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Overview of GPAW

Jussi Enkovaara
Department of Applied Physics
Aalto University School of Science
Finland

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GPAW

- Implementation of projector augmented wave method on
  - uniform real-space grids, atomic orbital basis, plane waves
- Density-functional theory, time-dependent DFT, many-body perturbation theory, ...
- Open source software licensed under GPL

wiki.fysik.dtu.dk/gpaw

J. J. Mortensen et al., Phys. Rev. B 71, 035109 (2005)

J. Enkovaara et al., J. Phys. Condens. Matter 22, 253202 (2010)

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Outline

- Basis sets in GPAW
- Overview of GPAW features
- Performance and parallelization

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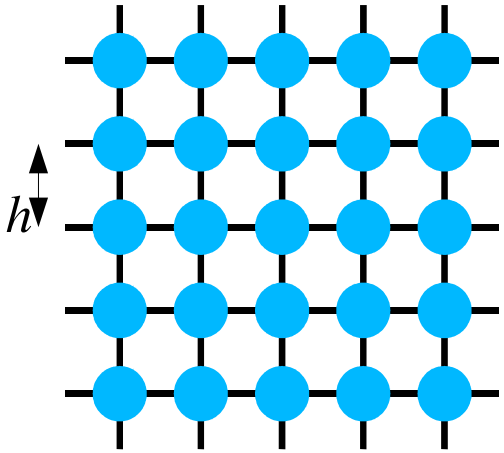
Real-space grids

- Wave functions, electron densities, and potentials are represented on grids.
- Single parameter, grid spacing h



- Accuracy of calculation can be improved systematically
- Derivatives by finite differences

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Boundary conditions

- Real-space description allows flexible boundary conditions
- Zero boundary conditions (finite systems)
- Periodic boundary conditions (bulk systems)
- Boundary conditions can be mixed
  - periodic in one dimension (wires)
  - periodic in two dimensions (surfaces)

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Localized basis set

- Linear combination of atomic orbitals (LCAO) provide compact basis set

$$\tilde{\psi}_n = \sum_\nu C_{n\nu}\Phi_\nu(\mathbf{r})$$

$$\Phi^a_{nlm}(\mathbf{r}) = R^a_{nl}(|\mathbf{r}-\mathbf{R}^a|)Y_{lm}(\mathbf{r}-\mathbf{R}^a)$$

- The atomic orbitals are obtained from a free atom in a confining potential well
- Possible to switch between localized basis and real-space grids
- Same boundary conditions as with real-space grid

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Plane wave basis

- Functions which are periodic with respect to unit cell can be written as sum of plane waves

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega^{1/2}} \sum_{\mathbf{G}} C_{\mathbf{G},n\mathbf{k}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}}$$

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \qquad V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

  where **G** are reciprocal lattice vectors

- The expansion is truncated according to

$$\frac{1}{2}|\mathbf{G}+\mathbf{k}|^2 < E_{cutoff}$$

- Only periodic cells (supercells)

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Comparison on basis sets

- Real-space grids
  - systematic convergence with single parameter
  - some integrals complicated in real-space
  - good parallelization prospects
- Localized basis set
  - compact basis
  - systematic convergence can be difficult
- Plane waves
  - systematic convergence with single parameter
  - some integrals simplified in reciprocal space
  - very efficient in small to medium size systems
  - parallelization more limited due FFTs

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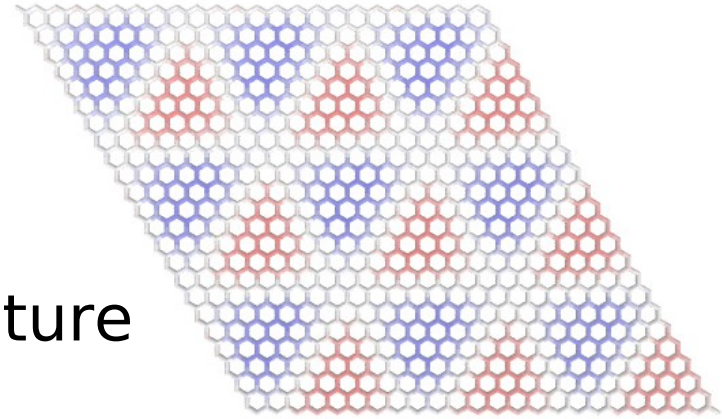
GPAW features

