Self-Documentation of ABINIT source

(How to avoid duplicated efforts for documentation ?)

Masayoshi Mikami (Mitsubishi Chemical Co.)

and the following developers (in alphabet order)
(CEA)
François Jollet, Marc Torrent, Gilles Zerah
(UCL)
Razvan Caracas, François Detraux,
Martin Fuchs (FHI-MPG), Xavier Gonze,
Luc Sindic, Matthieu Verstraete
(ULG)
Philippe Ghosez, Jean-Yves Raty (and their students)

Contents of this talk

1. Background (“Self-assembled(organized) way”)
2. Robodoc & Src2tex
3. Example (source code –> HTML & DVI(PS))
4. Future plan (Open discussion)
5. Summary

Background

In the long run :

a unique manual for the developers/contributors

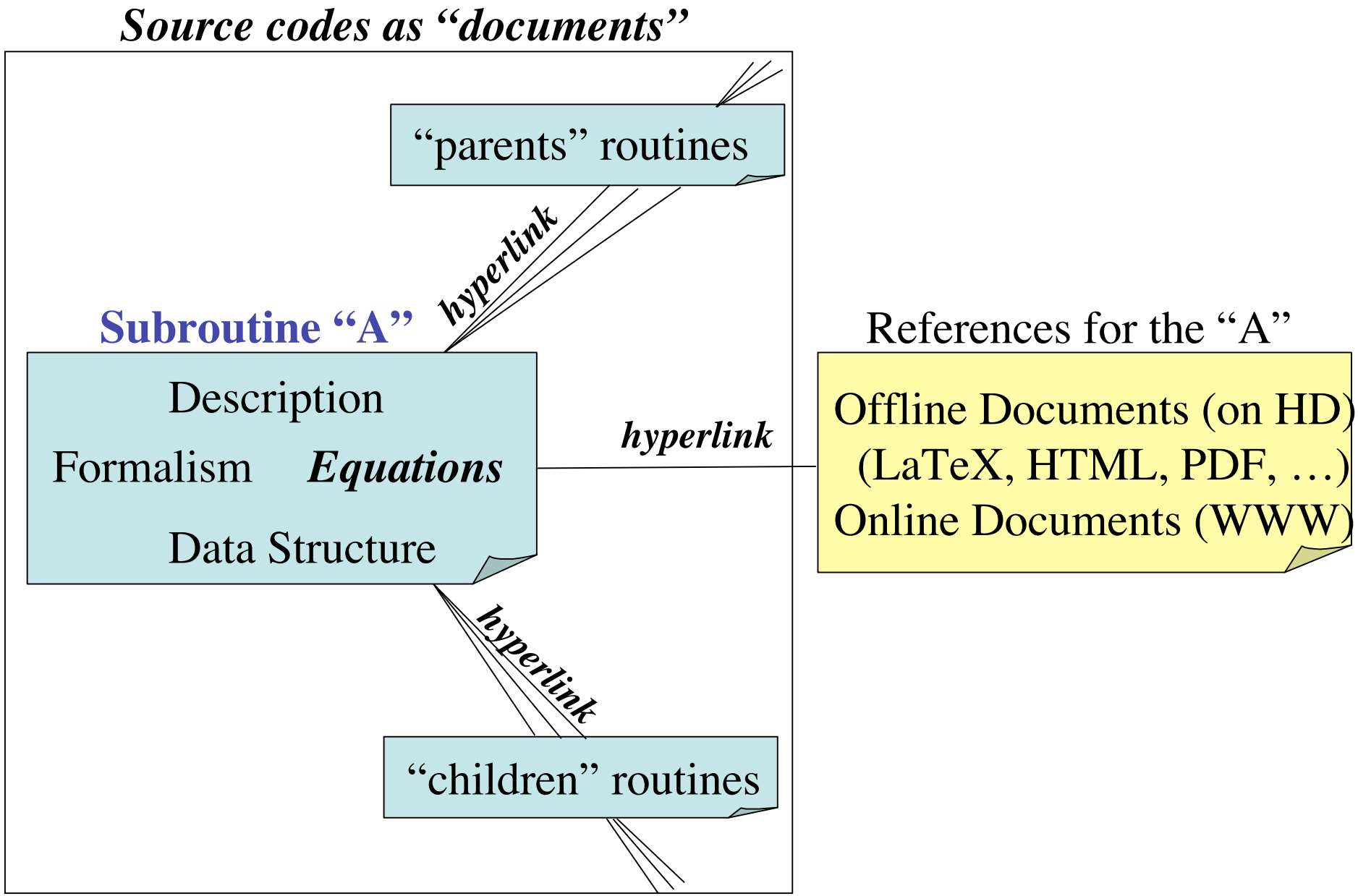
* nicely formatted (equations)
* explaining all the formalism
* explaining the data structures
* making references to the proper subroutines

