Massive plane-wave calculations in massive simulation cells

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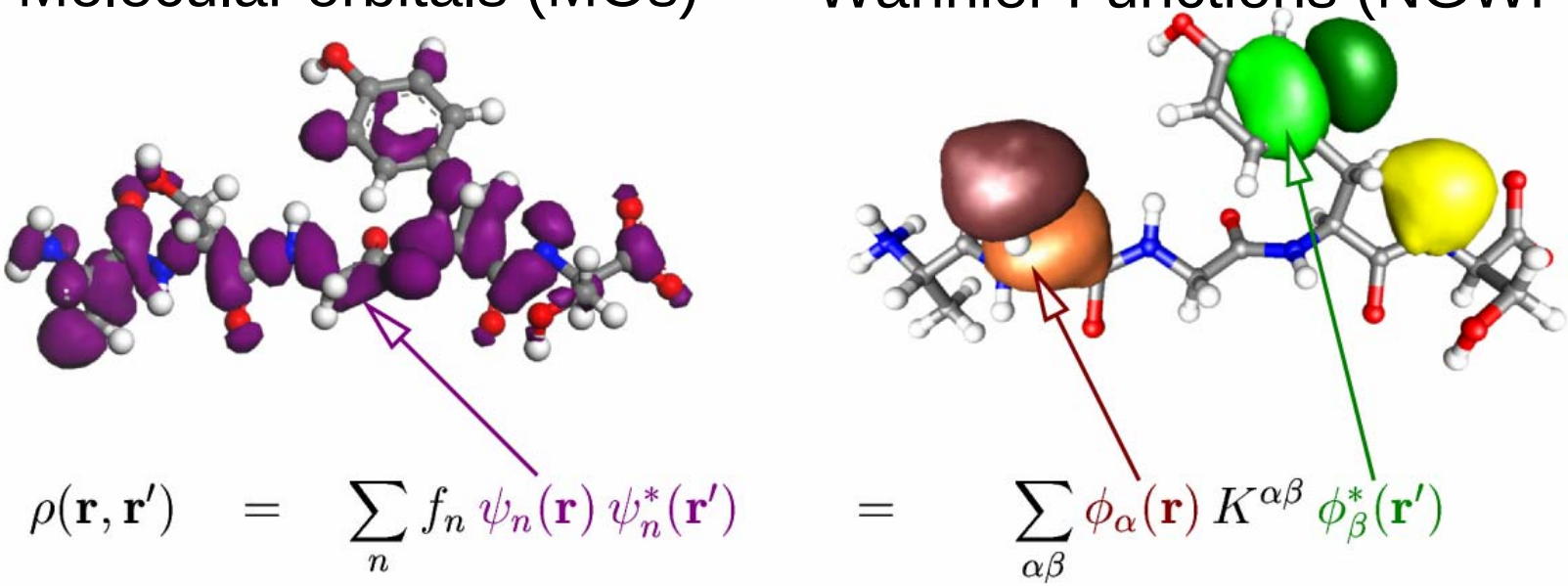
ONETEP: Density-matrix linear-scaling DFT

Molecular orbitals (MOs)

Non-orthogonal Generalised Wannier Functions (NGWFs)