- Ground state properties
  - Total energies, forces, magnetic moments
  - Structural optimization
  - Analysis of electronic structure
  - ...
- Wide range of XC-potentials (thanks to **libxc**!)
  - LDAs, GGAs, meta-GGAs, hybrids, DFT+U, vdW, RPA



Corrugation of BN sheet on Al surface (vdW functional)

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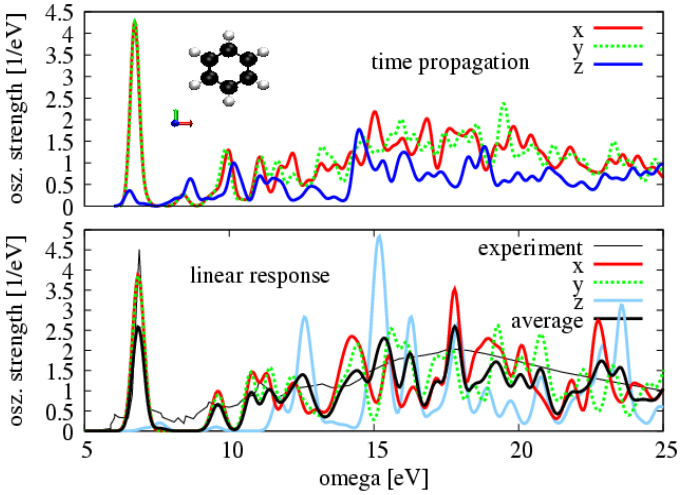
Time-dependent DFT

- Real-time propagation
  - Optical absoprtion spectra
  - Non-linear emission
  - Ehrenfest dynamics
- Linear response
  - Casida equation (finite systems)
  - Dyson equation (extended systems)
  - Excitation energies, optical absorption, electron energy loss spectra



M. Walter, L. Lehtovaara et al. J. Chem. Phys. 128 (2008)

J. Yan et al PRB 83, 245122 (2011)

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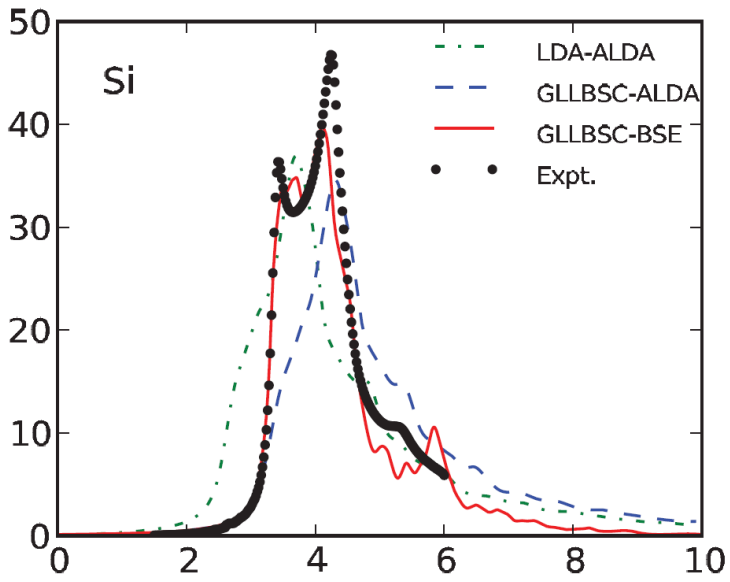
Many-body perturbation theory

- GW-approximation
  - Quasiparticle band structure
- Bethe-Salpeter equation
  - Excitonic effects in optical spectra



