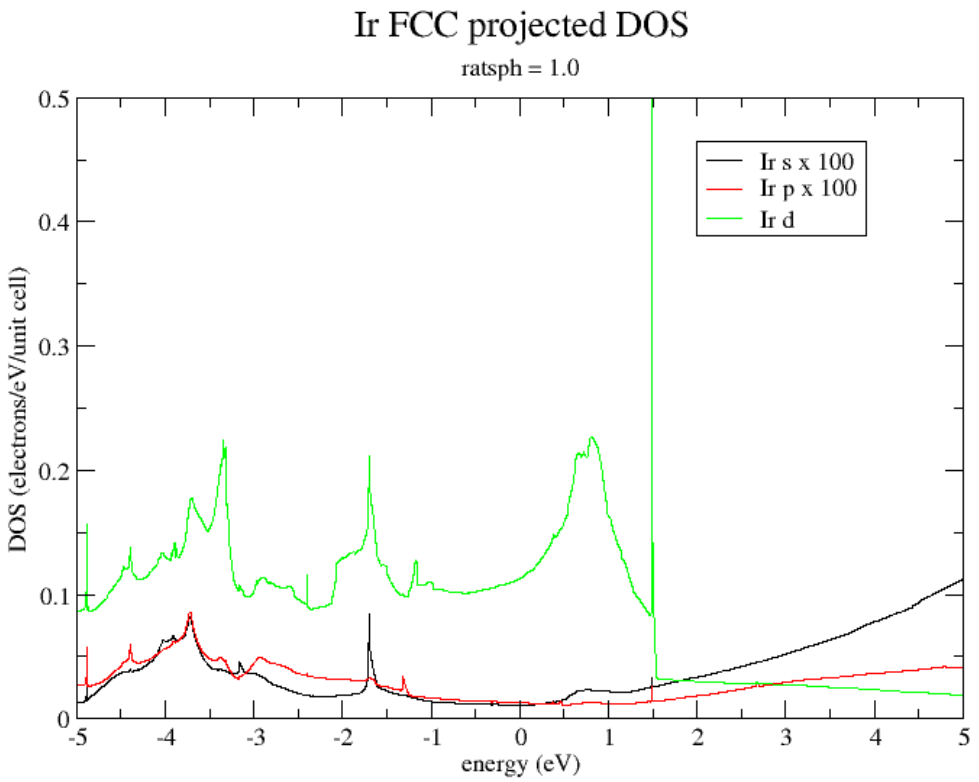
The tetrahedron method and angular momentum projection

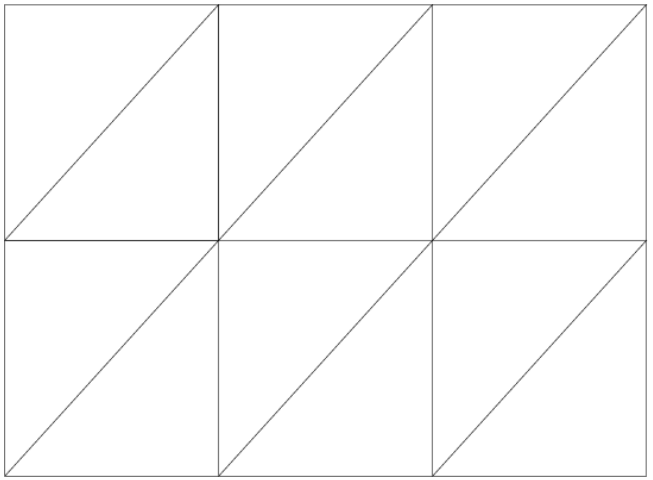


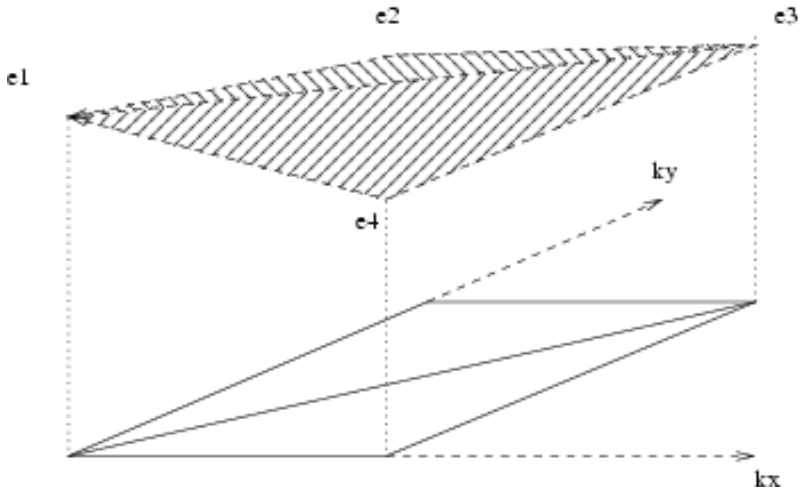
Overview

- General introduction: DOS and other uses
- Formalism
- Implementation
  - Subroutines
- Examples
- Conclusions

