Linear scaling fundamentals and algorithms

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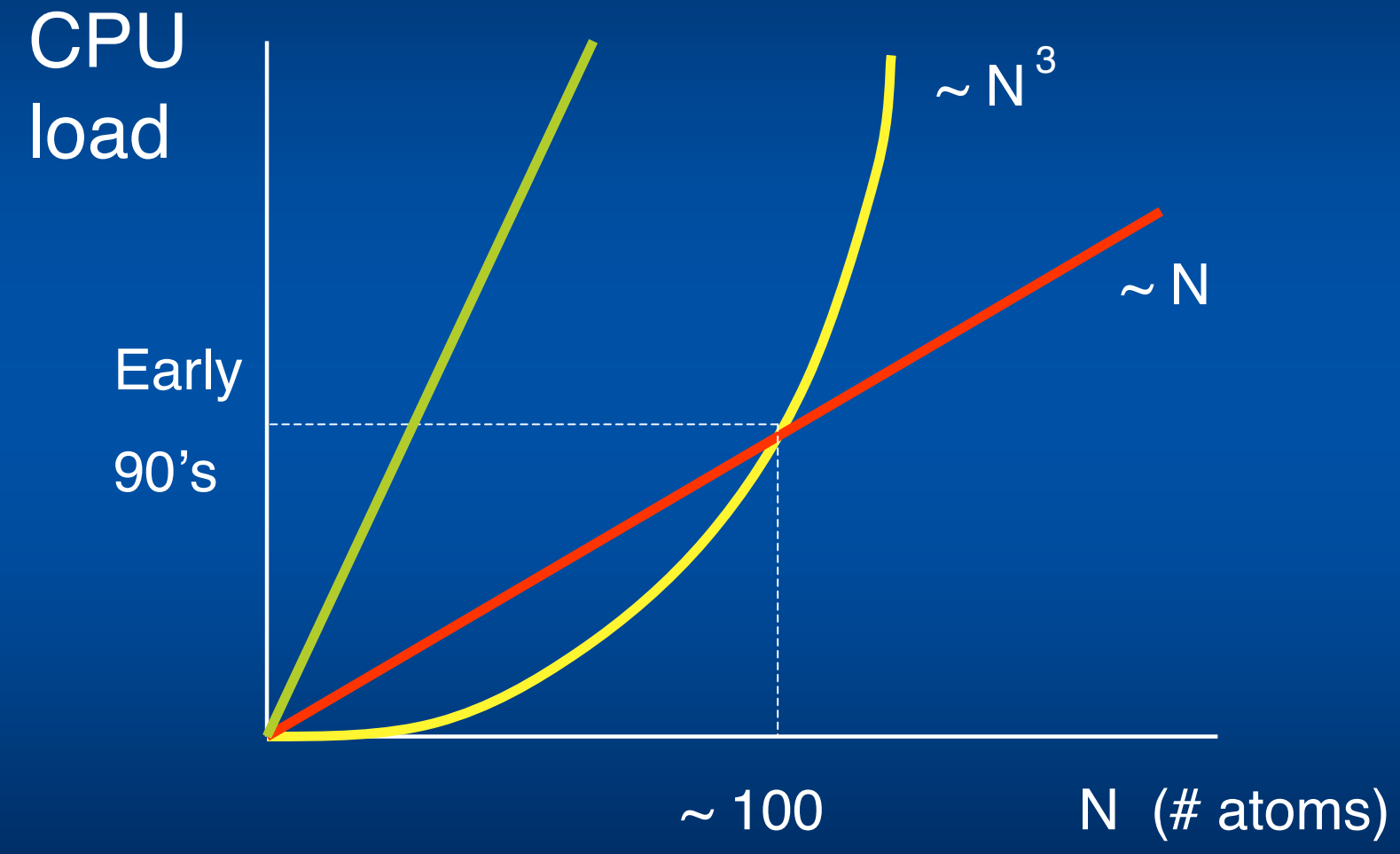
Linear scaling = Order(N)