For each subroutine:

* having ***locally*** the information on what it does
* having a list of related routines (***parents, children***)
  and having also ***hyperlinks*** to these routines
* being able to view the routine in a ***nicely formatted way***

As ***little duplication of the same information*** as possible
in order to ease ***maintenance*** and ***coherence***

Making documents by *self-assembled (self-organized) way*



Organization of the Self-Documentation

On Not Reinventing the Wheel,
"Laziness is an economic virtue"
(by Eric S. Raymond, "The Art of Unix Programming")

- as little human work as possible
- as few and simple rules as possible
- changes should be gradual to avoid useless efforts
- proper tools to automate boring tasks
  (maintenance and coherence of information)

=> ***Robodoc*** & ***src2tex*** way

Robodoc for HTML formatting (browsing)

Robodoc v. 3.2.3 (v.3.2.4 to be released soon on WEB)
(http://www.xs4all.nl/~rfsber/Robo/robodoc.html)

Src2tex for LaTeX formatting (printout)

http://www.eng.gunma-u.ac.jp/~amano version 2.13j (*obsolete*…)
modifications done by MM, to routines text2tex.c & modflag.c
to accept the Robodoc style.

“Template” for ABINIT source codes

```
!{\src2tex{texfont=tt}}                    | font setting for "src2tex"
!!****f* ABINIT/(subroutine name)          | Robodoc region starts
(package/name)
!!                                         |N.B. other "!!****..." are also available
!! NAME                                    | SUBROUTINE(or FUNCTION) NAME declaration
!! (subroutine name)                       |   (the name of the subroutine here)
!!                                         |
!! FUNCTION                                | FUNCTION declaration
!!  ...                                    |   (explanation of the routine here)
!!                                         |
!! COPYRIGHT                               | COPYRIGHT declaration
!! Copyright (C) ABINIT group (...)        |   (Authors and Date here)
!!                                         |
!! INPUTS                                  | INPUT variables declaration
!!  aa= ...                                |   (explanations for input variables)
!!  bb= ...                                |
!!                                         |
!! OUTPUT                                  | OUTPUTS variables declaration
!!  xx= ...                                |   (explanations for output variables)
!!  yy= ...                                |
!!                                         |
!! SIDE EFFECTS                            | SIDE EFFECTS declaration
!! Input/output                            |  if any variables may be changed
!!  ll= ...                                |  when exiting, explanation here
!!                                         |
```

“Template” for ABINIT source codes
(continued)

```
!! NOTES                                  | NOTES declaration
!!  (warning, etc.)                       |  If any annotations (e.g. warning)
!!                                        |  should be noticed, explanation here
!!                                        |
!! TODO                                   | TODO declaration
!!  ...                                   |  What to implement next & ideas (if any)
!!                                        |
!! SEE ALSO                               | References
!!  ...                                   |  References to other functions, man
!!                                        |  pages, other documentations (if any)
!!                                        |
!! PARENTS                                | PARENTS declaration
!!  ...                                   | Which modules use this one.
!!                                        |
!! CHILDREN                               | CHILDREN declaration
!!  ...                                   | What modules are used by this one
!!                                        |
!! BUGS                                   | BUGS declaration
!!  ...                                   |  Known bugs. (if any)
!!                                        |
!! SOURCE                                 | Source region (if it should be included.
                                          | If not, ends with "!!***" here.
```

“Template” for ABINIT source codes
(continued)

```
 subroutine ...

implicit none
!Arguments ------------------------------------------
  ....

!Local variables -------------------------------------
  ...

!*********************************************************************************
  ... (source code here)
  ...
  ...

 end subroutine
!!***                                    |   end of robodoc
```

Process for Self-documentation

The Perl script “parents” builds the list of “parents/children” routines.