Tetrahedron I

- Interpolate band structure linearly
- Calculate general integrals analytically
  and more precisely (Energy, DOS, others)
- A 2-D example



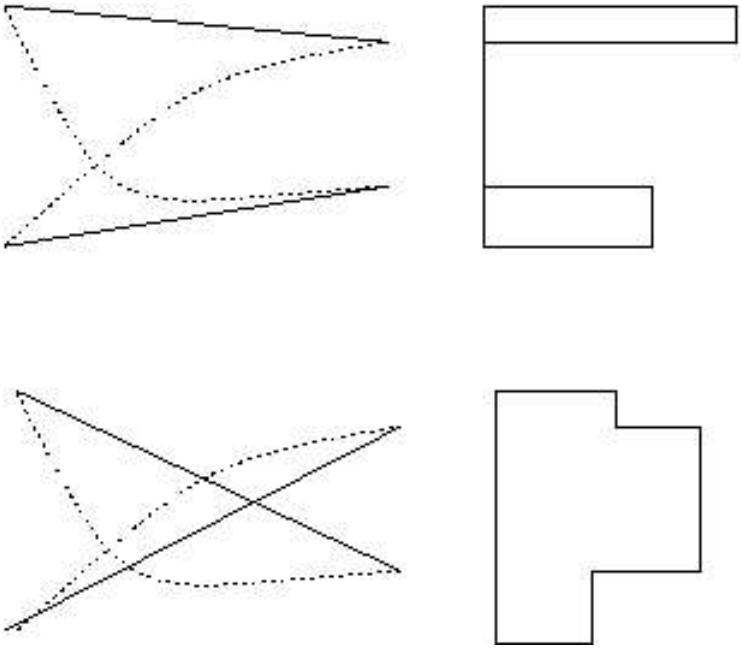


Tetrahedron II

- Several different versions
- Lehmann and Taut, phys stat sol (b) 54, 469
- Improved tetrahedron method
  (Blochl et. al. PRB 49, 16223)
- Other inter- or extra-polation methods
  are more risky
- Main issue: band crossings.

Tetrahedron III

- Distinguish between real crossings, anti-crossings and “close” bands
- The resulting DOS is very different
- No simple solution: either discontinuous bands or spurious crossings
- You still need a brute force convergence wrt kpts



Tetrahedron IV

- By integrating the linearized function, the integral over the full BZ is transformed into a sum.

- The contribution of each summit of the tetrahedron is separated, and the sum is reduced to one over inequivalent kpts.

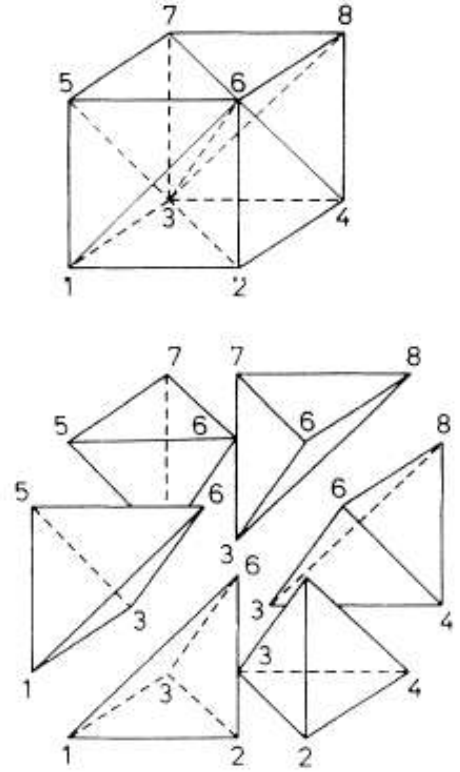


FIG. 5. Breakup of a submesh cell into six tetrahedra.

