WEST: Scalable Software for Materials by Design

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The poster in a nutshell

Petascale computational resources have provided the opportunity to perform quantum simulations of materials properties of unprecedented size, yielding results that complement experimental observations and may lead to the discovery of new materials, designed using the basic principles of quantum mechanics.

We describe the features of **WEST**, an open source massively parallel code developed to compute excited state properties of molecules and materials.

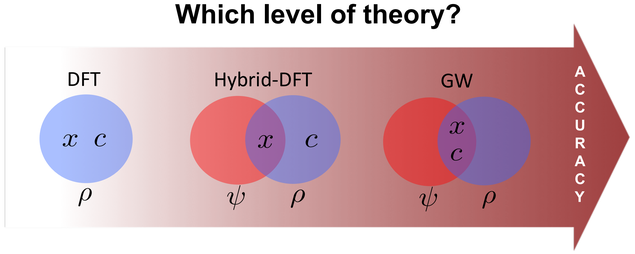
www.west-code.org

Motivation

Materials by design

1. Generate structural models with classical or Ab Initio Molecular Dynamics.
2. Carry out Density Functional Theory (DFT) electronic structure calculations with semi-local or hybrid functionals.
3. Use DFT input to carry out Many Body Perturbation Theory (MBPT) calculations and obtain quasiparticle energies (GW) and absorption properties (BSE).

Which level of theory?



Understanding materials at the nanoscale and building predictive capabilities require high accuracy.

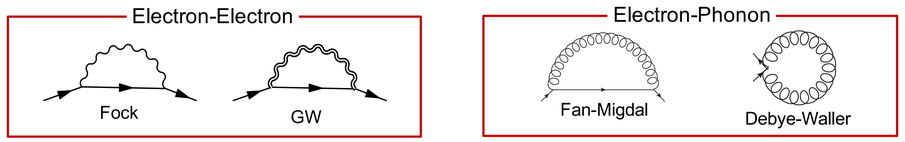
Many-Body Perturbation Theory

In a fashion similar to DFT, quasiparticle (QP) states and energies may be obtained replacing the exchange-correlation potential with the electronic self-energy Σ .

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

Kinetic energy — Electron-ion — Hartree — Self-energy

The self-energy can be derived using Many-body Perturbation Theory



Improved calculation of response functions: non-locality, retardation effects.

Scalability

Midway2 @ RCC

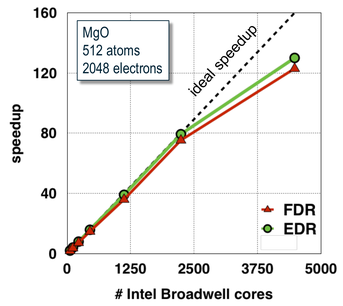
Intel Broadwell

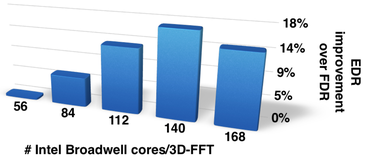
Mira @ ALCF

IBM BG/Q

Theta @ ALCF

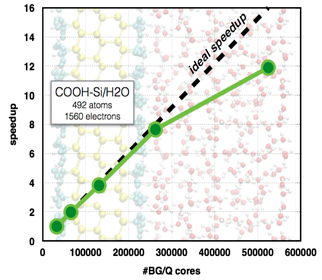
Intel Knights Landing



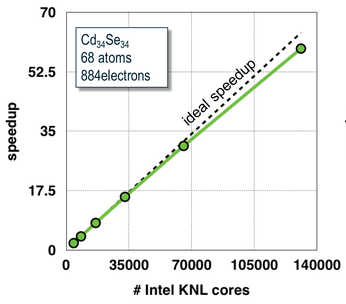


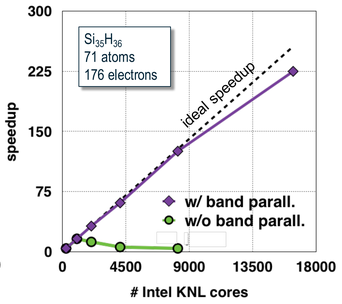
EDR interconnect shows better strong scaling of 3D-FFT than FDR.

Interconnect	Signal rate (Gbps)	Latency (μs)
FDR	54.40	0.7
EDR	96.97	0.5

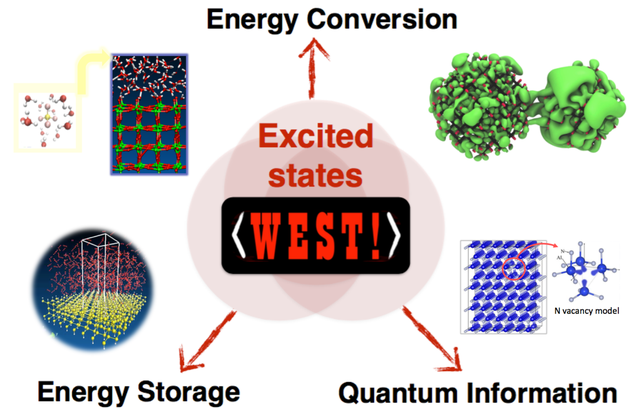


WEST enables massive parallelization of computation and the efficient distribution of data structures. The scalability was measured up to ~500k cores.

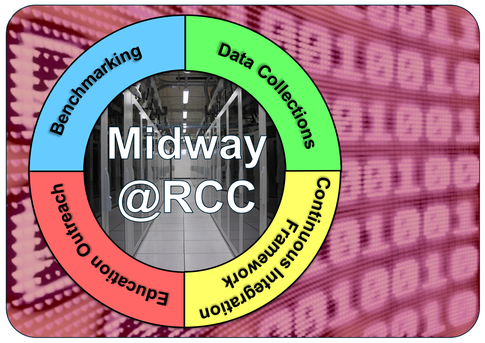




Impact



Leveraging RCC resources



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Future directions

Thanks to Early Science Programs at ANL and NERSC we plan to adapt the software to leverage the next generation of HPC machines.

Many integrated cores architectures

References

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