

Systematics



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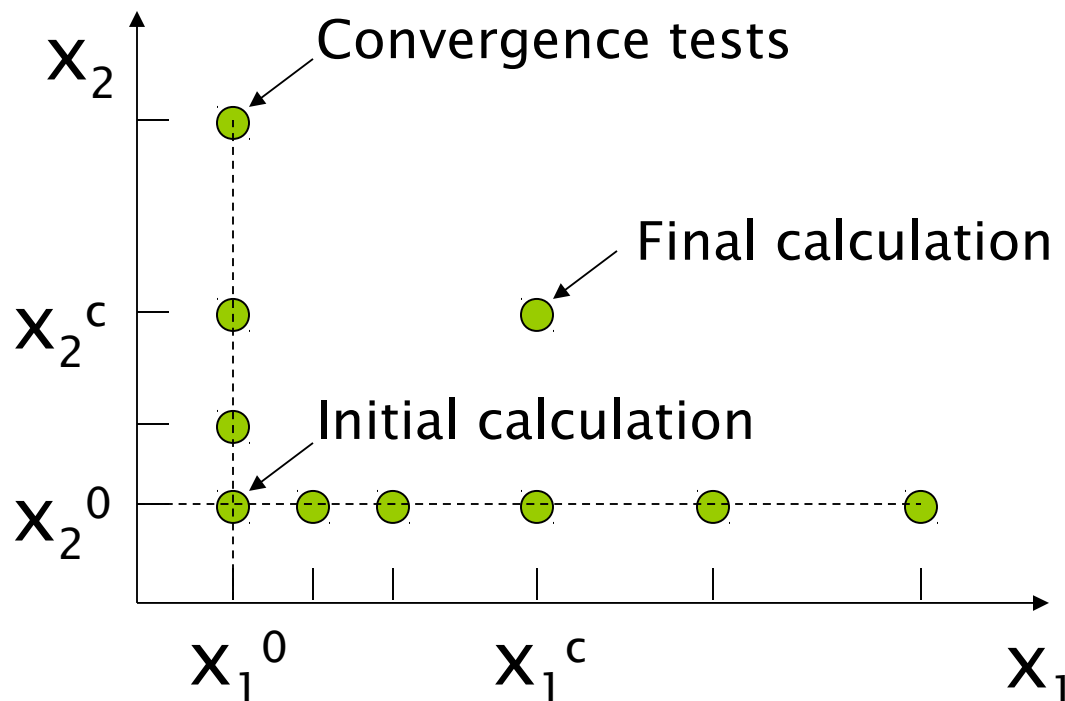
Basic strategy

- Exploratory-feasibility tests
- Convergence tests
- Converged calculations

A fully converged calculation is impossible without convergence tests

Convergence tests

- Choose relevant magnitude(s) A of the problem (e.g. an energy barrier or a magnetic moment)
- Choose set of qualitative and quantitative parameters x_i (e.g. xc functional, number of k-points, etc)



