Linear−scaling density−functional theory with plane−waves

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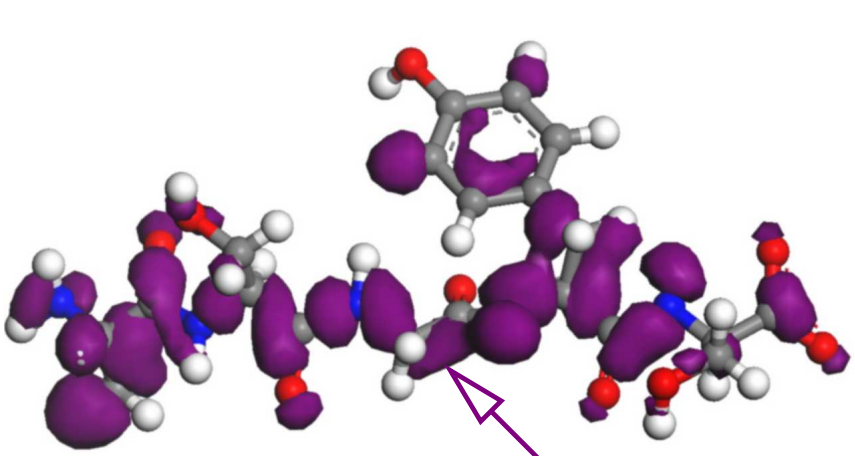
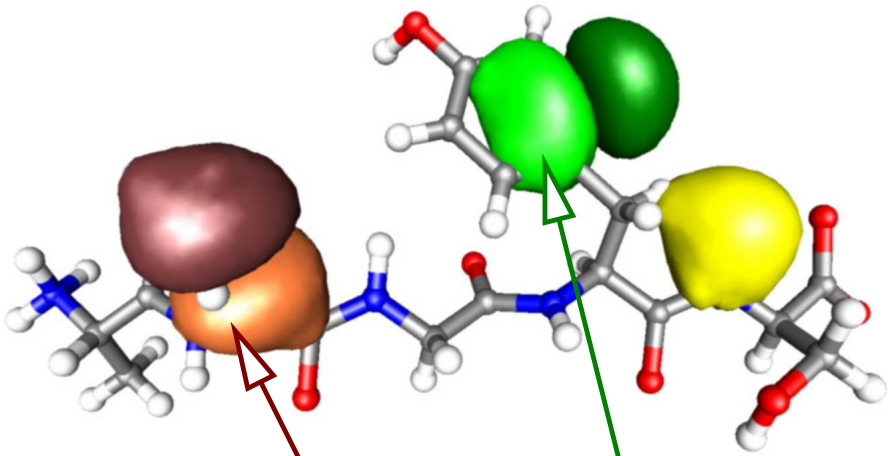
Density−matrix linear−scaling methods





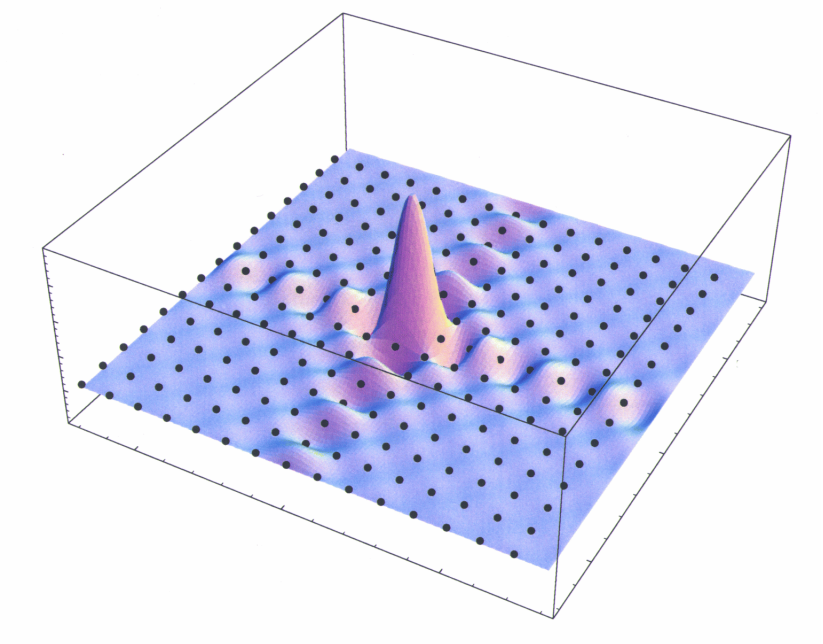
$$\rho(\mathbf{r},\mathbf{r}') \quad = \quad \sum_n f_n \, \psi_n(\mathbf{r}) \, \psi_n^*(\mathbf{r}') \quad = \quad \sum_{\alpha\beta} \phi_\alpha(\mathbf{r}) \, K^{\alpha\beta} \, \phi_\beta^*(\mathbf{r}')$$

