

# Discussion session - Distribution of the code

## Open Session

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# Discussion

- ① Building lattice models for magnetic systems  
Reference state?
- ② Relaxing the constraints on the reference state  
Metallic systems?
- ③ Other issues?

# Future developments - Priorities?

## ▶ Major implementations

### ① Defects (Medium term)

Chemical inhomogeneity

Impurities

### ② TDDFT (Short term)

### ③ Spin-orbit (Medium-long term)

### ④ Integration of electron-model building in FP (ABINIT, SIESTA)

## ▶ Minor implementations

### ① Nudged band optimization

### ② Separated chemical potentials for electrons and holes

### ③ Constrained DFT ( $\delta$ SCF?)

Suggestions?