Documentation and Beautification

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Outline

Documentation
and
Beautification

J. W.
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Code
Beautification

Code Docu-
mentation

Tutorials

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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

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- PAW/NCPP
- Positrons
- Berry's Phase

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ROBODOC Header Style

- 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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1 Code Beautification

2 Code Documentation

3 Tutorials

- 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 funcionality should include writing tutorials to use it
- Are any of the current tutorials "obsolete"?

Planning new tutorials

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- 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?