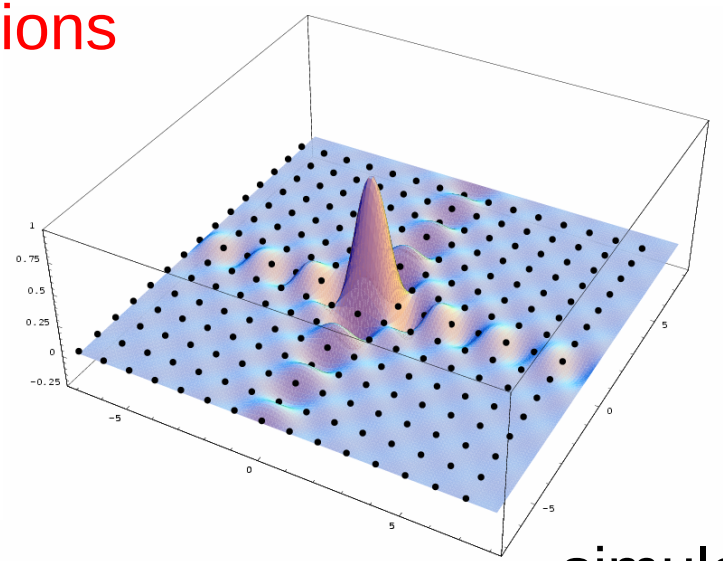


$$\rho(\mathbf{r},\mathbf{r}') = \sum_n f_n\,\psi_n(\mathbf{r})\,\psi_n^*(\mathbf{r}') = \sum_{\alpha\beta}\phi_\alpha(\mathbf{r})\,K^{\alpha\beta}\,\phi_\beta^*(\mathbf{r}')$$

- 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

Our basis set consists of plane-waves combined into spike-like “psinc” functions

$$D(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{G}}^{\mathbf{G}_{max}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

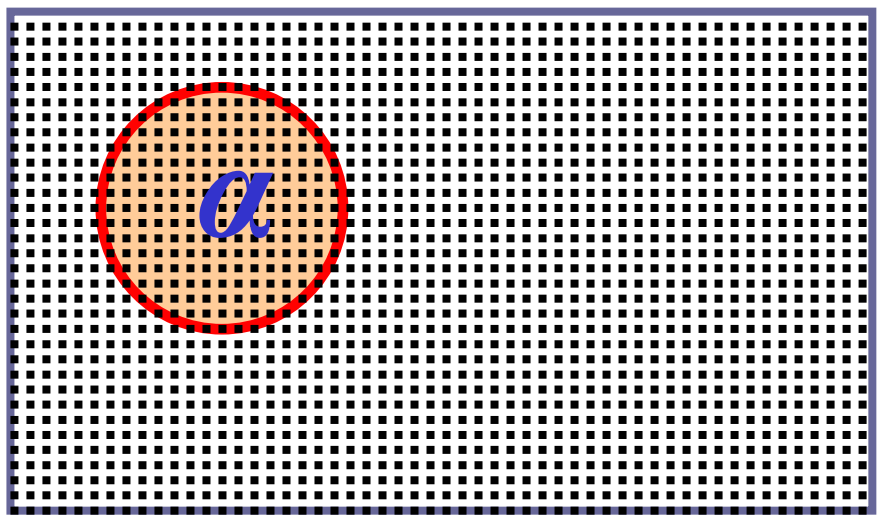


$$\phi_\alpha(\mathbf{r}) = \sum_{m}^{\text{sim. cell}} D_m(\mathbf{r}) C_{m\alpha}$$

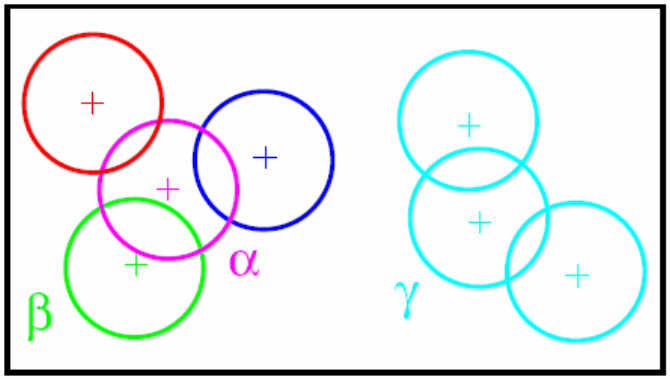
$$= \sum_{m}^{\text{sim. cell}} D(\mathbf{r} - \mathbf{r}_m) C_{m\alpha}$$

$$C_{m\alpha} = 0 \text{ if } m \notin \text{sphere of } \alpha$$

simulation cell



Linear-scaling formulation



$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha\beta} \phi_\alpha(\mathbf{r})\, K^{\alpha\beta}\, \phi^*_\beta(\mathbf{r}')$$

