Organization of software for the computational design of new materials

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This talk describes the somewhat disorganized state of computer software in a typical University research program (my own) to advocate for more coordination between the various large code development groups. Our research studies the fundamental physics of a range of novel materials including multiferroics (which are simultaneously ferromagnetic, ferroelectric and ferroelastic), magnetic semiconductors and materials for molecular spintronics. The questions we investigate are varied and require a range of tools, and we are currently using the following software packages:

- ABINIT, for its linear response capability
- SIESTA, since the local orbital basis set allows us to study large systems
- an in-house ultra-soft pseudopotential code which we have modified to include self-interaction corrections to the exchange-correlation functional
- the Stuttgart-LMTO package, for its visualization tools, and
- VASP, for its speed and LDA+U capabilities.

We outline some of the factors, both technical and historical, that have led to this untidy diversification and suggest some ideas for future improvement. Finally we describe one application, the investigation of grain boundaries in cobalt-doped anatase TiO_2, for which we are using the ABINIT code.