Tetrahedron V

- Special care must be taken if:
- The tetrahedron is degenerate (e1=e4)
  - Replace contrib by a gaussian
  - NB: you need at least 2 kpts!

- Or only partially (e1, e2=e4)
  - The slope of the BS on either side can be different, and the DOS will jump.

- Integrated DOS is analytical too

Angular momenta I

- Angular momenta $Y_{lm}(\theta,\varphi)$ are a complete basis (angular variables)
- Atomic-like orbitals: project full Ψ close to nucleus to determine character
- Not real point group character, but usually good enough to distinguish bands
- Density in sphere:

$$n(r_{max}) = \sum_{G \neq 0} \frac{1}{|G|^3} e^{i 2\pi \vec{G} \vec{R}_\tau} n_k(\vec{G})\, Int0(|\vec{G_{max}}| r_{max}) + n_k(\vec{G}=0) \frac{4\pi r_{max}^3}{3}$$

$$Int0(Y) = \int_0^Y 4\pi y^2 j_0(y)\, dy$$

Angular momenta II

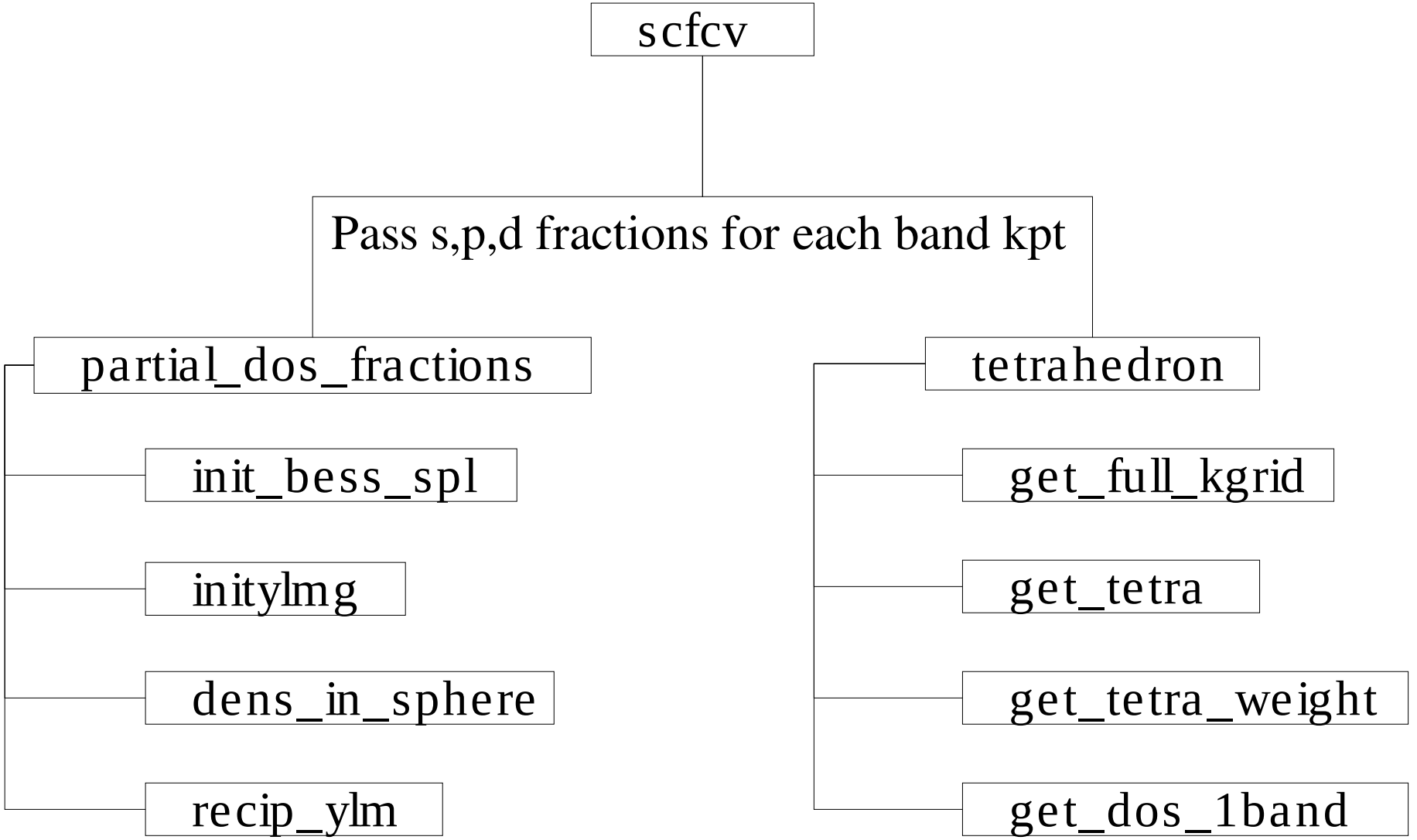
- Angular momentum decomposition:

