DFT Plane Wave Code

— Do It Yourself

Self-consistent loop in CPMD

- Calculate electron density $n(\mathbf{r}) = \sum_i f_i \left|\phi(\mathbf{r})\right|^2$
- Calculate local potential $V_{\text{local}}(\mathbf{r})$
- Calculate projectors $F_{I,i}^{\alpha}$
- Calculate forces on the orbital coefficients $= \frac{1}{f_i}\frac{\partial E_{\text{total}}}{\partial c_i^*(\mathbf{G})}$
- Propagate wave function coefficients
- Orthonormalise them

Components of Kohn-Sham energy

$$\boxed{E_{\text{total}} = E_{\text{kin}} + E^{\text{PP}}_{\text{local}} + E^{\text{PP}}_{\text{nonlocal}} + E_{\text{xc}} + E_{\text{ES}}}$$

$$\begin{aligned}
E_{\text{kin}} &= \sum_i f_i \sum_{\mathbf{G}} \frac{1}{2} \mathsf{G}^2 \left| c_i \left(\mathbf{G} \right) \right|^2 \\
E^{\text{PP}}_{\text{local}} &= \sum_I \sum_{\mathbf{G}} \Delta V^I_{\text{local}} \left(\mathbf{G} \right) S_I \left(\mathbf{G} \right) n^* \left(\mathbf{G} \right) \\
E^{\text{PP}}_{\text{nonlocal}} &= \sum_i f_i \sum_I \sum_{\alpha,\beta \in I} \left(F^\alpha_{I,i} \right)^* h^I_{\alpha\beta} F^\beta_{I,i} \\
E_{\text{xc}} &= \Omega \sum_{\mathbf{G}} \epsilon_{\text{xc}} \left(\mathbf{G} \right) n^* \left(\mathbf{G} \right) \\
E_{\text{ES}} &= 2\pi\Omega \sum_{\mathbf{G} \neq 0} \frac{\left| n_{\text{tot}} \left(\mathbf{G} \right) \right|^2}{\mathsf{G}^2} + E_{\text{ovrl}} - E_{\text{ovrl}}
\end{aligned}$$

$$F^\alpha_{I,i} = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}} P^I_\alpha \left(\mathbf{G} \right) S_I \left(\mathbf{G} \right) c^*_i \left(\mathbf{G} \right)$$

$$P^I_\alpha \left(\mathbf{G} \right) = \frac{4\pi}{\sqrt{\Omega}} \left(-\mathsf{i} \right)^l \int_r r^2 P_k \left(r \right) j_l \left(Gr \right) Y_{lm} \left(\theta, \phi \right)$$

Force on wave function coefficient

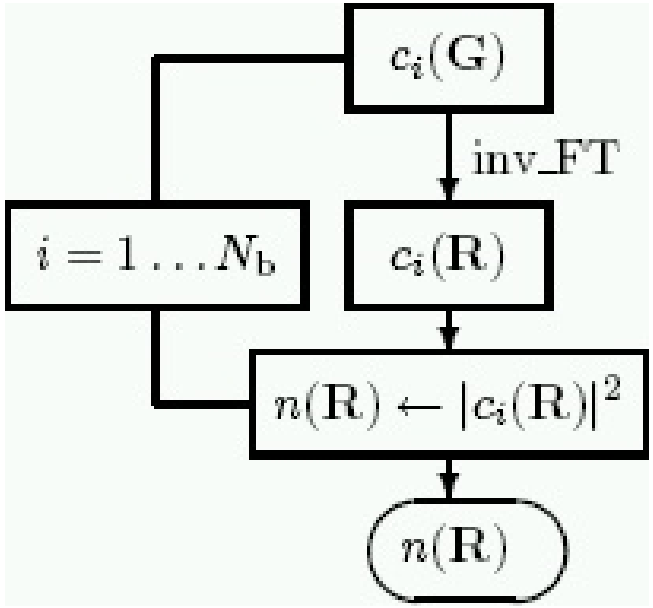
$$\boxed{E_{\text{total}} = E_{\text{kin}} + E^{\text{PP}}_{\text{local}} + E^{\text{PP}}_{\text{nonlocal}} + E_{\text{xc}} + E_{\text{ES}}}$$