- Optimise non−orthogonal localised functions $\{\phi_\alpha(\mathbf{r})\}$
  instead of orthogonal extended wavefunctions $\{\psi_n(\mathbf{r})\}$ } linear scaling
- Aim: to achieve the same accuracy as traditional plane−wave methods

Basis set

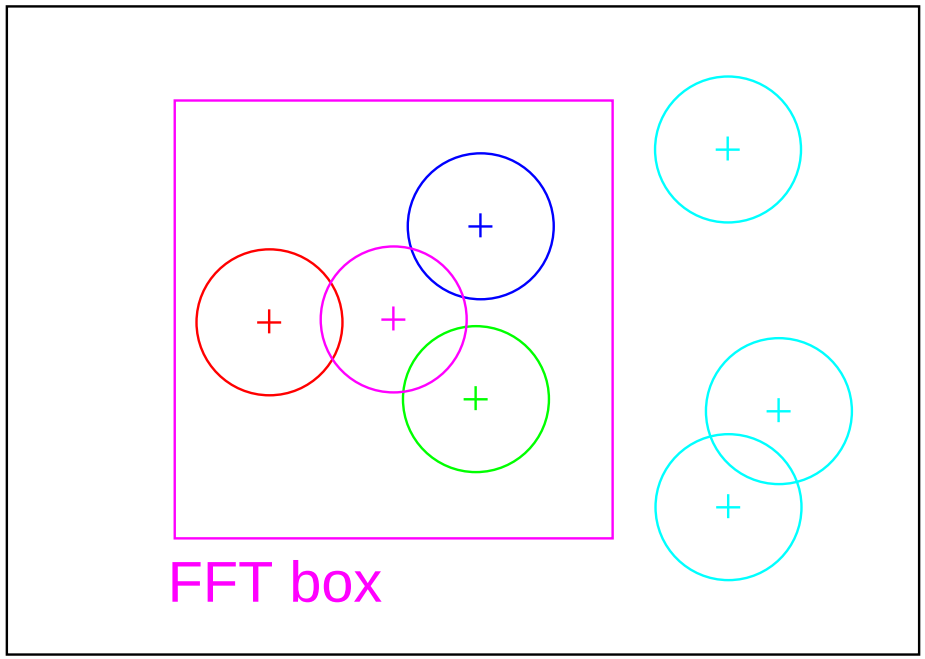
PSINC orthogonal basis:

(Periodic Cardinal Sine)



- Orthogonal
- Localised
- Linear combination of plane−waves

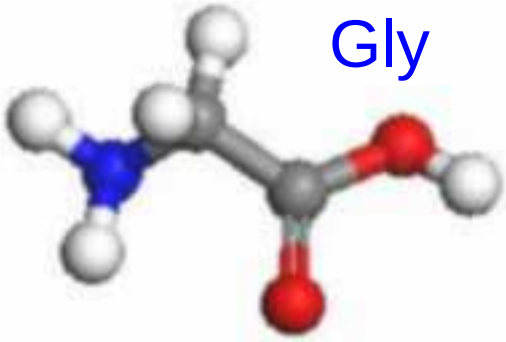
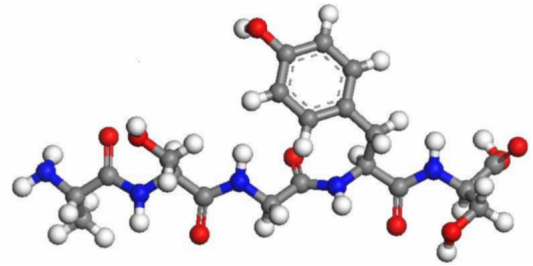
FFT box technique:



