Implementation of the PAW formalism in ABINIT: present features and perspectives

F. Jollet, M. Torrent, F. Bottin, and G. Zerah

Commissariat à l'Energie Atomique, Centre d'Etudes de Bruyères-le-Chatel, BP 12, F-91680 Bruyères-le-Chatel

In this presentation, we shall review all the new features added since the first ABINIT workshop. We shall especially focus on the following points:

- What has been added or modified for PAW implementation?
- How does a PAW calculation work?
- What about accuracy and efficiency?
- Physical examples