Order-N DFT

1. Find density and hamiltonian (80% of code)
2. Find “eigenvectors” and energy (20% of code)
3. Iterate SCF loop

Steps 1 and 3 spared in tight-binding schemes

DFT: successful but heavy

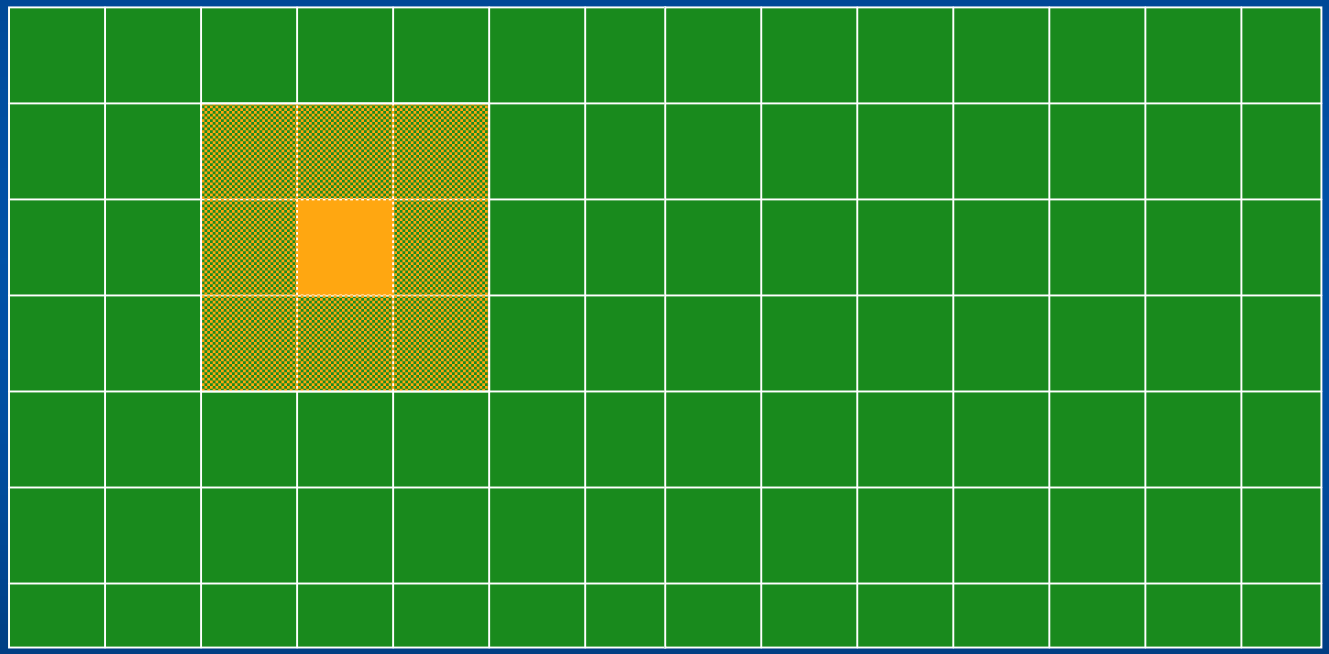
- *Computationally much more expensive than empirical atomic simulations*
- *Several hundred atoms in massively parallel supercomputers*

- *Computational load* $\sim N^3$

$$\langle \psi_n | \psi_m \rangle = \int \psi_n^*(\vec{r}) \psi_m(\vec{r}) d^3\vec{r} = \delta_{n,m}$$

Key to O(N): locality

Large system



``Divide and conquer'' *W. Yang, Phys. Rev. Lett. 66, 1438 (1992)*

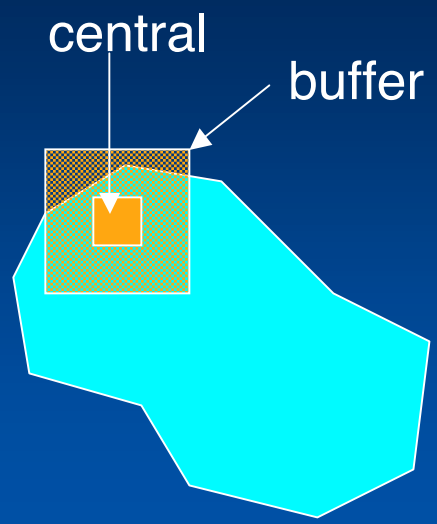
``Nearsightedness'' *W. Kohn, Phys. Rev. Lett. 76, 3168 (1996)*