Density $n(\mathbf{r}) = 2\,\rho(\mathbf{r},\mathbf{r})$

Energy $E[n] = E[\{K^{\alpha\beta}\},\{\phi_\alpha(\mathbf{r})\}] = E[\{K^{\alpha\beta}\},\{C_{m\alpha}\}]$

Short−ranged: $\rho(\mathbf{r},\mathbf{r}') \longrightarrow 0$ as $|\mathbf{r}-\mathbf{r}'| \longrightarrow \infty$

$\Rightarrow$ impose cutoffs: $\phi_\alpha(\mathbf{r}) = 0$ when $|\mathbf{r}-\mathbf{R}_\alpha| > R_{\rm reg}$

$K^{\alpha\beta} = 0$ when $|\mathbf{R}_\alpha - \mathbf{R}_\beta| > R_{\rm cut}$

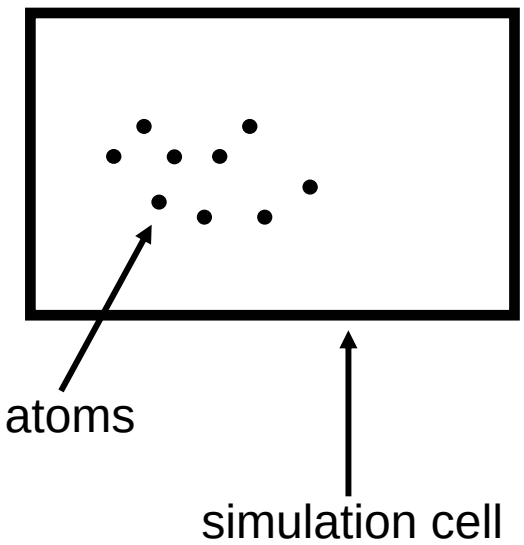
Idempotent:

$$\rho^2(\mathbf{r},\mathbf{r}') = \int \rho(\mathbf{r},\mathbf{r}'')\,\rho(\mathbf{r}'',\mathbf{r}')\,d^3r'' = \rho(\mathbf{r},\mathbf{r}')$$

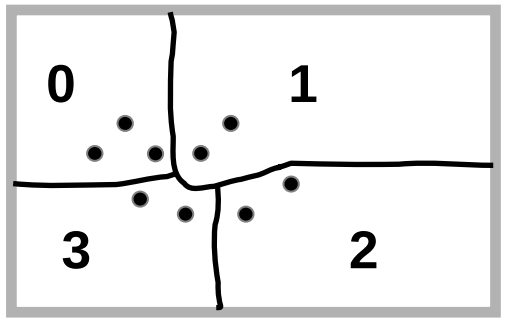
Parallelisation Strategy

Demonstration with four processors (0 to 3)

Serial calculation



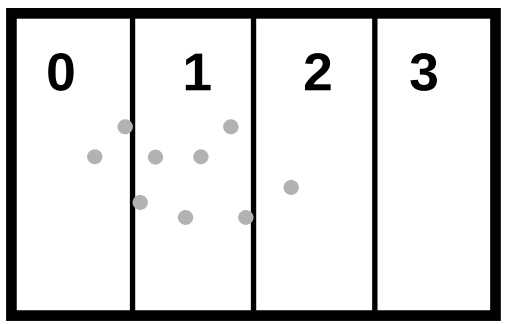
Parallel calculation



Phase 1

Distribution of atomic data (each processor holds **only a subset** of the $\{\varphi\alpha\}$)

