Systematic testing

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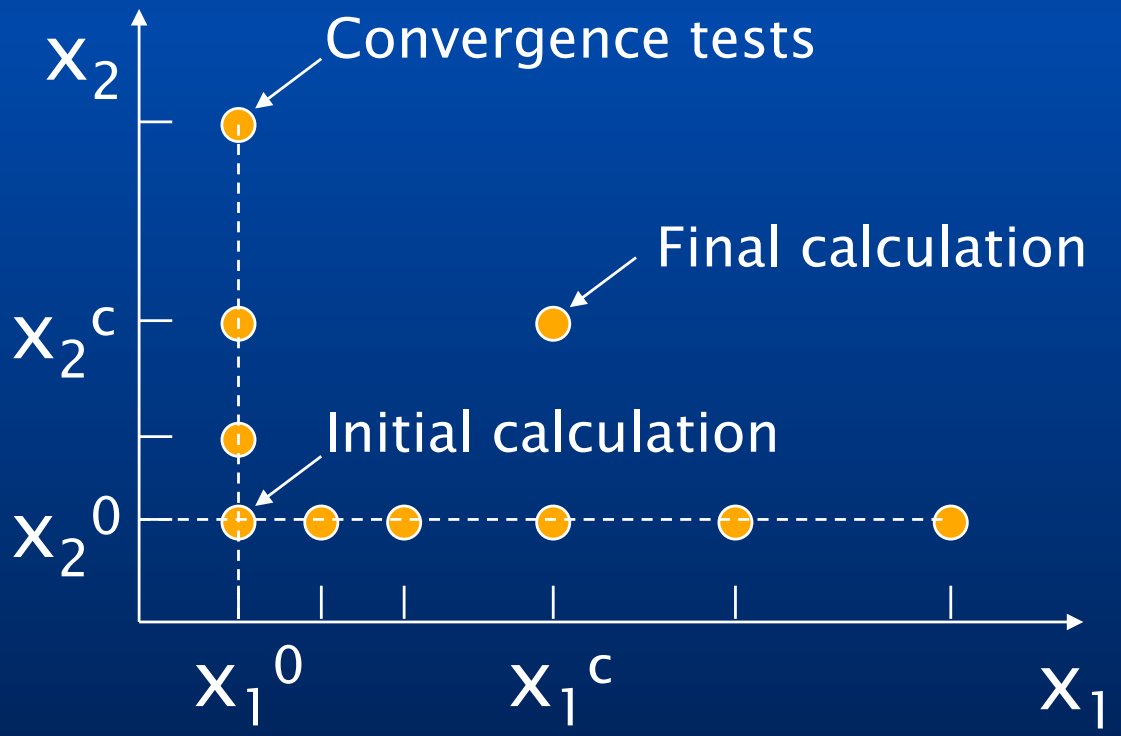
Basic strategy

- Exploratory–feasibility tests
- Convergence tests
- Converged calculations

A reliable result 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)



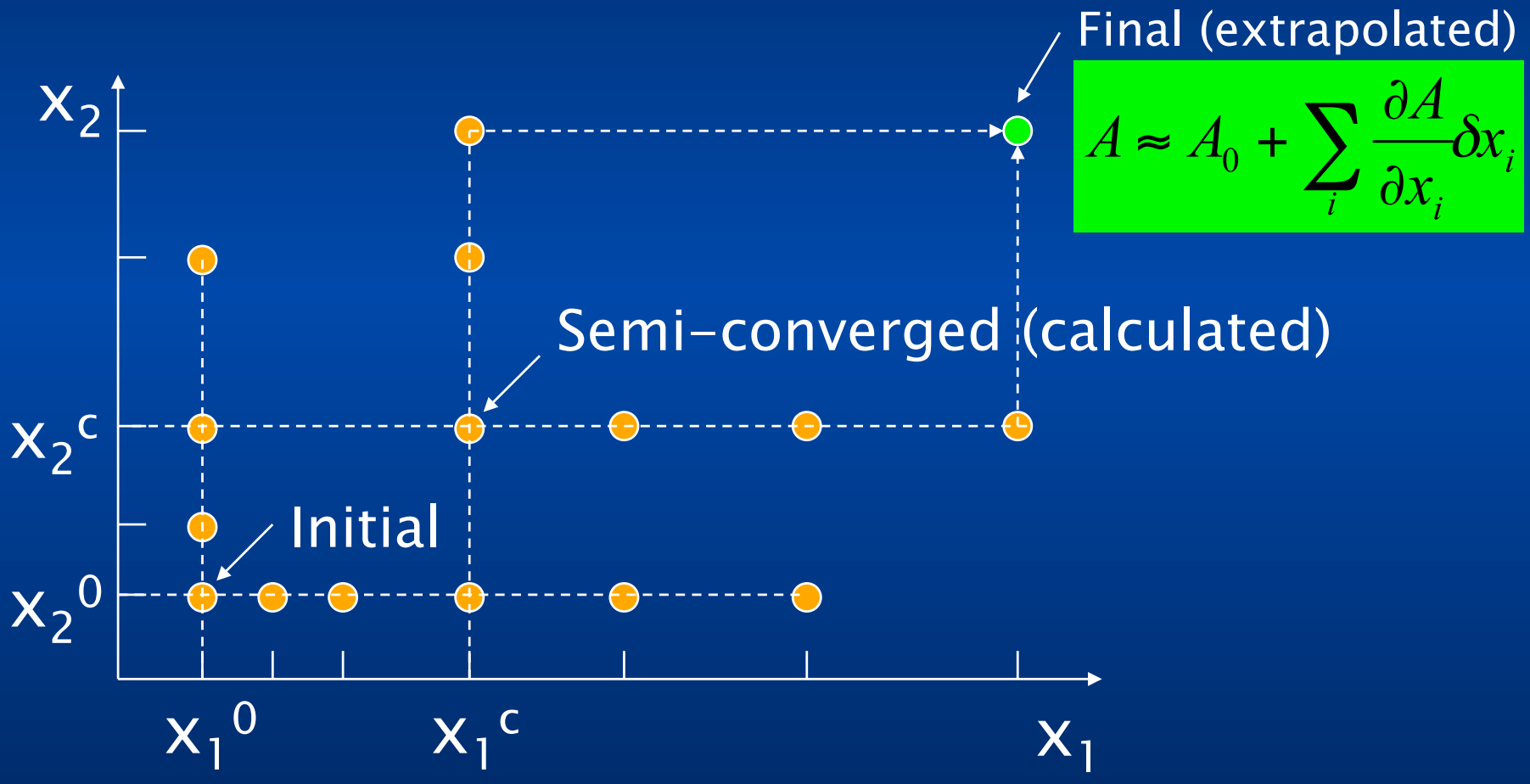
Parameter independence

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

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”

Short parameter list

- XC functional: LDA, GGAs, vdWs
- Pseudopotential
- Basis set
    - Number of functions
        - Highest angular momentum
        - Number of zetas
    - Range
- Real space mesh cutoff
- Number of k-points
- Spin polarization
- SCF convergence tolerance
- System size (atoms & vacuum)
- Geometry relaxation tolerance
- MD time step & duration

Parameter interactions

$$\partial^2 A / \partial x_i \partial x_j \neq 0$$

Number of k-points:

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

Mesh cutoff:

- Pseudopotential
- Nonlinear core corrections
- Basis set
- GGA