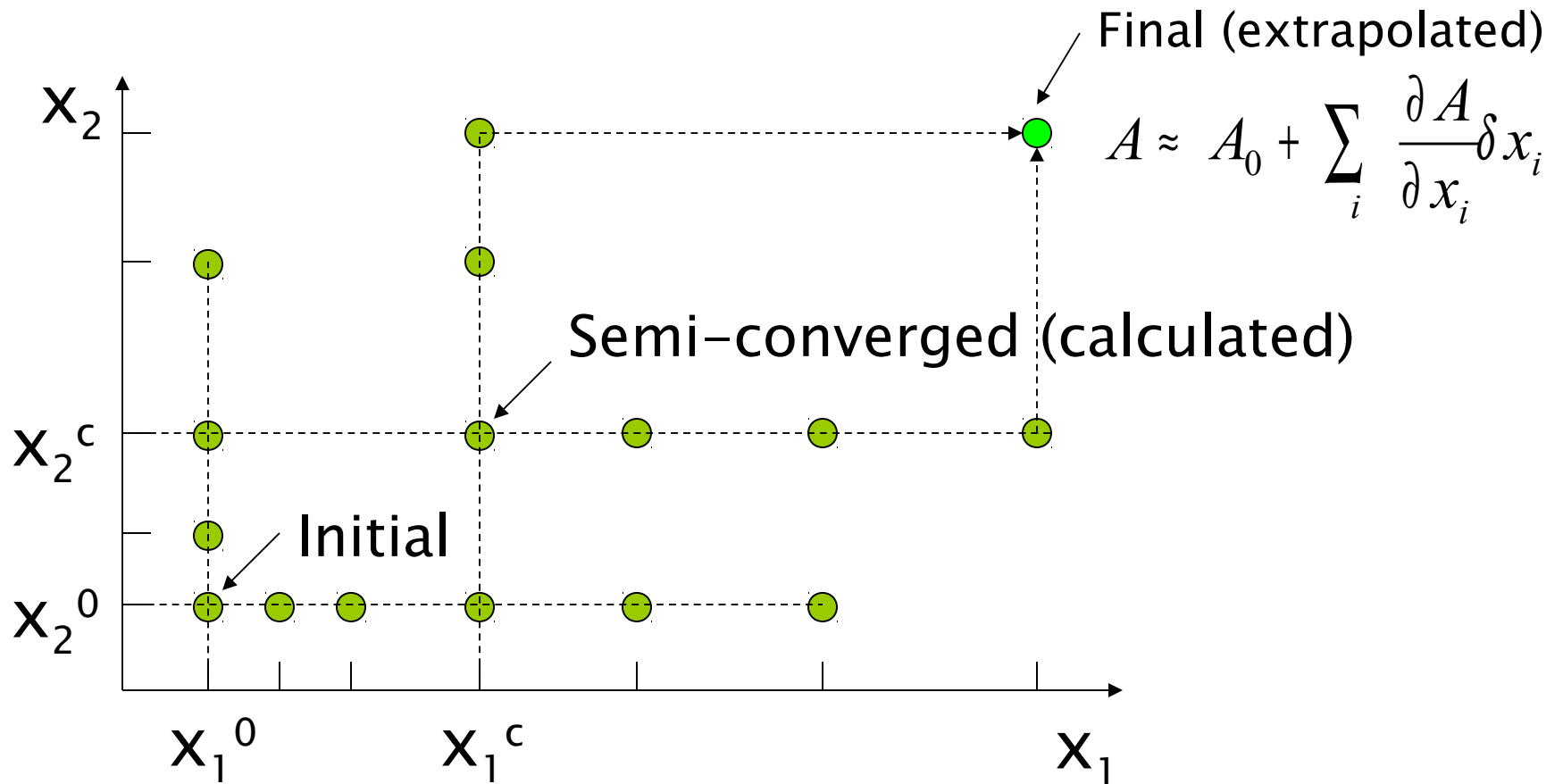
Parameter independence

$$A \approx A_0 + \sum_i \frac{\partial A}{\partial x_i} \delta x_i$$

Monitor:

- Convergence
- CPU time & memory

Multi-stage convergence



Practical hints

- Ask your objective: find the truth or publish a paper?
- Do not try a converged calculation from the start
- Start with minimum values of all x_i
- Do not assume convergence for any x_i
- Choose a simpler reference system for some tests
- Take advantage of error cancellations
- Refrain from stopping tests when results are “good”

Parameters list

- Pseudopotential
 - Method of generation
 - Number of valence states
 - Number of angular momenta
 - Core radii
 - Nonlinear core corrections
- Number of k-points
- Electronic temperature
- XC functional: LDA, GGAs
- Harris functional vs SCF
- Spin polarization
- SCF convergence tolerance
- Supercell size (solid & vacuum)
- Geometry relaxation tolerance
 - Check of final stability
- Basis set
 - Number of functions
 - Highest angular momentum
 - Number of zetas
 - Range
 - Shape
 - Sankey
 - Optimized
- Real space mesh cutoff
 - Grid-cell sampling
- Neglect nonoverlap interactions
- O(N) minimization tolerance