⇒ **Large number of atoms**

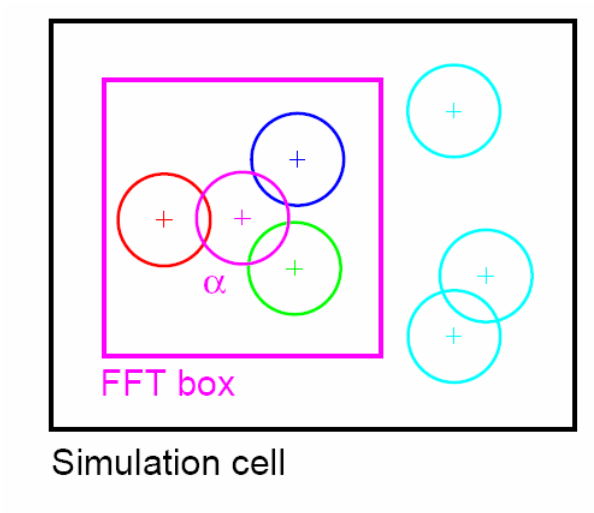


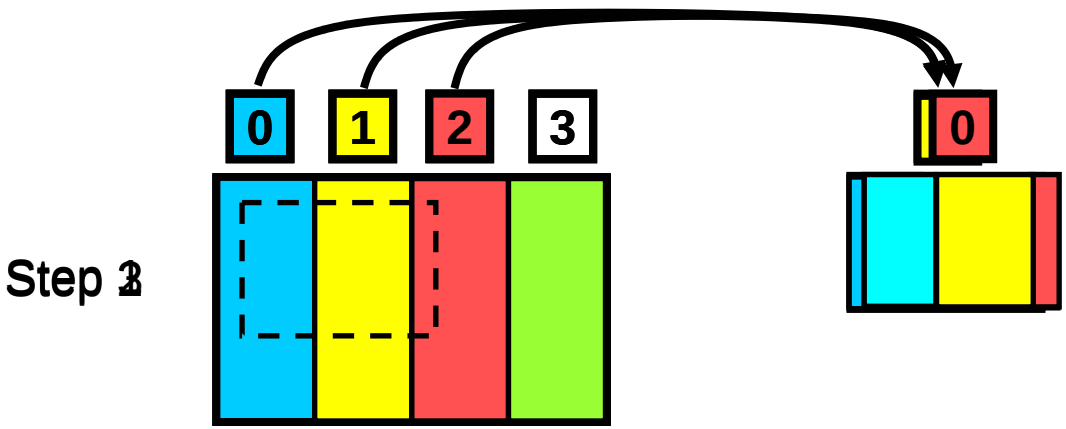
Phase 2 (**New work - completed in July 2004**)

Distribution of simulation cell data (each processor holds **only a slice** of the charge density and local potentials)

⇒ **Large simulation cells**

Phase 2: Most challenging aspect - the FFTbox technique

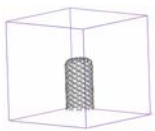
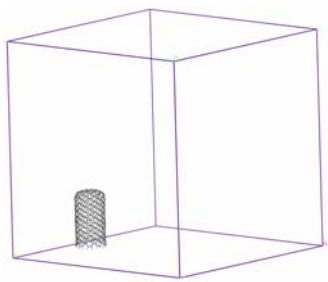
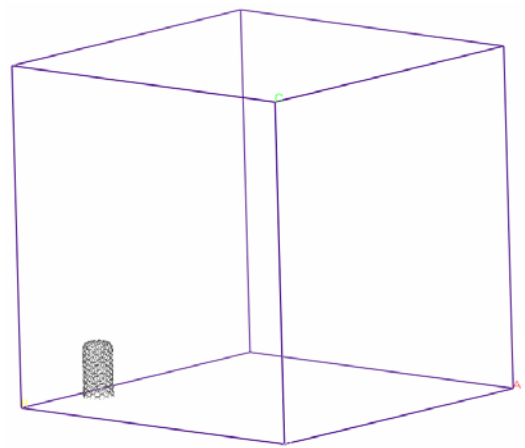