$$\Psi_{lm}(\Delta r) = 4\pi i^l \sum_G c_k(\vec{G}) e^{i2\pi(\vec{k}+\vec{G})\vec{R}_\tau} j_l(2\pi|\vec{k}+\vec{G}||\Delta r|) Y_l^{m*}(\Omega_{\vec{k}+\vec{G}})$$

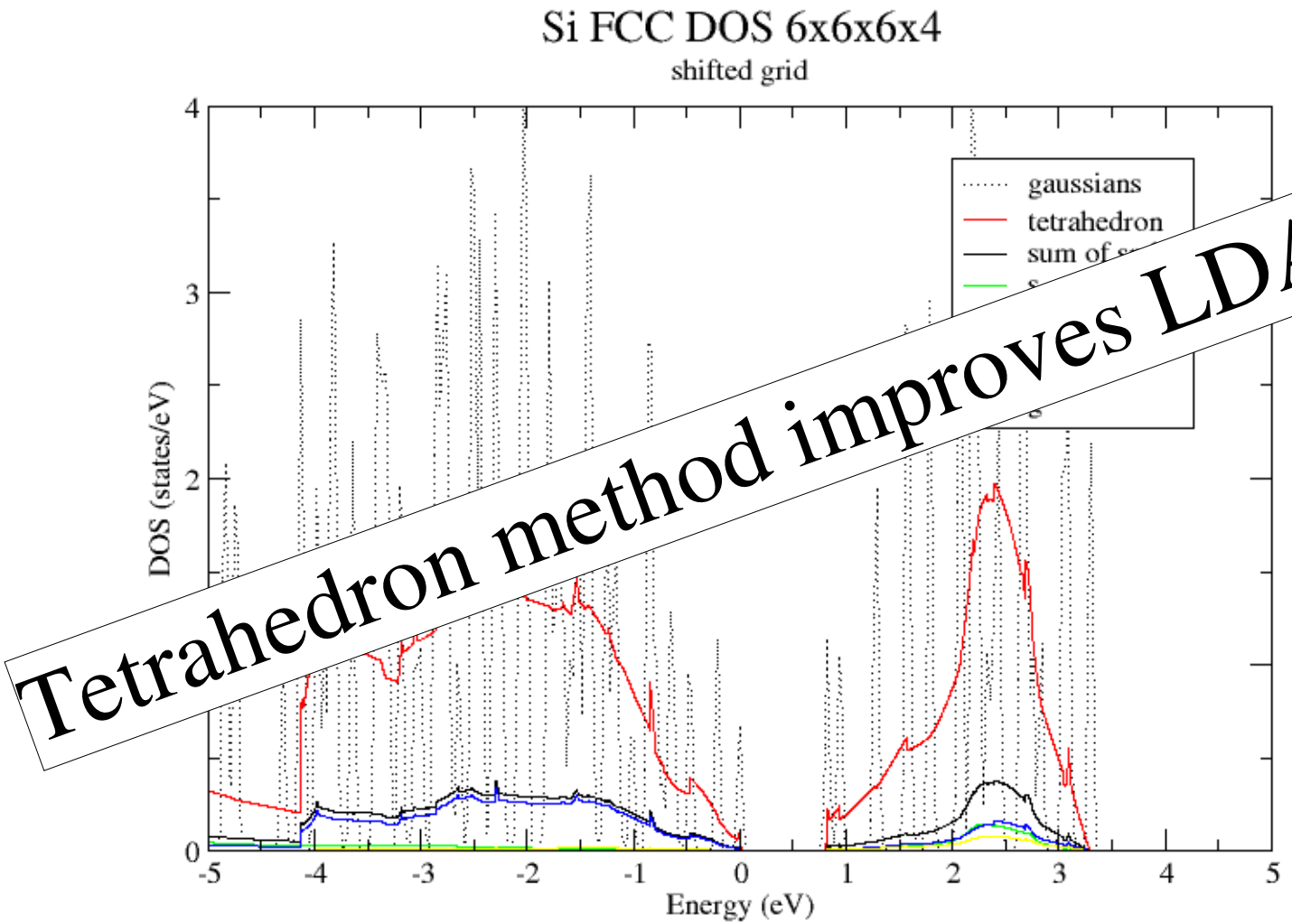
$$c_{lm}(r_{max}) = \frac{1}{\Omega_0} \int_0^{r_{max}} \Psi_{lm}^*(\Delta r) \Psi_{lm}(\Delta r) (\Delta r)^2 dr$$