Simulation cell

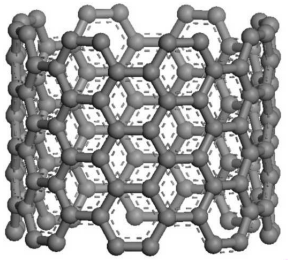
- Same FFT box for all functions guarantees:
  - Hermitian Hamiltonian matrix
  - consistent action of operators
- Equivalent to a coarse reciprocal−space sampling

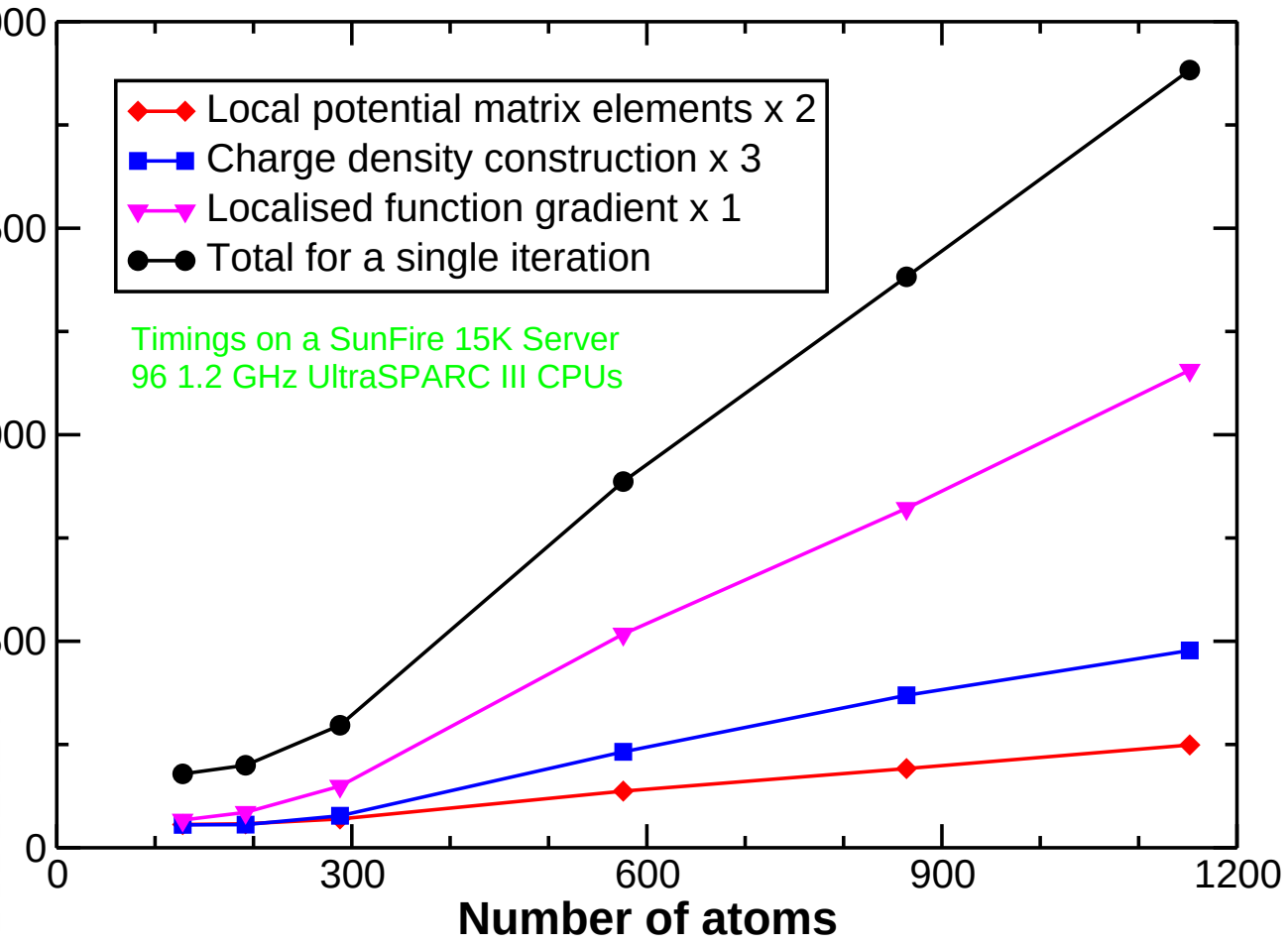
Comparison with traditional plane−wave code