J. Yan et al. PRB 86, 045208 (2012)

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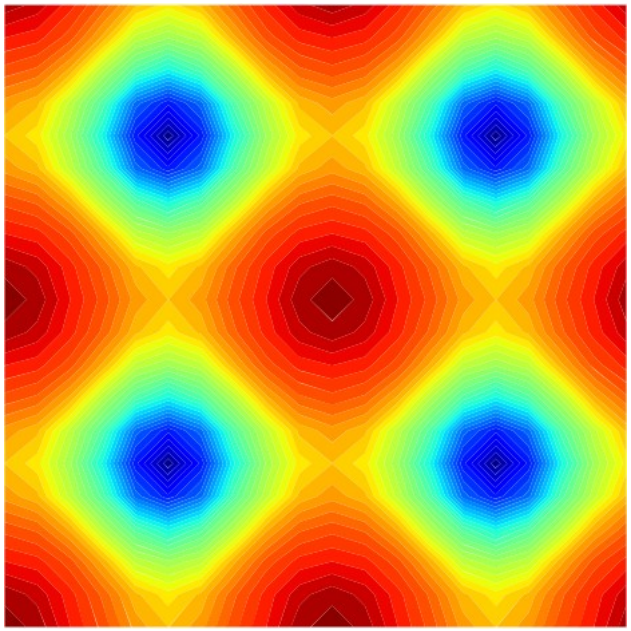
Other features

- Transport (Non-equilibrium Green functions)
- XAS spectra
- STM simulations
- ΔSCF
- Wannier functions
- …



STM image of
Al (100) surface

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Usage features

- Simple but flexible Python scripting interface via Atomic Simulation Environment
- Modular design helps implementing new features
- Runs on wide variety of computer architectures from simple Linux workstations to big supercomputers (Blue Gene P/Q, Cray, ...)
  - experimental GPGPU support
- Efficient parallelization, system sizes up to thousands of electrons

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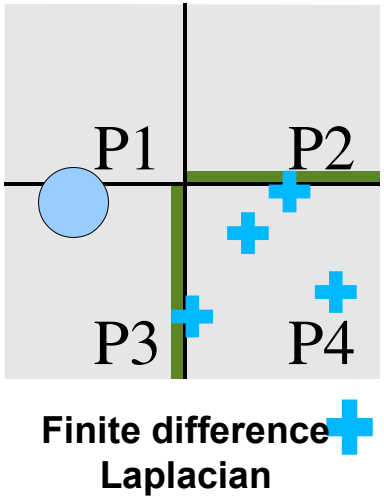
Parallelization in GPAW

$$H_{k,s}\psi_{i,k,s}(r) = e_i S\psi_{i,k,s}(r)$$

$$n(r) = \sum_{i,k,s} |\psi_{i,k,s}(r)|^2$$

- Parallelization over several degrees of freedom
- Domain decomposition (real-space, LCAO)
  - only local communication
- Parallelization over k-points and spin
  - periodic and magnetic systems
- Parallelization over electronic states



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Parallelization in GPAW

- Some GPAW features have additional parallelization possibilities
- Real-time TDDFT: trivial parallelization over electronic states
- Linear response TDDFT, Bethe-Salpeter: parallelization over electron-hole pairs
- GW: parallelization over energy