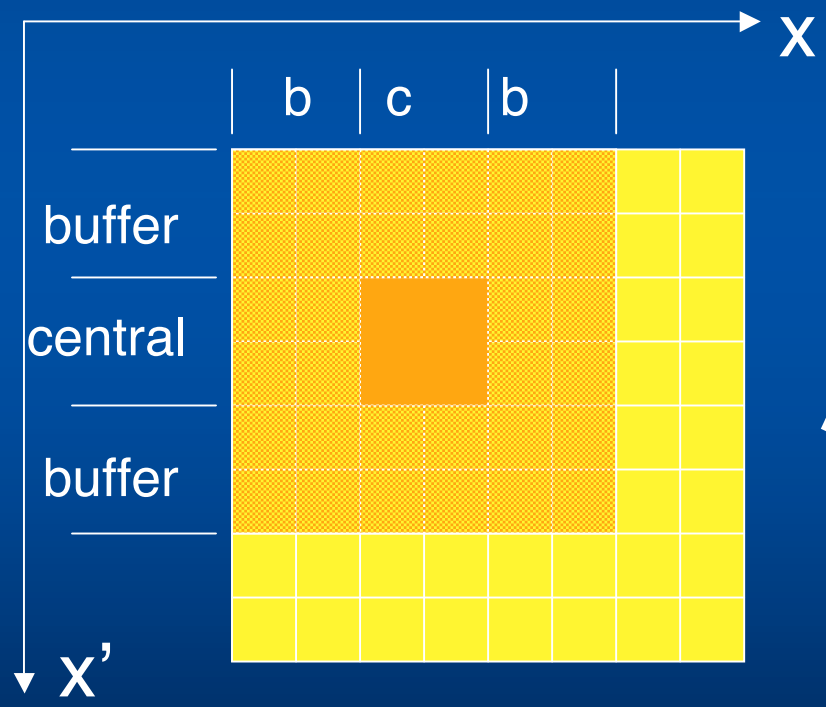
Basis sets for linear-scaling DFT

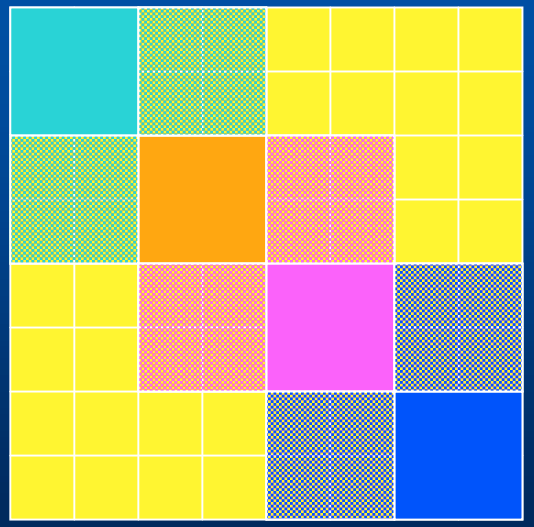
- *LCAO:* - Gaussian based + QC machinery
  G. Scuseria (GAUSSIAN),
  M. Head-Gordon (Q-CHEM)
  - Numerical atomic orbitals (NAO)
  SIESTA
  S. Kenny &. A Horsfield (PLATO)
  - Gaussian with hybrid machinery
  J. Hutter, M. Parrinello
- *Bessel functions in ovelapping spheres*
  P. Haynes & M. Payne
- *B-splines in 3D grid*
  D. Bowler & M. Gillan
- *Finite-differences (nearly O(N))* *J. Bernholc*

Divide and conquer

Weitao Yang (1992)