Harris functional

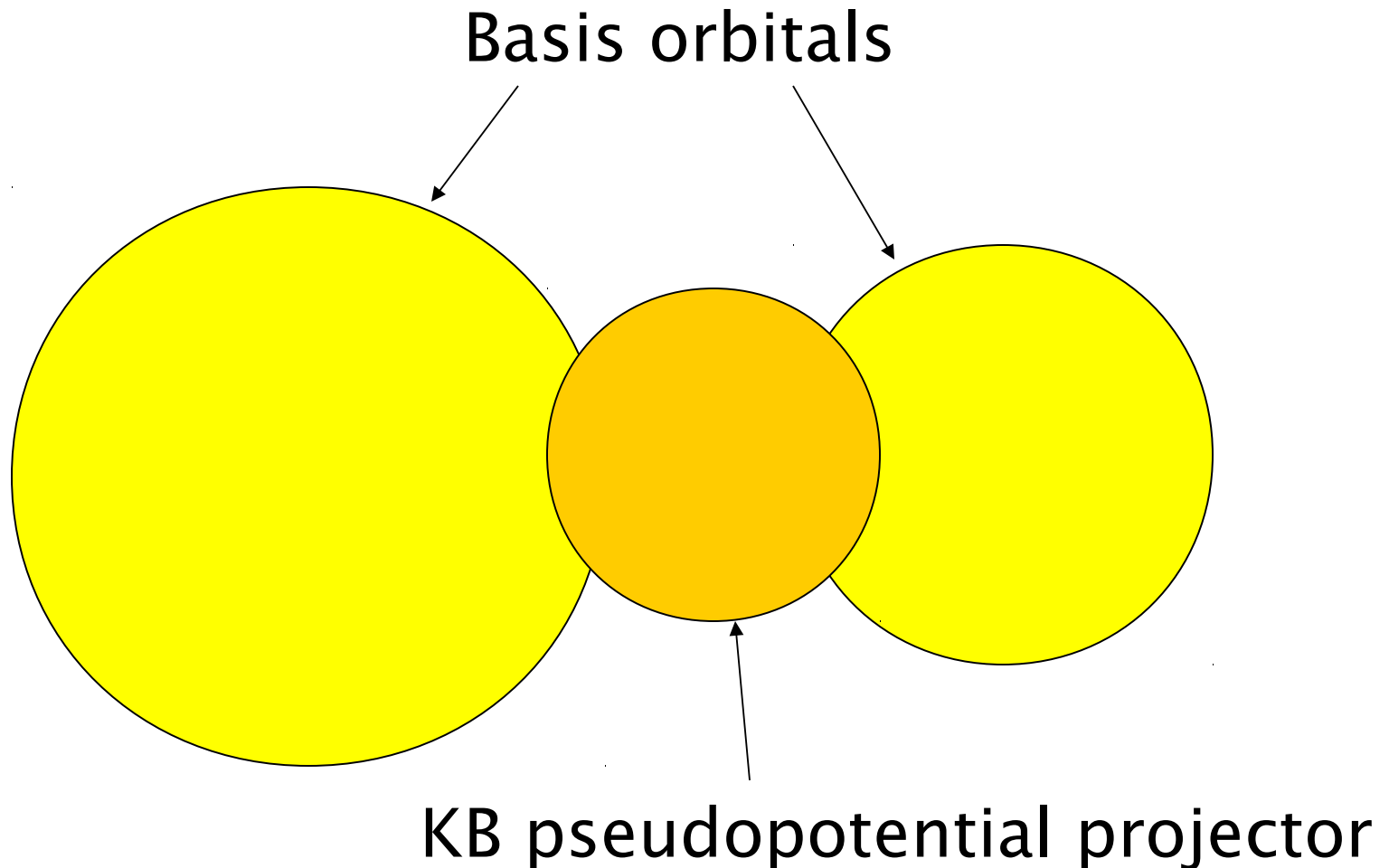
$$\rho(r) = \sum_i |\psi_i(r)|^2$$

$$E_{KS}[\rho] = -(1/2) \sum_i |\nabla \psi_i(r)|^2 + \int V_{\text{ext}}(r) \rho(r) dr \\ + (1/2) \int V_H(r) \rho(r) dr + \int \epsilon_{xc}(r) \rho(r) dr$$