$$\begin{aligned}\frac{1}{f_i}\frac{\partial E_{\text{total}}}{\partial c_i^*(\mathbf{G})} &= \frac{1}{2}\mathrm{G}^2 c_i(\mathbf{G}) \\ &\quad + \sum_{\mathbf{R}} V_{\text{loc}}(\mathbf{R})\, c_i(\mathbf{R}) + \sum_I \sum_{\alpha,\beta\in I} \left(F^{\alpha}_{I,i}\right)^* h^I_{\alpha\beta} P^I_{\beta}(\mathbf{G})\, S_I(\mathbf{G})\end{aligned}$$

where the local potential $V_{\text{loc}}(\mathbf{R})$ is the Fourier transform of

$$V_{\text{loc}}(\mathbf{G}) = 4\pi\frac{n_{\text{tot}}(\mathbf{G})}{\mathrm{G}^2} + V_{\text{xc}}(\mathbf{G}) + \sum_I \Delta V_{\text{local}}(\mathbf{G})\, S_I(\mathbf{G})$$

Calculation of density

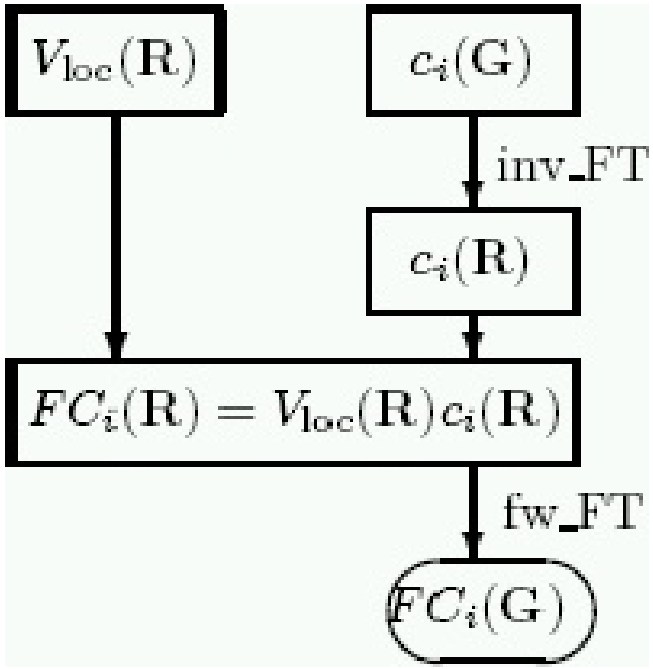


Calculation of density

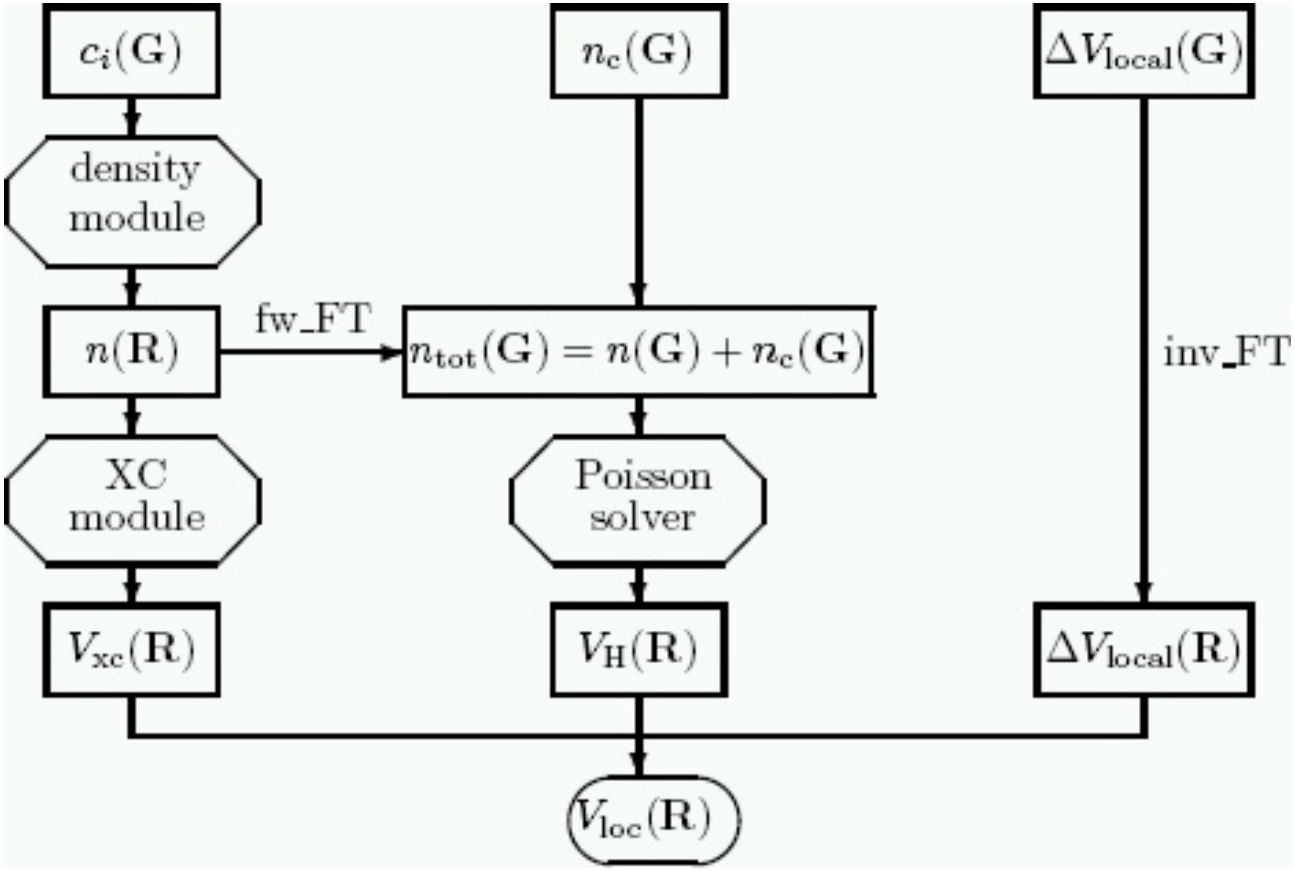
Implementation in *Faust*

- The calculation of the density is done in routine `rhoofr`
- The wave function coefficients $c_{i\mathbf{k}}(\mathbf{G})$ come in in the array `psi[;;]`; the dimensions are 1.: $\mathbf{G}$, 2.: state i, 3.: $\mathbf{k}$ point (please note: spin polarisation is currently not implemented in *Faust*!)
- 3D-FFT performed in `bwfft()`
- Also kinetic energy calculated
- Density collected into 3D real-space array `rhoes[;;]`

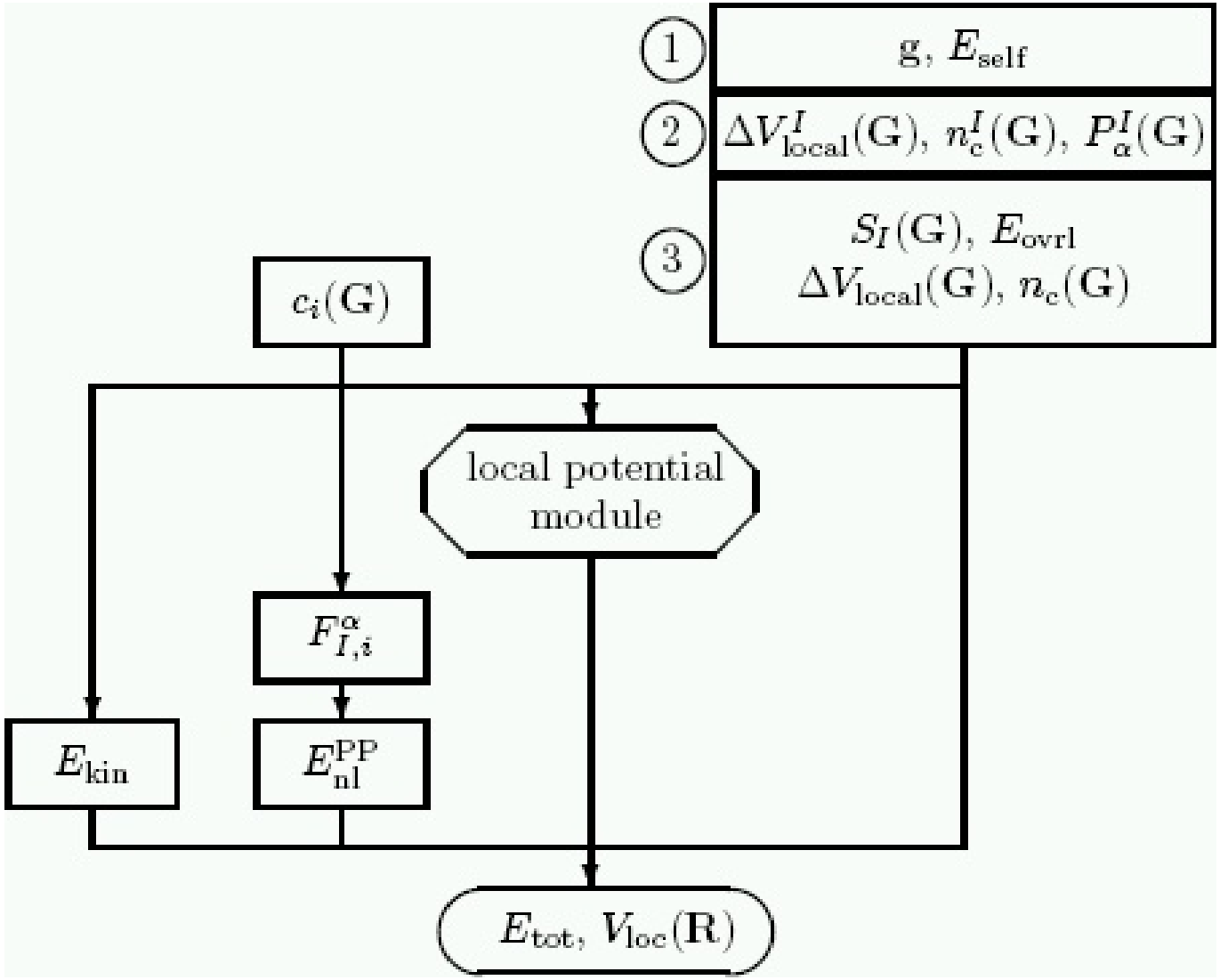
Local part of potential on force on orbital