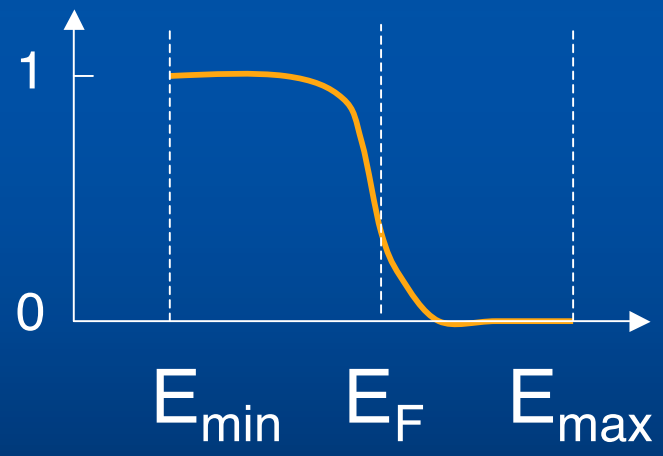




Fermi operator/projector

Goedecker & Colombo (1994)

$$f(E) = 1/(1+e^{E/kT}) \approx \sum_n c_n E^n$$

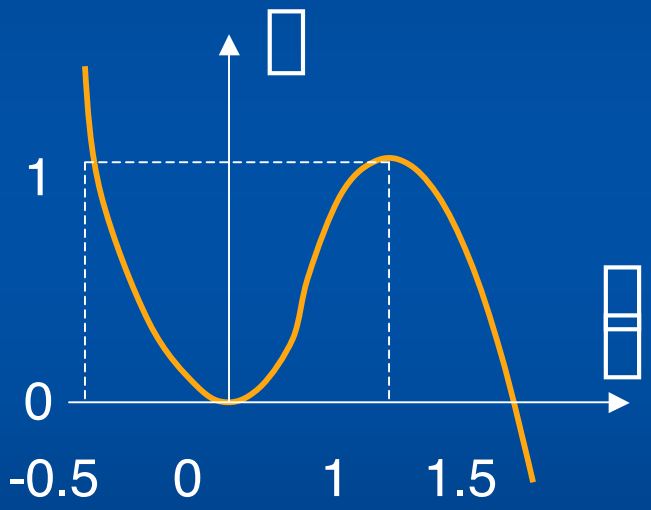


$$\hat{F} \approx \sum_n c_n \hat{H}^n$$

$$E_{tot} = Tr[\hat{F}\hat{H}]$$

Density matrix functional

Li, Nunes & Vanderbilt (1993)



$$\rho_{ij} = 3\rho^2_{ij} - 2\rho^3_{ij}$$