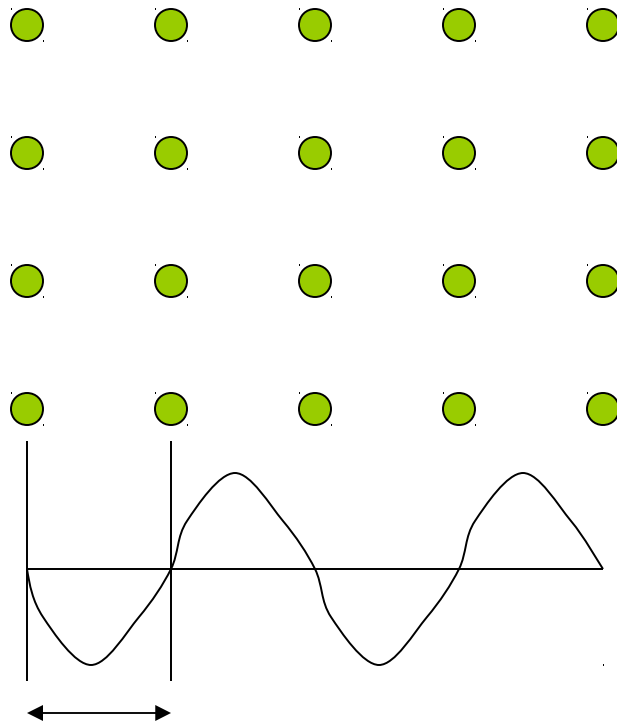
$$E_{\text{Harris}}[\rho_{\text{in}}] = E_{KS}[\rho_{\text{in}}] + \text{Tr}[(\rho_{\text{out}} - \rho_{\text{in}})H_{\text{in}}]$$

- Much faster SCF convergence
- Usually $\rho_{\text{in}} = \sum \rho_{\text{atoms}}$ and no SCF

Neglect of non-overlap interactions

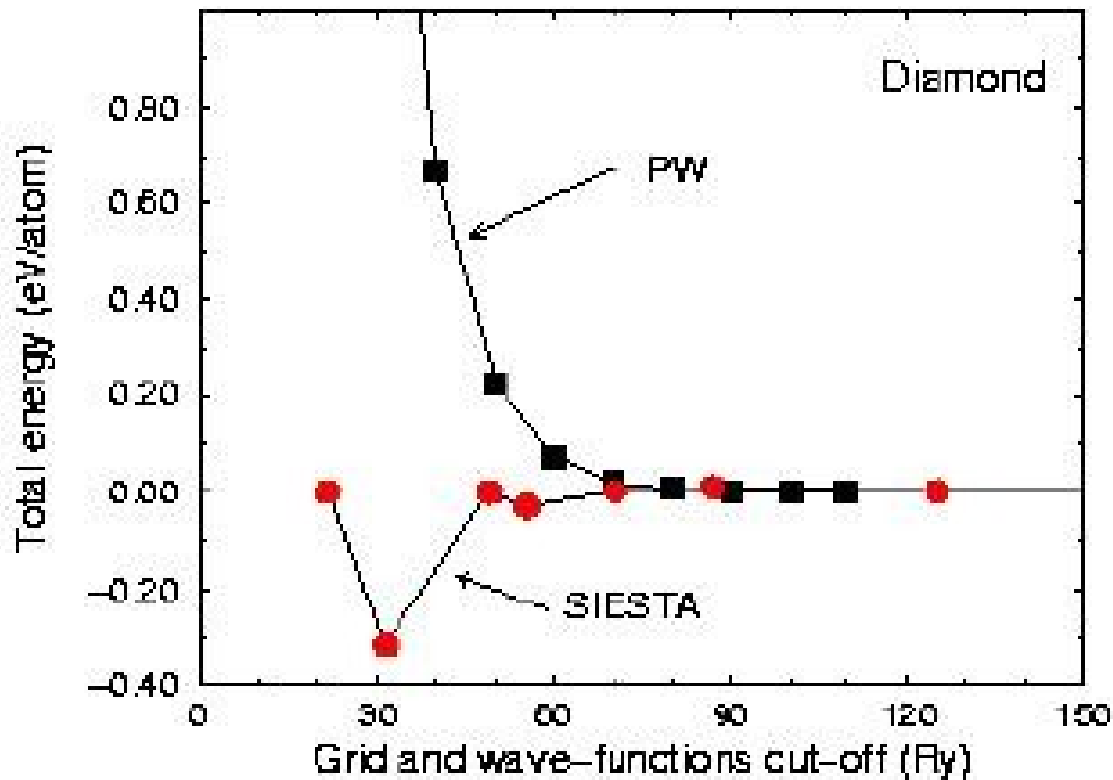


Mesh cutoff



$$\Delta x \Rightarrow k_c = \pi / \Delta x \Rightarrow E_c = \hbar^2 k_c^2 / 2m_e$$