- Fourier transforms in **small regions** of the simulation cell, **independent of system size**
- Each processor has **its own** FFTbox
- Construction of the Hamiltonian matrix requires **"filling" the FFTbox with "slices" of local potential** from different processors
- Construction of the **charge density needs the opposite**: **"Deposit" the contents of each FFTbox to "slices"** on different processors
- A complex yet efficient **algorithm for communication** between processors has been developed

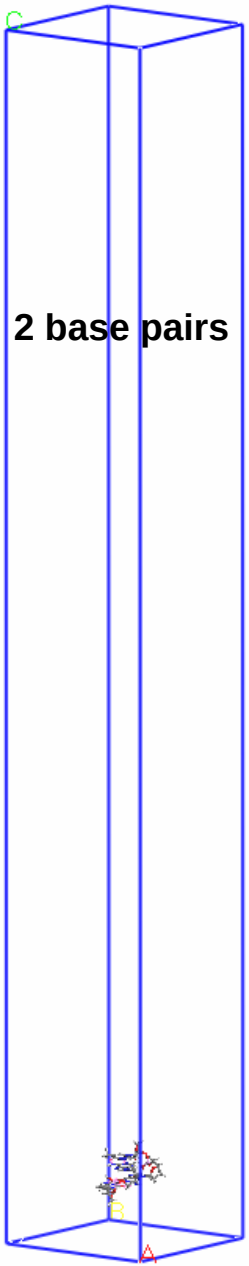
Example: Plane-wave calculations in massive simulation cells!

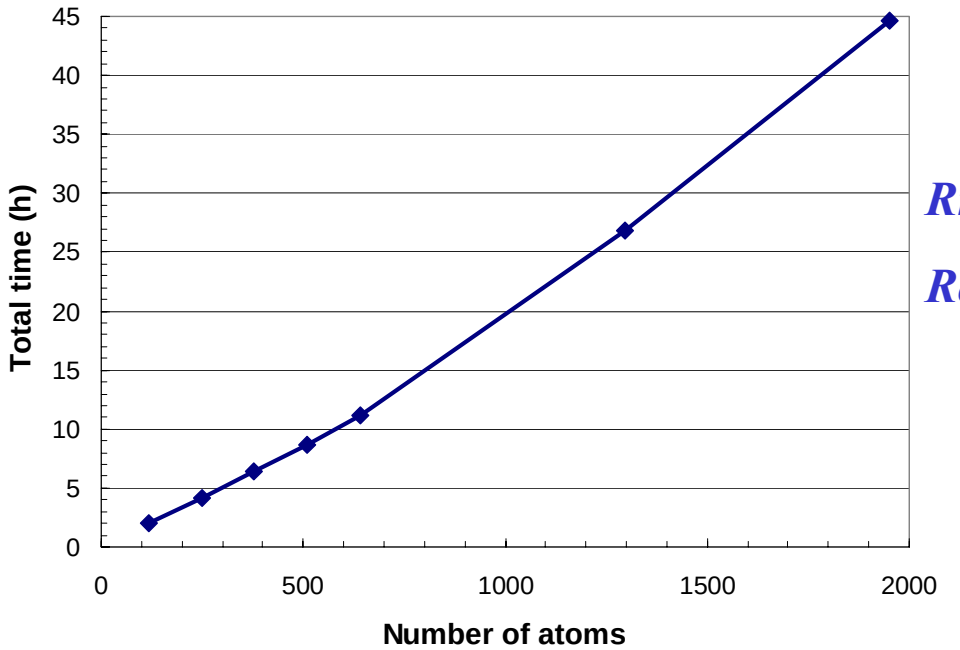
Test - supercell approximation for a 500-atom capped nanotube.
KE Cutoff 574eV. $Rreg$ =8.0 a0. $Rcut$=∞. 96 processors (Franklin).