$$E_{tot}(\rho_{ij}) = \rho_{ij}\rho_{ij}H_{ij} = \min$$

Wannier O(N) functional

- Mauri, Galli & Car, PRB **47**, 9973 (1993)
- Ordejon et al, PRB **48**, 14646 (1993)

$$S_{ij} = \langle \phi_i | \phi_j \rangle \qquad | \phi'_k \rangle = \phi_j | \phi_j \rangle S_{jk}^{-1/2}$$

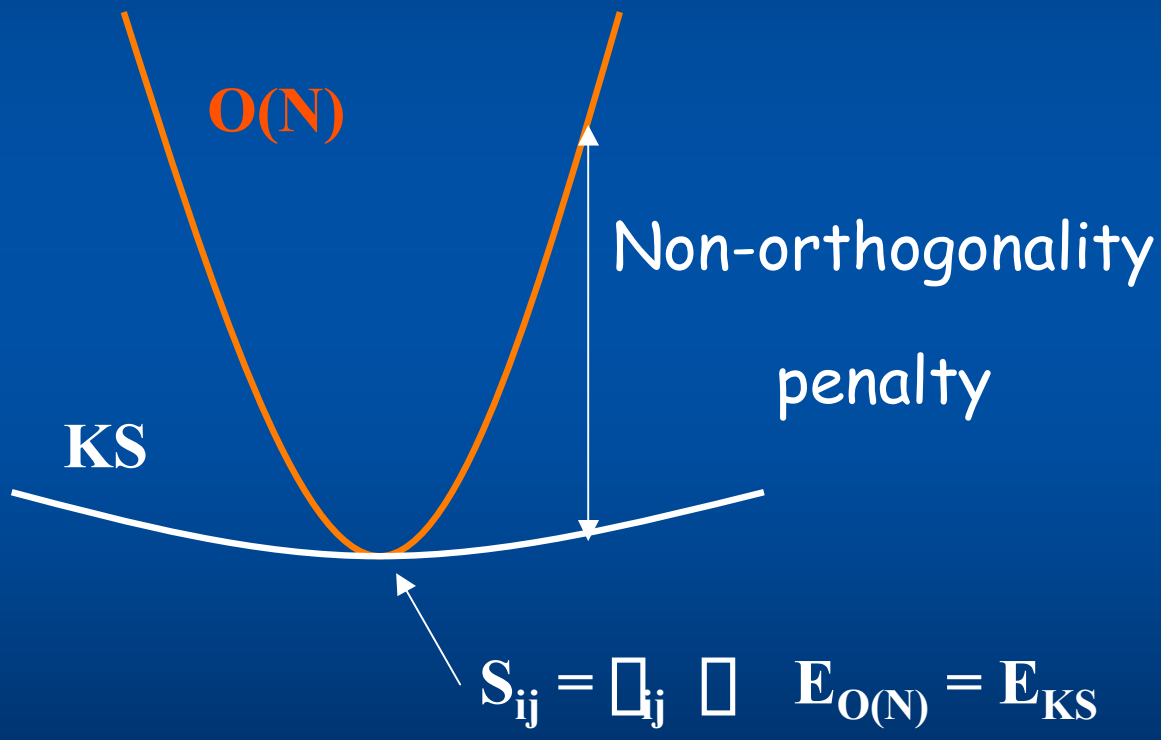
$$E_{KS} = \phi_k \langle \phi'_k | \hat{H} | \phi'_k \rangle$$