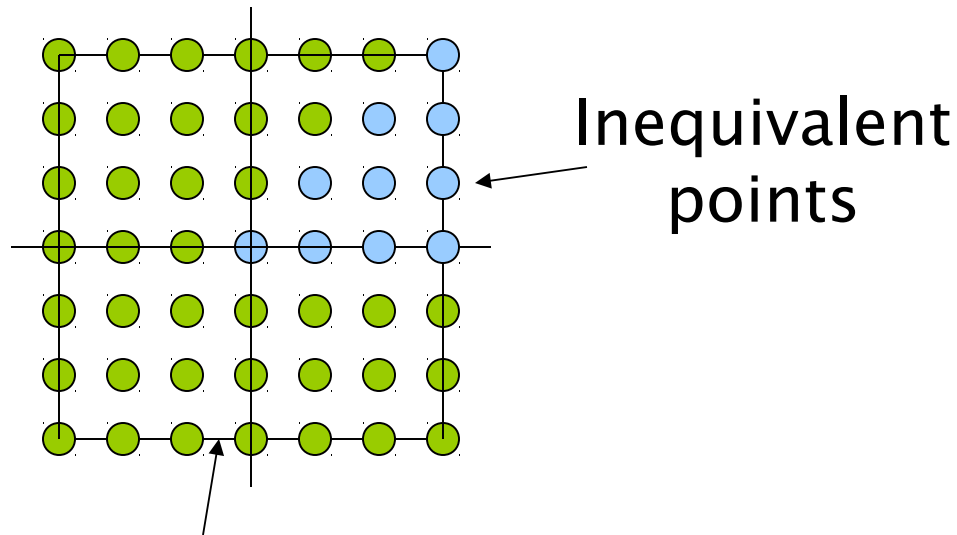
Grid fineness convergence



$$E_{cut} = (\pi / \Delta x)^2$$

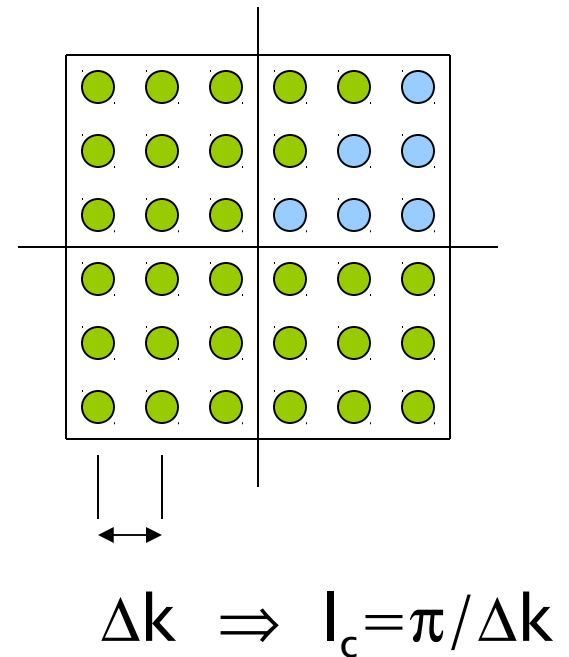
K-point sampling

Regular k-grid



First Brillouin Zone

Monkhorst-Pack



Miminal initial parameters

- Smaller system (e.g. Si(111)3x3 vs Si(111)7x7)
- Small supercell (e.g. 2-layer slab)
- Fixed geometry (no relaxation)
- Harris functional (no selfconsistency)
- Minimum pseudo-valence states (e.g. Ti 3s3p3d)
- No nonlinear core correction
- Minimal basis set (single zeta)
- Small basis range (e.g. Eshift=0.5eV)
- Gamma point
- Large electronic temperature (e.g. 3000 K)
- LDA
- Neglect non-overlap interactions

Parameter interactions

Number of k-points:

- Supercell size
- Geometry
- Electronic temperature
- Spin polarization
- Harris vs SCF

Mesh cutoff:

- Pseudopotential
- Nonlinear core corrections
- Basis set
- GGA

Surface (slab) calculations

