

A Personal History of the ABINIT Project

Douglas C. Allan

Corning Incorporated



CORNING

Discovering Beyond Imagination

On shoulders of giants: DFT, LDA, pseudopots

- 1964 -- Hohenberg + Kohn “Inhomogeneous electron gas” Phys. Rev. **136**, B864
- 1965 -- Kohn + Sham “Quantum Density Oscillations in an Inhomogeneous Electron Gas” Phys. Rev. **137**, A1697
- ... etc. laying foundation for DFT and LDA

- 1979 -- “Norm-Conserving Pseudopotentials” Hamann, Schlüter, Chiang PRL **43**, 1494
- 1982 -- “Pseudopotentials that work: From H to Pu” Bachelet, Hamann, Schlüter PRB **26**, 4199 (1982)

- **“Erratum: Pseudopotentials that sometimes work: From H to Pu”** PRB **29**, 2309 (1984)

Beginnings

- 1985 – Corning Glass Works – quantum mechanics for much larger and more complex systems (glasses) – mostly LDA-based ideas – get beyond matrix diagonalization
- 1985 – Car and Parrinello PRL **55**, 2471 – “A unified approach for molecular dynamics and density-functional theory” – **local pseudopotentials only**
- 1986 – Focus on separately diagonal operators T and V, disregard “unified approach” – PRL (Comment) **56**, 2656 (focus on FFT and iterative minimization concepts)
- 1987 – Linear response theory in LDA – PRL **58**, 1861
- 1987 – “Efficacious” nonlocal pseudopotentials rescued from obscurity – PRL **59**, 1136
 - uses Kleinman & Bylander PRL **48**, 1425 (1982)
 - forerunner of Vanderbilt ultrasoft pseudopotentials

Beginnings, continued

- circa 1987-1994 Cornell Electronic Structure group (Ken Wilson, John Wilkins, Mike Teter, Me, others)
- 1989 – Variational formulation for response functions – Gonze and Vigneron PRB **39**, 13120
- 1989 – Preconditioned conjugate gradient – PRB **40**, 12255
 - (by this time other strategies being pursued at Corning/ Cornell were abandoned in favor of plane waves)
- 1989 onward – “Corning code” has a small user base
- 1989 – “fast diagonalization” Gonze, Vigneron, Mechenaud J.Phys:Cond.Matt. **1**, 525 (1989)
- 1990 -- Ghost states and Kleinman-Bylander pseudopotentials: Gonze et al, PRB **41**, 12264

Code and algorithm developments

- 1990: Collaborate with Gonze or get scooped; Xavier to Cornell (July 1990)
- 1992: “Iterative minimization techniques” fully developed with nonlocal pseudopotentials in RMP **64**, 1045
- 1992: By now corning.f has a dozen or more users who try remarkable things – code grows more defensive or “idiot proof” (and idiots become more clever)
- **1990-1992** – First development of Respfn, built on top of Corning code, by Gonze while at Cornell (response functions)
- Coding rules developed and refined for shared subroutines – notably, variational DFT allows re-use of same *algorithms*

The real ABINIT

- 1993 – “Corning code” rewritten into “Plane_Wave”, marketed by Biosym
- 1993 – Xavier Gonze back to Louvain-la-Neuve
- 1995 -- Biosym merges with MSI, now called Accelrys, and Plane_Wave is retired in favor of CASTEP
- 1996 – Initiated a brand new code, destined to be ABINIT, intended to be *freely distributed* (gnu public license)
 - Merge all functionality of Respfn and Plane_Wave
 - Entirely written in F90 with all new source lines
 - Adopt best of methods for pseudopotentials, algorithms, and functionality (especially for response functions)
- 1996 – Work proceeds on ABINIT, with center of gravity now in **Belgium** (story now gets hazier to me)

ABINIT goes live

- 1998(?) – ABINIT named and urgently requested by users; a few special testers are allowed access
- 1999(?) – ABINIT goes live with its own web site hosted by Louvain-la-Neuve
- 2000 – ABINITv3.0 first covered by GNU public license
- -2002 – Developments continue up through version 3.4.3 with developers and users throughout the world
- New users continue to find remarkable ways to run the code (see email)

Some keys

- Defensive coding
 - checking input reasonability
 - checking array dimensions, etc.
- Coding standards spelled out
- Automated testing
- Planning and organizing – now global of course!
- Benchmarking and testing against other codes where possible

- Focus always on results: see web site for citation list
- Also see “short presentation of the ABINIT project” pdf file on web site

Conclusions

- Glass chemistry still too complex
- Typical result: value (ABINIT) created even without solving original problem
- Next: keep momentum!