Simulation cell volume:	**50Å x 50Å x 50Å**	**100Å x 100Å x 100Å**	**160Å x 160Å x 160Å**
			
	Maximum possible simulation cell size before Phase 2 parallelisation		
Total energy (Hartree):	-2526.007305	-2526.006203	-2526.010921

Single-point total energy calculations on DNA

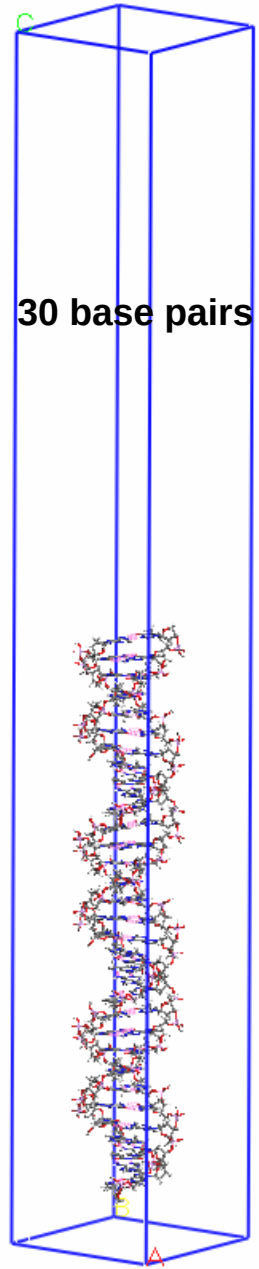
64 processors, simulation cell of 30Åx30Åx220Å. Wannier function RMS gradient convergence threshold 1.0E-6 Eh*a0^(3/2)





Rreg=6.3a0

Rcut=25.0a0

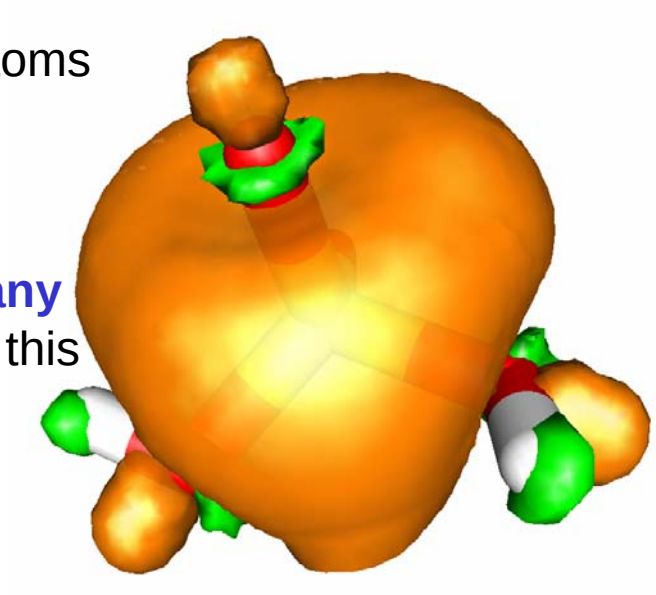


N base pairs	N atoms	N iterations	Total time (h)	DeltaE/atom (Eh)
2	117	26	2.0	1.3E-8
4	248	29	4.2	9.6E-9
6	379	29	6.4	6.6E-9
8	510	29	8.7	6.5E-9
10	641	29	11.2	7.6E-9
20	1296	30	26.9	1.1E-8
30	1951	28	44.6	1.1E-8

Conclusions

ONETEP is a pseudopotential DFT method with Plane-wave accuracy

- **Linear-scaling** w.r.t. to the number of atoms
- Now also able to treat **extremely large simulation cells**
- These simulation cell volumes can fit **many thousands of atoms**, so calculations of this size should now be possible
- Speedups should result from future **improvements** in the new “Phase 2 parallelisation” code



Acknowledgments

Cambridge-Cranfield High Performance Computing Facility (CCHPCF) for access to “Franklin”, their SUN-Fire 900-processor parallel supercomputer