$$= \phi_{ijk} S_{ki}^{-1/2} \langle \phi_i | \hat{H} | \phi_j \rangle S_{jk}^{-1/2}$$

$$= \mathrm{Tr}[\, S^{-1} H \,] \qquad \textbf{Kohn-Sham}$$

$$E_{O(N)} = \mathrm{Tr}[\, (2I-S) H \,] \qquad \textbf{Order-N}$$

Order-N vs KS functionals



Chemical potential

Kim, Mauri & Galli, PRB **52**, 1640 (1995)

$\rho(r) = 2\Omega_{ij}\,\phi_i(r)\,(2\Omega_{ij}-S_{ij})\,\phi_j(r)$

$E_{O(N)} = Tr[\,(2I-S)\,H\,]$ # states = # electron pairs

- Local minima

$E_{KMG} = Tr[\,(2I-S)\,(H-\mu S)\,]$ # states > # electron pairs

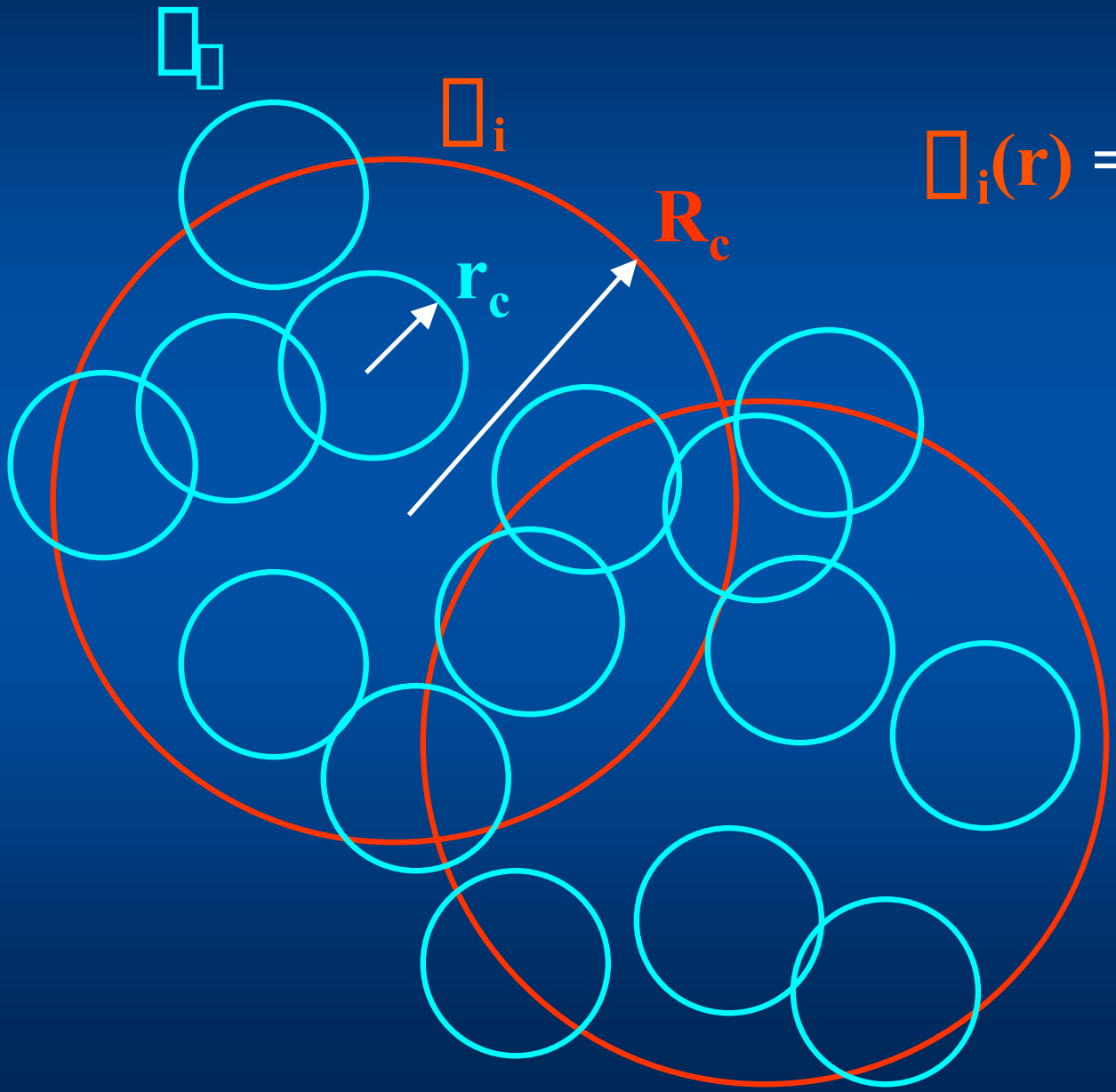
- μ = chemical potential (Fermi energy)

