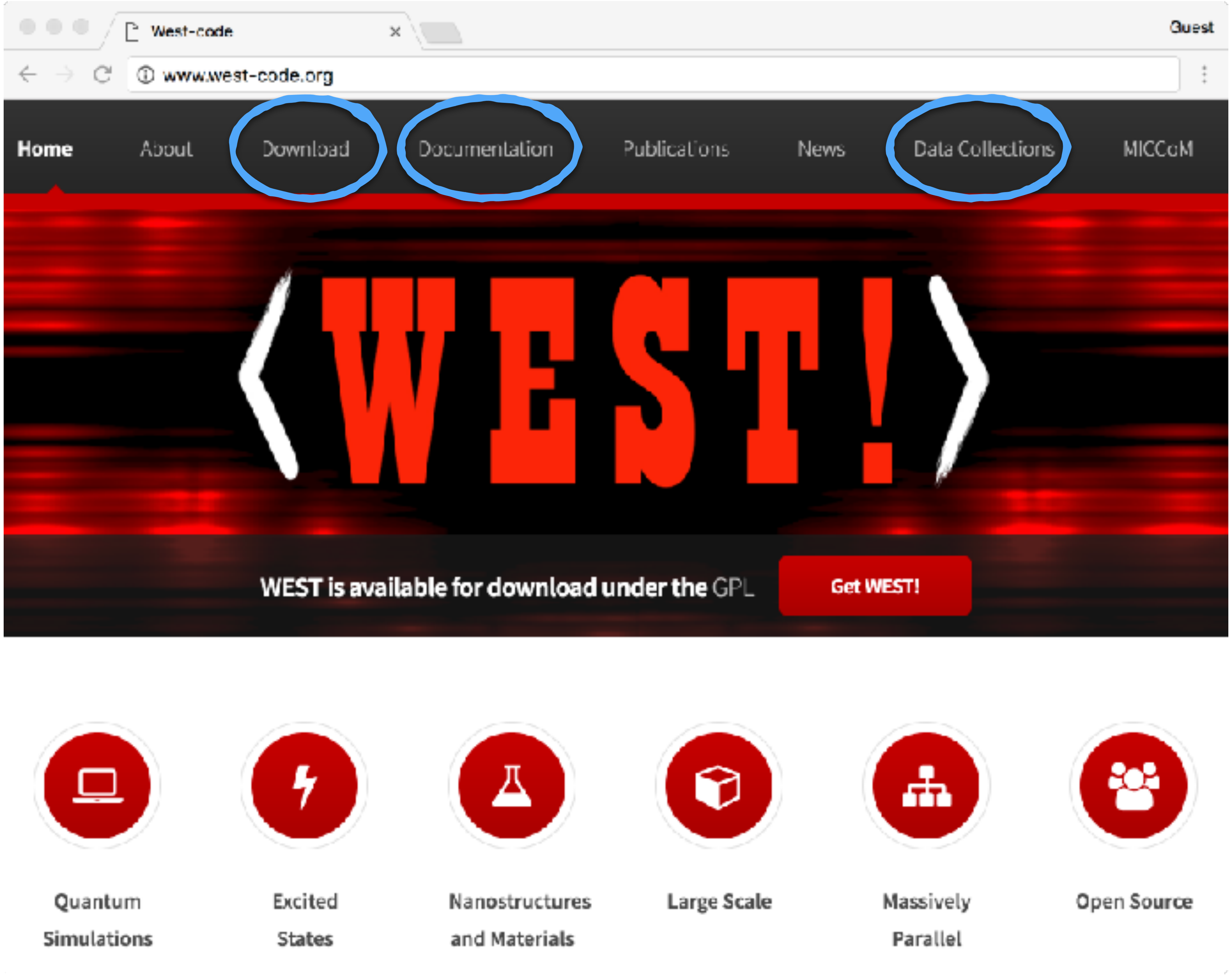
The computation is diversified in order to keep frequent communication bound to small number of cores

✔ **Improved scalability**

mpirun -n 6 wstat.x -nimage 2 -i wstat.in



WEST: website



WEST: Hands-on!

Wednesday, July 19th

Morning Session: University of Chicago, William Eckhardt Research Center, Room ERC 161

8:00am	Continental Breakfast (ERC 161)
8:30am – 12:30pm	Hands-on: WEST
12:30 – 1:30pm	Lunch (ERC 161)

jupyter

Let’s look at a summary of what we will learn!