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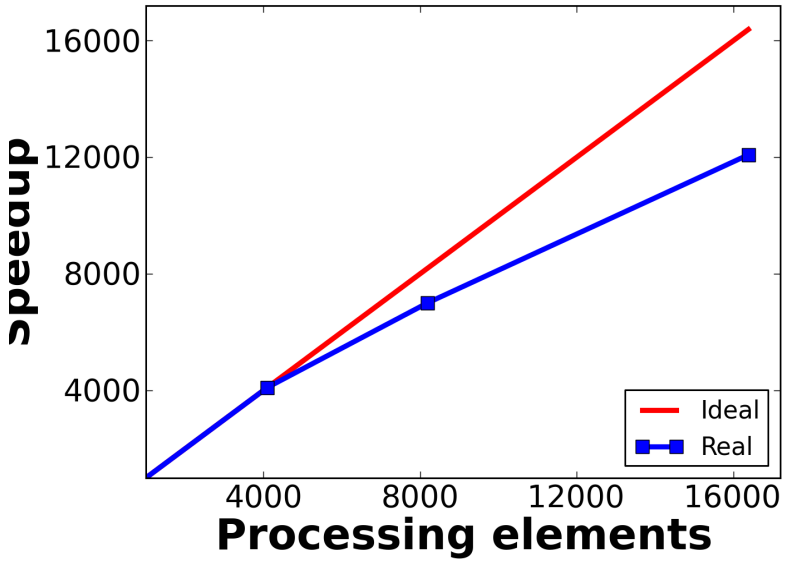
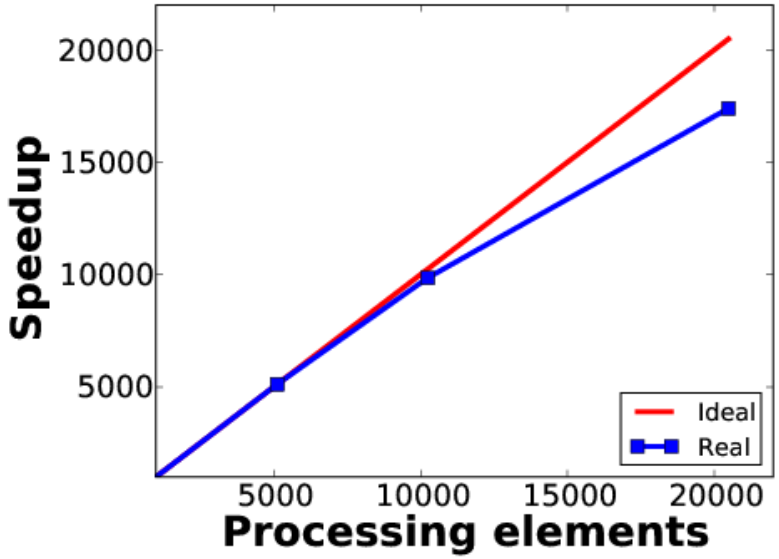
Parallel scalability





- Ground state DFT
  - 561 Au atom cluster
  - ~6200 electronic states
  - Blue Gene P, Argonne
- TD-DFT
  - 702 Si atom cluster
  - ~2800 electronic states
  - Cray XT5 Jaguar

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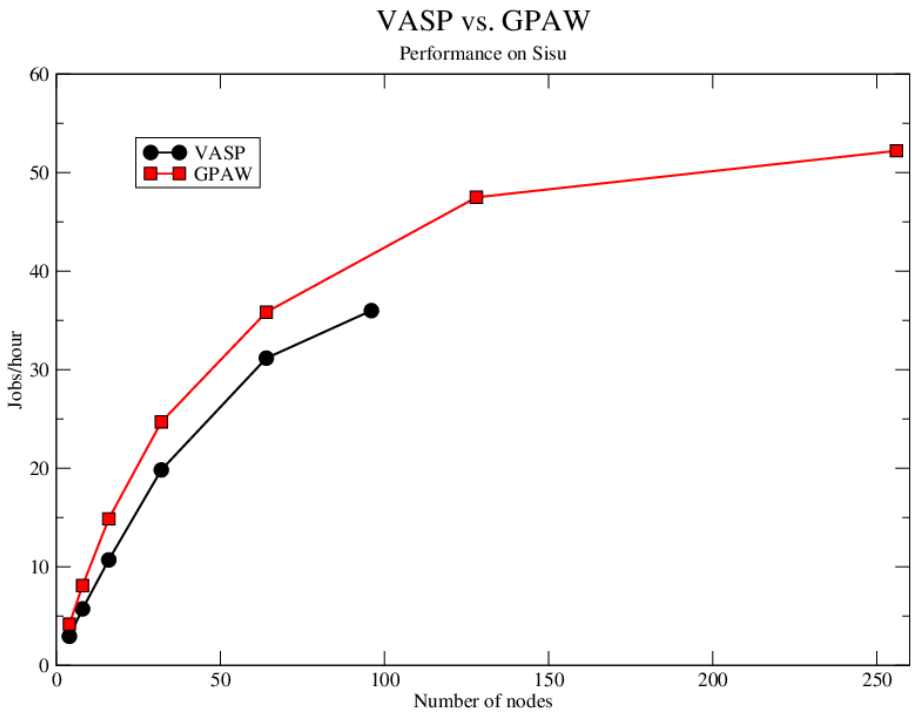
GPAW performance

- Generally, GPAW has similar performance to equivalent DFT packages



1269 atom MgH2 system, courtesy of T. Björkman

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Summary

- GPAW is a versatile program package for electronic structure calculations
- Different basis sets
- Vast set of features
- Well suitable for large scale calculations on massively parallel computers

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