$E_i < \mu \quad \mu \quad |\Omega_i| \to 0$

$E_i > \mu \quad \mu \quad |\Omega_i| \to 1$

Difficulties	Solutions
Stability of $N(\mu)$	Initial diagonalization
First minimization of E_{KMG}	Reuse previous solutions

Orbital localization

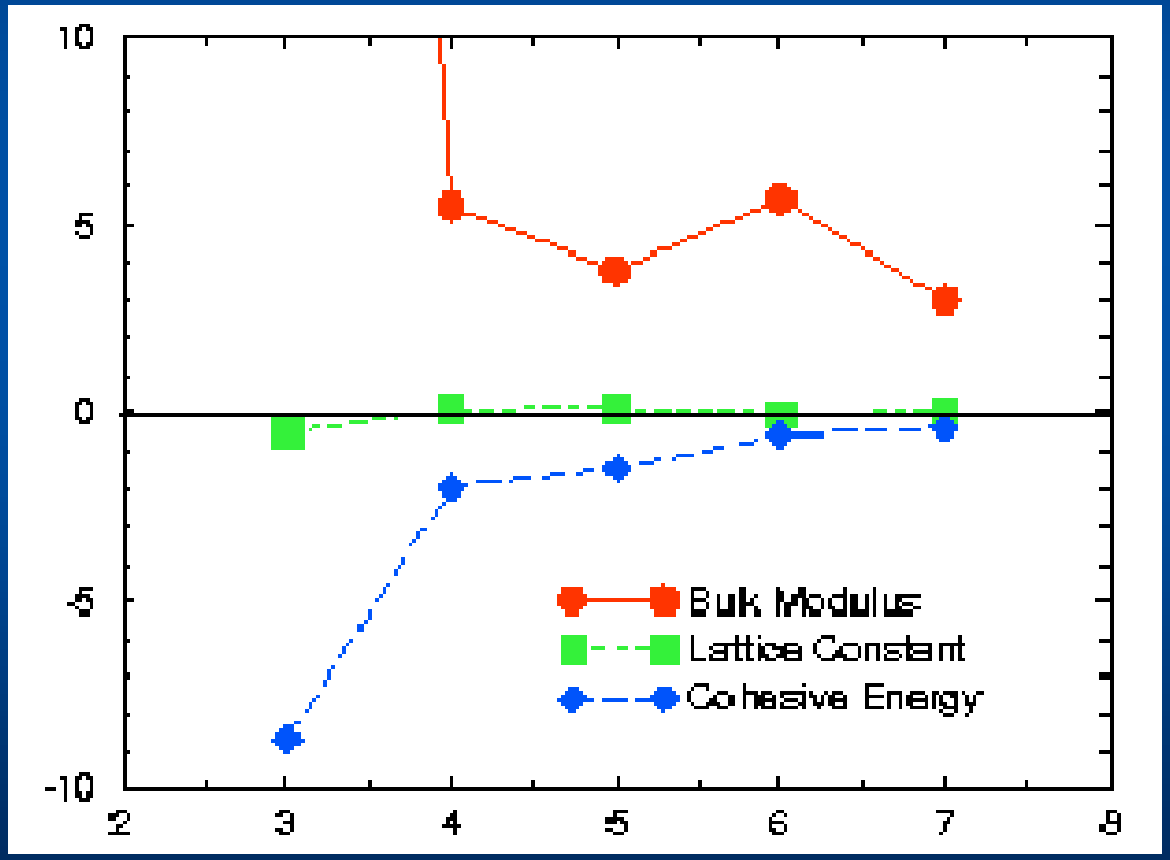


$$\psi_i(\mathbf{r}) = \sum_\mu c_{i\mu}\,\phi_\mu(\mathbf{r})$$

Convergence with localisation radius

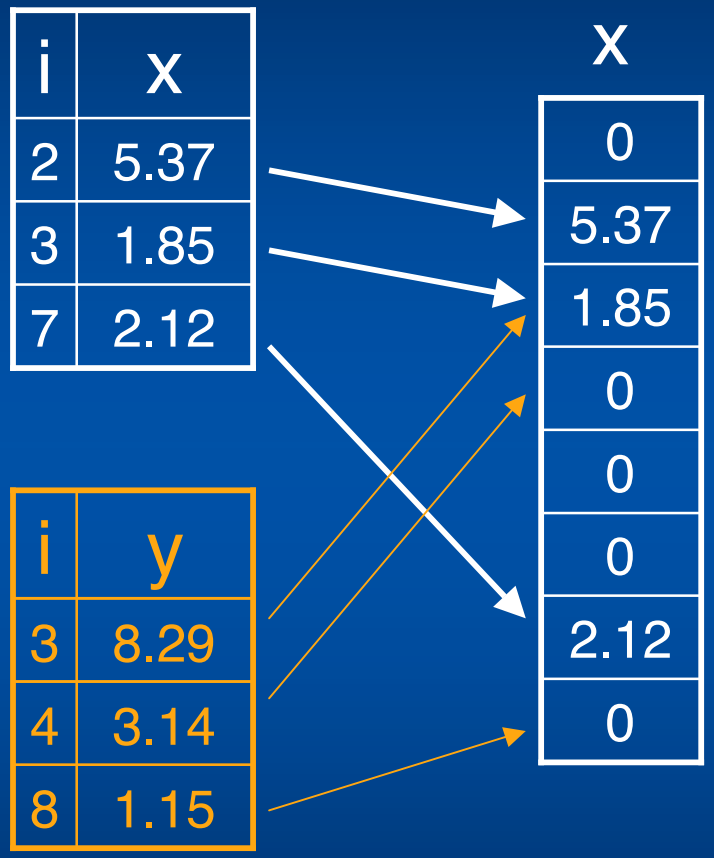
Si supercell, 512 atoms

Relative Error (%)



R_c (Ang)