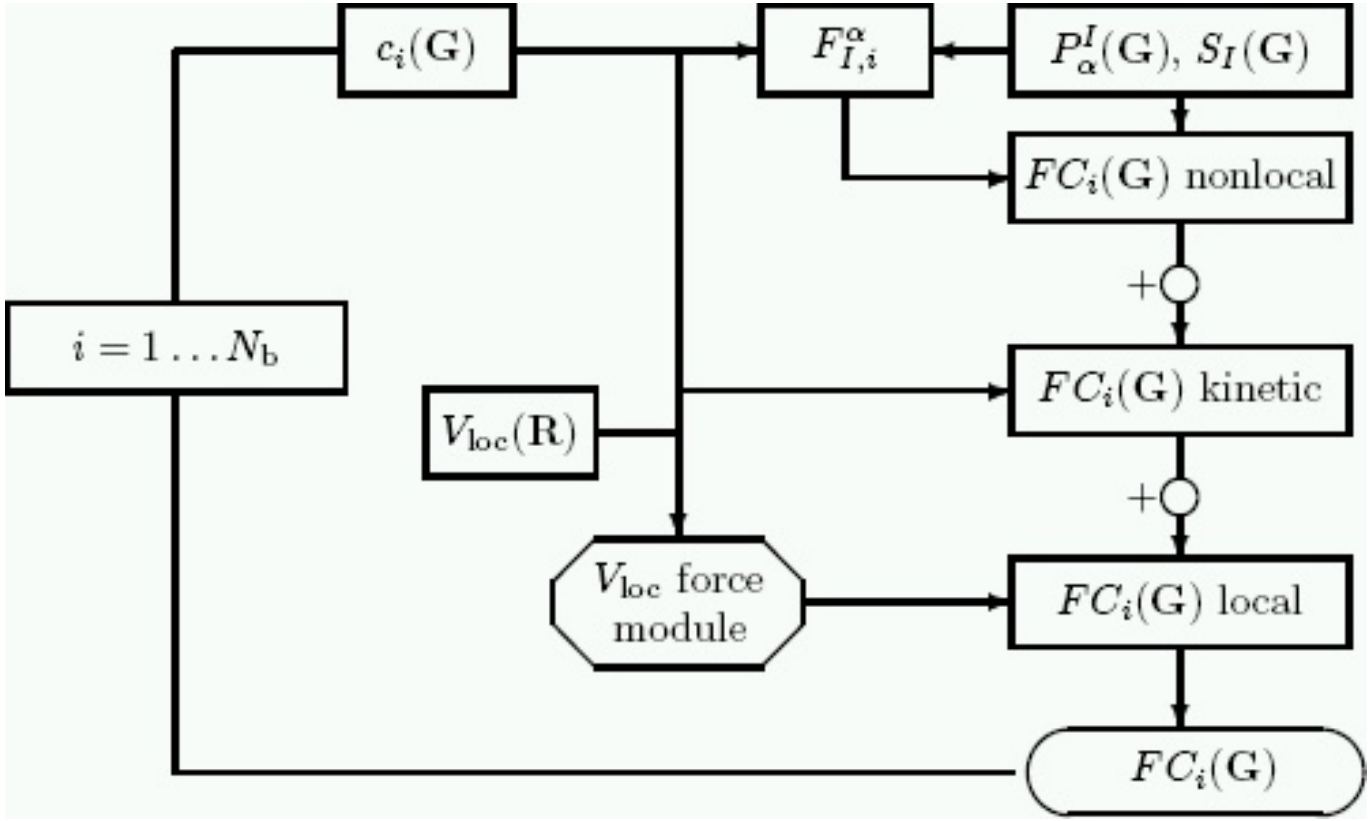
Local part of potential from orbitals



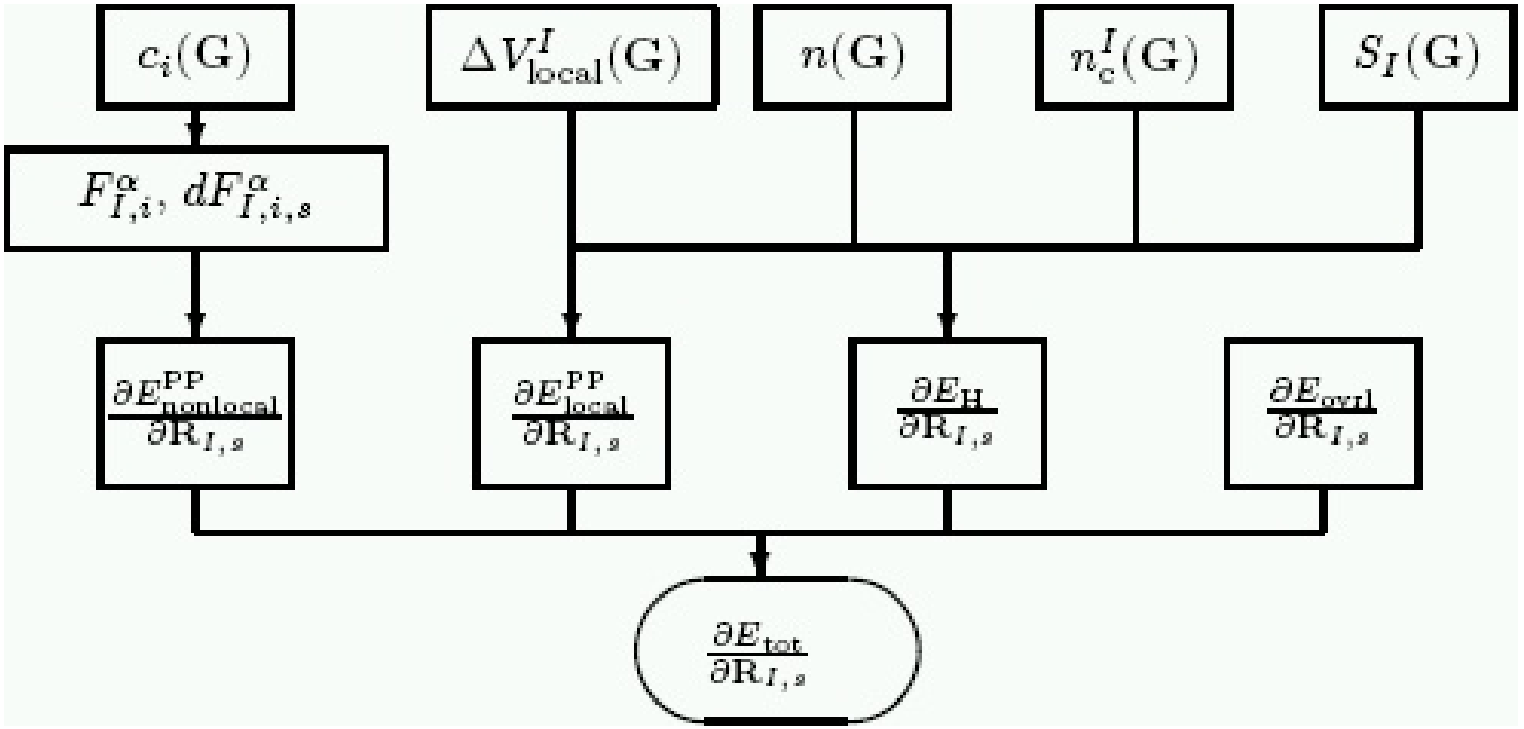
Local part of potential and total energy



Forces on wave function coefficients



Forces on nuclei



Local part of potential and total energy