- Repeat for each band and kpoint
- Sum over all l and m should give full density
- Multiplicative factor for each irred kpt in tetrahedron method
- 1 atom at a time: only do inequivalent ones (iatsph, natsph)

Implementation

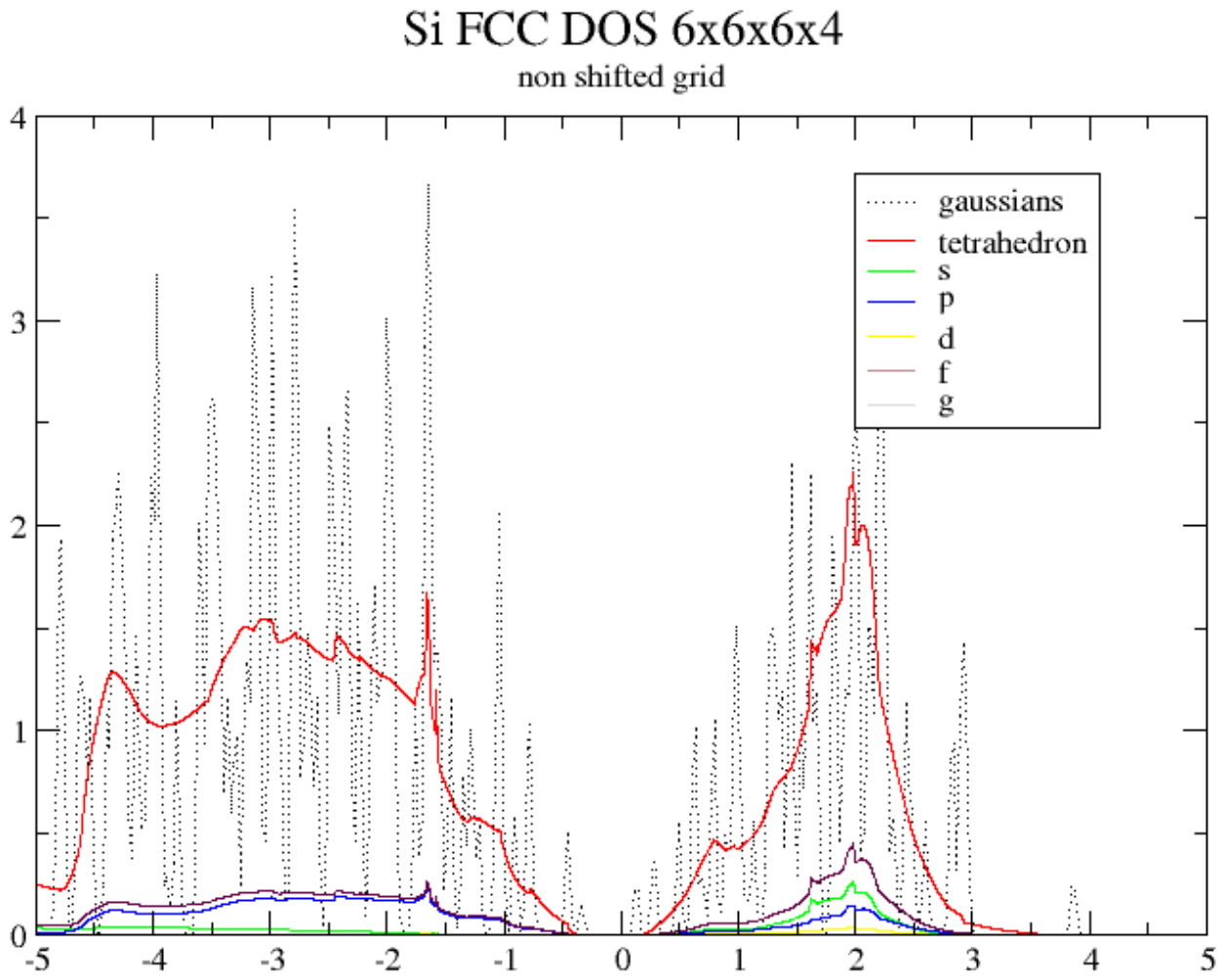


An Example I

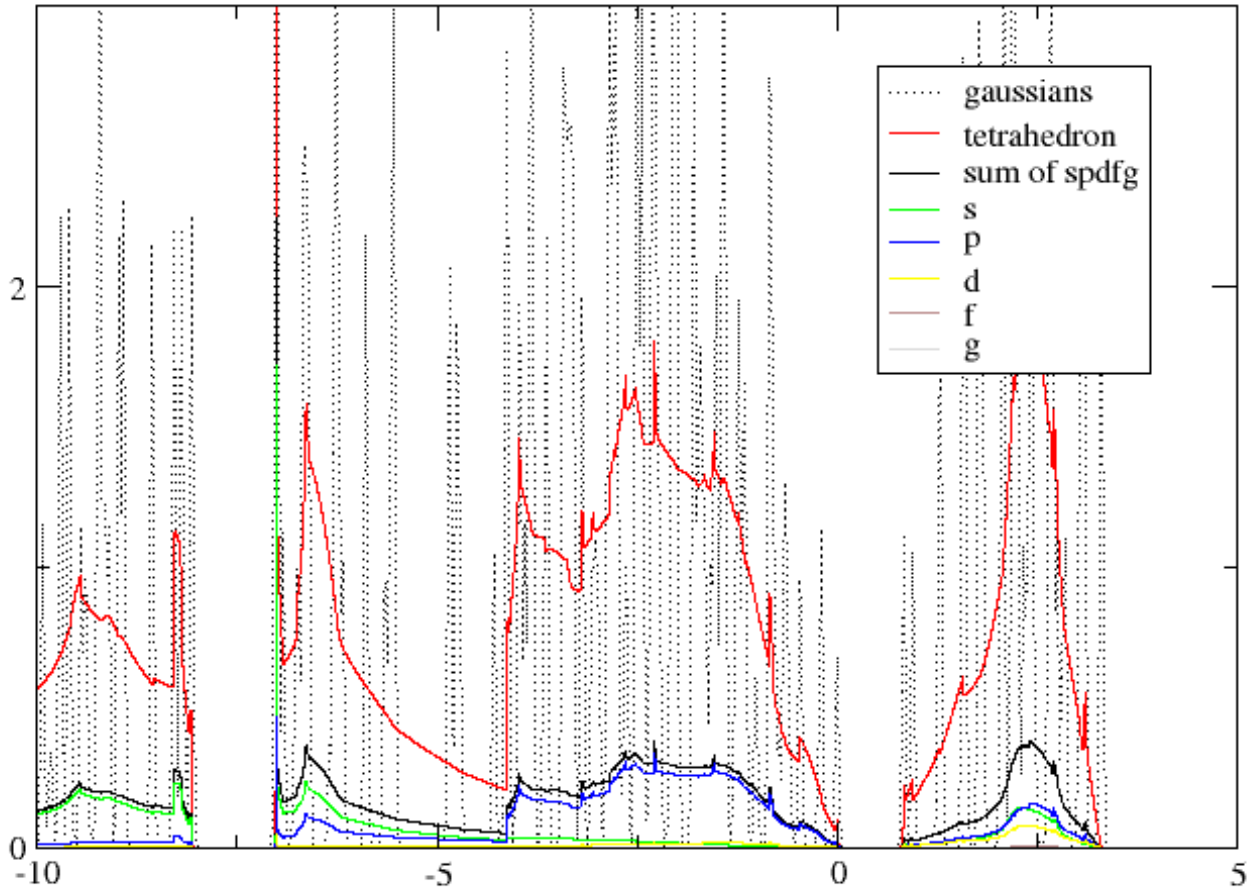


Tetrahedron method improves LDA gap!

An Example II



An Example III



The lesson

- The tetrahedron method is sensitive to the presence of degenerate points on the kpt grid. Use a non-shifted grid containing a maximal number of special points
- Method is not yet parallelized for angular momentum projection
- The value of the projected DOS is proportional to the integrated density in the sphere! Not directly comparable.

Conclusions

- Tetrahedron method and projections work decently well for production
- To be parallelized
- Only calculate dens_in_sphere for irred atoms (memory can explode)

- Extend to other types of partial DOS: spatial criteria, 1st layer of a slab...