Sparse vectors and matrices



8.29 □ 1.85 = 15.34

3.14 □ 0 = 0

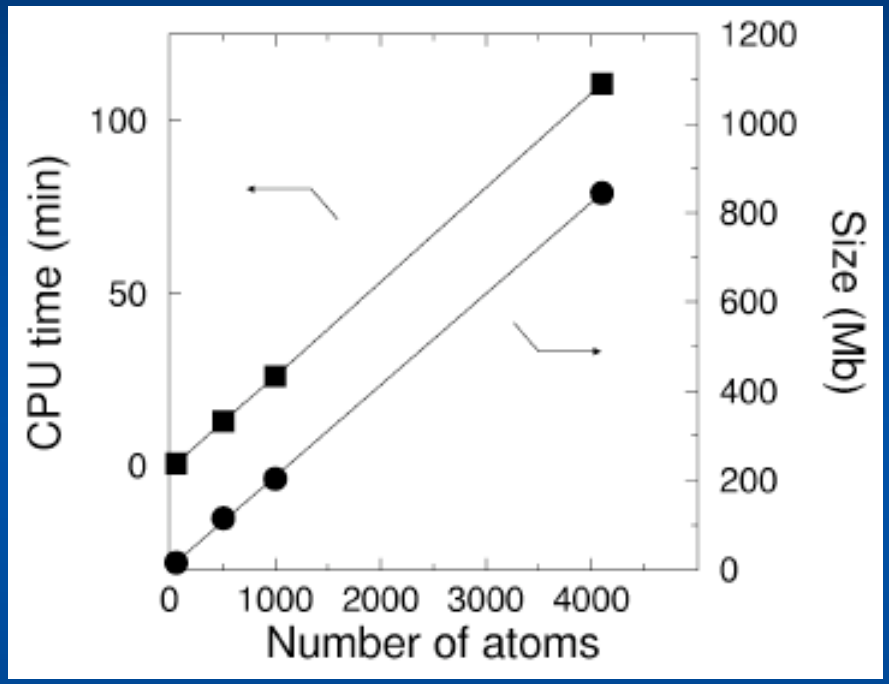
1.15 □ 0 = 0

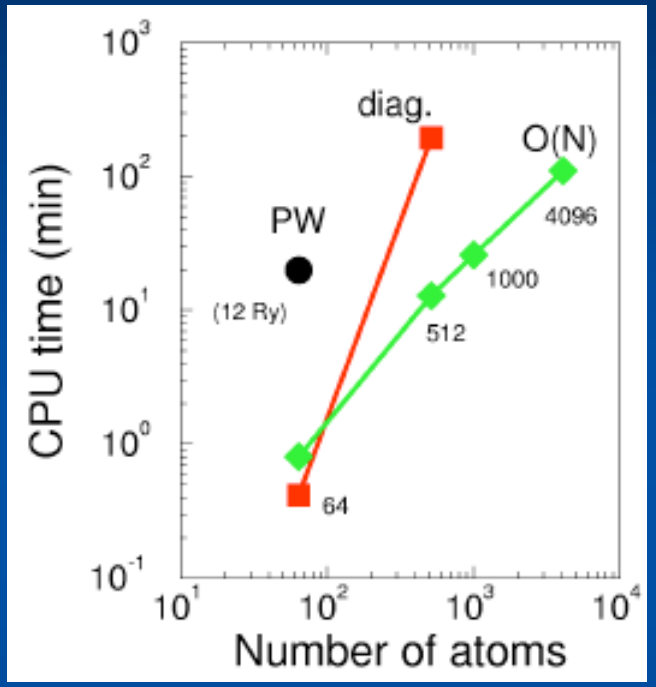
Sum 15.34

Restore to zero $x_i \neq 0$ **only**

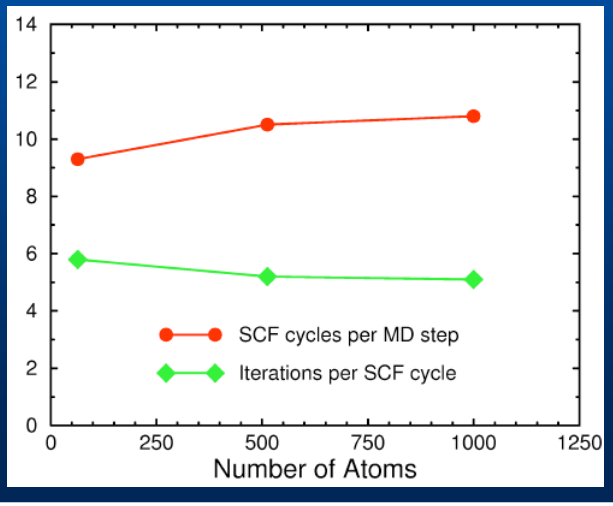
Actual linear scaling

c-Si supercells, single-□





Single Pentium III 800 MHz. 1 Gb RAM



132.000 atoms in 64 nodes