Documentation and Beautification

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Outline

1. Code Beautification
2. Code Documentation
3. Tutorials
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1  Code Beautification

2  Code Documentation

3  Tutorials
2009 Code Cleaning Exercise

- Removed unused variables—ABILINT checks for these, and test fails if present
  - How to run ABILINT test on own branch before pushing?
- Did 2009 exercise verify presence of proper documentation in each subroutine?
Going forward

- Code beautification: what should be done?
- Code style: use of modules and OOP methodology?
Code and Feature Creep

- gstate.F90
- scfcv.F90
- vtorho.F90
- vtowfk.F90
- cgwf.F90

And, foo3.F90 variants for response functions.
Potential Opportunities

- PAW/NCPP
- Positrons
- Berry’s Phase
1 Code Beautification

2 Code Documentation

3 Tutorials
Most but not all subroutines have proper ROBODOC style documentation

Many but not all have up-to-date documentation

Need to check (by script?) and correct documentation for:

- Function
- Inputs, Outputs, Side Effects
- Notes
- Parents, Children (automatically generated?)

Improve information content of failure/error/warning output lines
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I see this as a real strength of ABINIT compared to many other packages

Current suite contains a mix of old and new

Implementation of major new functionality should include writing tutorials to use it

Are any of the current tutorials "obsolete"?
Planning new tutorials

- PAW near-nucleus properties: electric field gradient, Fermi contact, density
- From CIF to Abinit
- Extend response function tutorials to PAW case?
- Need more GW tutorials or expansion of current offerings?