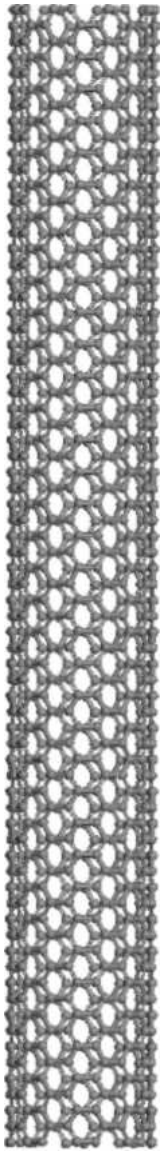
Energy differences between nonionic and zwitterionic forms	CASTEP	**ONETEP**
 Gly	1.21 eV (28.0 kcal mol^{-1})	1.20 eV (27.7 kcal mol^{-1})
 AlaSerGlyTyrSer	1.07 eV (24.7 kcal mol^{-1})	1.08 eV (24.9 kcal mol^{-1})

- Same energy cutoff: 40 Ry
- Same simulation cell
- Same pseudopotentials: Troullier−Martins norm−conserving
- Same XC functional: LDA

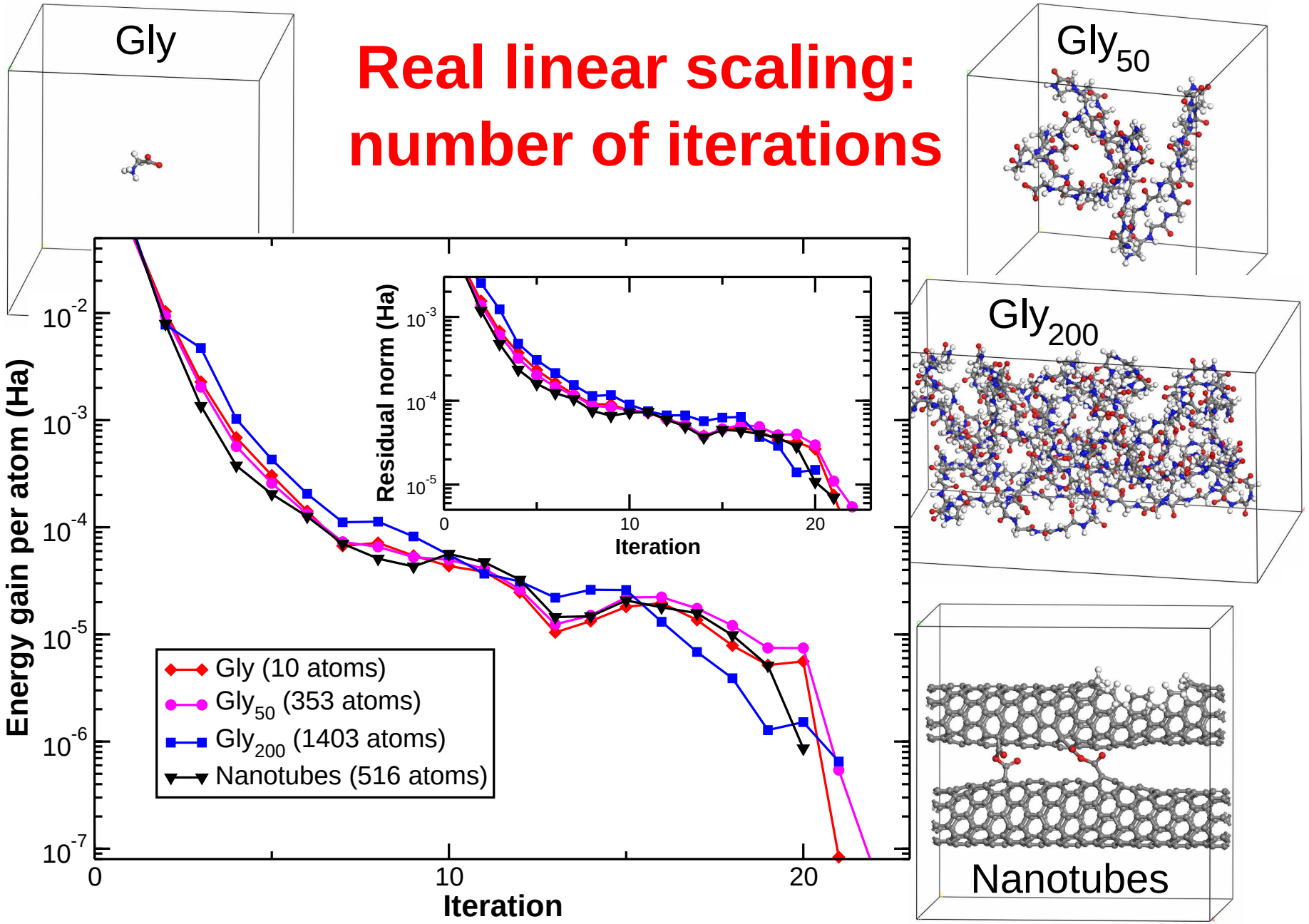
Linear scaling with system−size



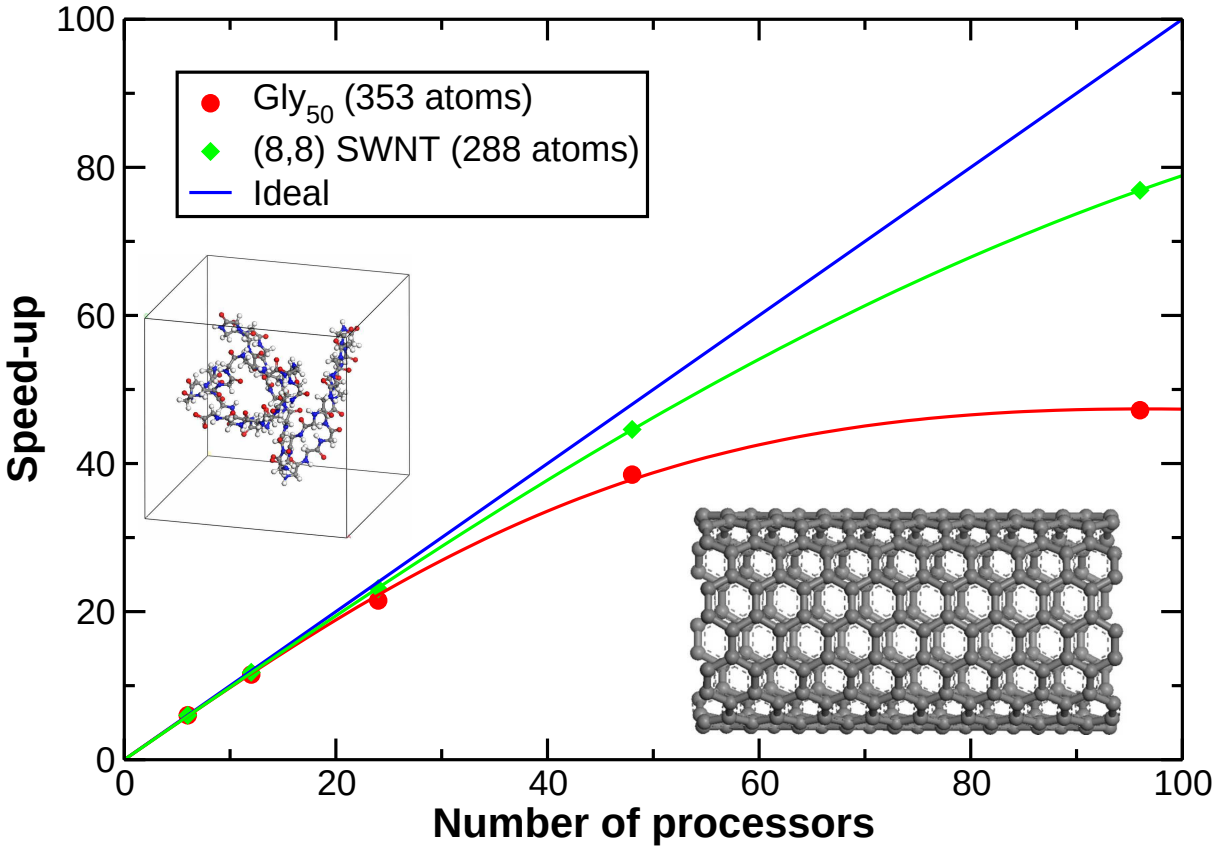




