Implementing the Relaxed Core PAW Method into ABINIT

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Therefore an intermediate method is necessary.
Relaxed Core PAW

- Method proposed by Marsman and Kresse\(^a\)
- General idea, relax cores in between SCF cycles:
  - Solve atomic problem with fixed (DFT) valence charge density to obtain new AE core density.
  - Calculate new core AE partial waves.
  - Calculate new PS partial waves, that remain dual to the original projectors.
  - Recalculate dependent parameters.

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- We will modify the pawtab data structure in an unobtrusive way (e.g. pointers) to allow for changes.
Algorithm

- Enter relax core routine during SCF cycle, after valence densities have been updated.
**Model and Implementation**

**Algorithm**

- Enter relax core routine during SCF cycle, after valence densities have been updated.
- Adapt ATOMPAW functions to solve atomic problem with fixed (radially averaged) valence density (possibly used as library).

Recalculate $D_{ij}$ and $Q_{ij}$. Introduce suitable mixing. Resume SCF cycle.
Enter relax core routine during SCF cycle, after valence densities have been updated.

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Reuse pseudoization parameters from input core wave function (modifications might be necessary).
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ATOMPAW as a Library

- Pro:
  - Reuse of already existing code.

- Contra:
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- For many applications one relaxed atom might be sufficient.
- However, if all atoms should be relaxed, a more efficient approach might be necessary, e.g. separate again between per atom and per atom-type data.
- Downside: More coding and more potential for unexpected interactions with the rest of ABINIT.