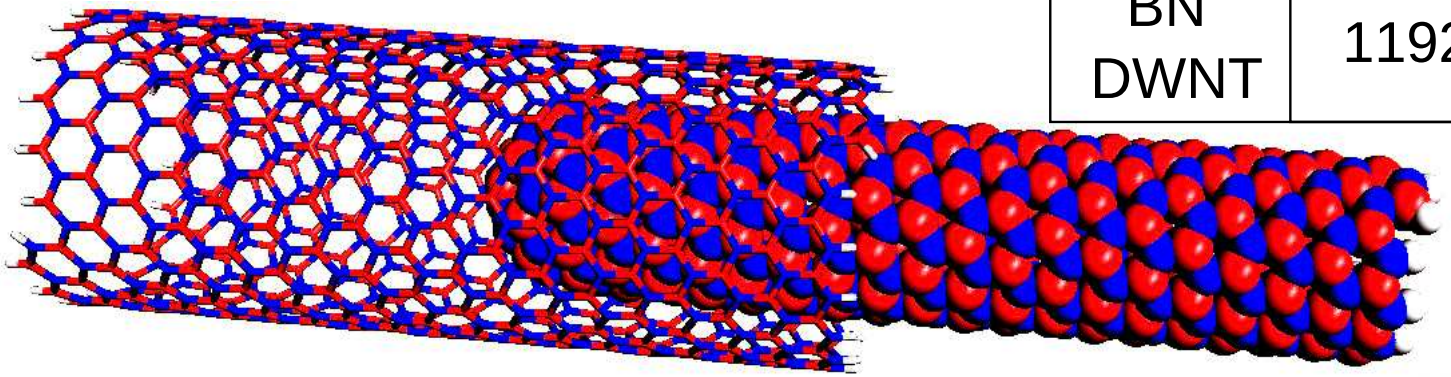
Real linear scaling: number of iterations



Parallel scalability



System	Number of atoms	Speed−up on 96 procs
Gly_{50}	353	47.2
Gly_{100}	703	88.8
Gly_{200}	1403	80.0
(8,8) SWNT	288	76.9
BN DWNT	1192	71.5



Conclusions

We have demonstrated a linear−scaling DFT method with:

- plane−wave accuracy
- excellent convergence properties
- good parallel scalability

- Nonorthogonal generalized Wannier function pseudopotential plane−wave method
  Phys. Rev. B **66**, 035119 (2002)
- Preconditioned iterative minimisation for linear−scaling electronic structure calculations
  J. Chem. Phys. **119**, 8842 (2003)
- Total−energy calculations on a real space grid with localized functions and a plane−wave basis
  Comput. Phys. Commun. **147**, 788 (2002)
- Comparison of variational real−space representations of the kinetic energy operator
  Phys. Rev. B **66**, 073103 (2002)
- Accurate kinetic energy evaluation in electronic structure calculations with localized functions...
  Comput. Phys. Commun. **140** , 315 (2001)