To make the sources (HTML format), at ~ABINIT directory, type

1) “make parents”
   parents -s

2) “ make robodoc”
   ./makemake.ROBODOC (to complete “Makefile.ROBODOC”)
   make -f Makefile.ROBODOC xhtml (“xref” files)
   make -f Makefile.ROBODOC html (html files)

(The scripts were devised by L. Sindic. Merci !)

Example file (psp1cc.f)

```
!! and
!! $ xx=¥frac{r}{rchrg}=¥frac{r}{xcccrc/3.0d0}=3*¥frac{r}{xcccrc}=3*yy $
!!
!! Code for gg(xx), gp(xx), and gpp(xx) has been tested by numerical
!! derivatives--looks ok. gpp(x) should still be rewritten.
!! The argument of xccc1d is assumed to be normalized, and to vary
!! from yy=0 to 1 (from r=0 to r=xcccrc, or from xx=0 to 3)
!! Thus :
!!{{¥ ¥begin{equation}
!! xccc1d(yy)=fchrg*[¥frac{¥sin(2*¥pi*(3yy))}
!! {(6*¥pi*(3yy))(1-4*(3yy)^2)(1-(3yy)^2)}]^2
!!¥end{equation} }}
!!
!! WARNINGS
!! Warning : the fifth derivative is not yet delivered.
!!
!! PARENTS
!!      psp1in,psp5in
!!
!! CHILDREN
!!      gg1cc,gp1cc,gpp1cc,leave_new,spline,wrtout
!!
!! SOURCE

 subroutine psp1cc(fchrg,n1xccc,xccc1d)
```

$ xx=¥frac{r}{rchrg}=¥frac{r}{xcccrc/3.0d0}=3*¥frac{r}{xcccrc}=3*yy $

Converted HTML file

Code for gg(xx), gp(xx), and gpp(xx) has been tested by numerical
derivatives--looks ok. gpp(x) should still be rewritten.
The argument of xccc1d is assumed to be normalized, and to vary
from yy=0 to 1 (from r=0 to r=xcccrc, or from xx=0 to 3)
Thus :
{{¥ ¥begin{equation}
xccc1d(yy)=fchrg*[¥frac{¥sin(2*¥pi*(3yy))}
{(6*¥pi*(3yy))(1-4*(3yy)^2)(1-(3yy)^2)}]^2
¥end{equation} }}

WARNINGS

```
Warning : the fifth derivative is not yet delivered.
```

PARENTS

psp1in,psp5in

CHILDREN

gg1cc,gp1cc,gpp1cc,leave_new,spline,wrtout

SOURCE

```
subroutine psp1cc(fchrg,n1xccc,xccc1d)

use defs_basis
implicit none
```

Converted LaTeX (dvi) file

!!
!! NOTES
!! density(r)=fchrg*gg(xx)
!! with
!! $gg(xx) = (\frac{\sin(2\pi xx)}{(2\pi xx)(1-4xx^2)(1-xx^2)})^2$
!! and
!! $xx = \frac{r}{rchrg} = \frac{r}{xcccrc/3.0d0} = 3 * \frac{r}{xcccrc} = 3 * yy$
!!
!! Code for gg(xx), gp(xx), and gpp(xx) has been tested by numerical
!! derivatives--looks ok. gpp(x) should still be rewritten.
!! The argument of xccc1d is assumed to be normalized, and to vary
!! from yy=0 to 1 (from r=0 to r=xcccrc, or from xx=0 to 3)
!! Thus :
!!

$$xccc1d(yy) = fchrg * [\frac{\sin(2 * \pi * (3yy))}{(6 * \pi * (3yy))(1 - 4 * (3yy)^2)(1 - (3yy)^2)}]^2 \qquad (1)$$

!!
!! WARNINGS
!! Warning : the fifth derivative is not yet delivered.
!!
!! SOURCE

```
 subroutine psp1cc(fchrg,n1xccc,xccc1d)

 use defs_basis
 implicit none
```

Future Plan (Open Discussion)

1) Linking to references on WWW (HTML)

Robodoc latest version (v. 3.2.4) enables us to do :

http://someaddress.somewhere
file:/fullpath/to/file
href:localpathtofile (relative paths allowed)

2) Linking to available document files (e.g. LaTeX)

a) LaTeX –> **PDF** (by **dvipdfm**)

"hyperref.sty" work for hyperlinks (URL, *links inside PDF*)
good display/printout for Math equations
Most browsers can treat PDF (using "plug-in")

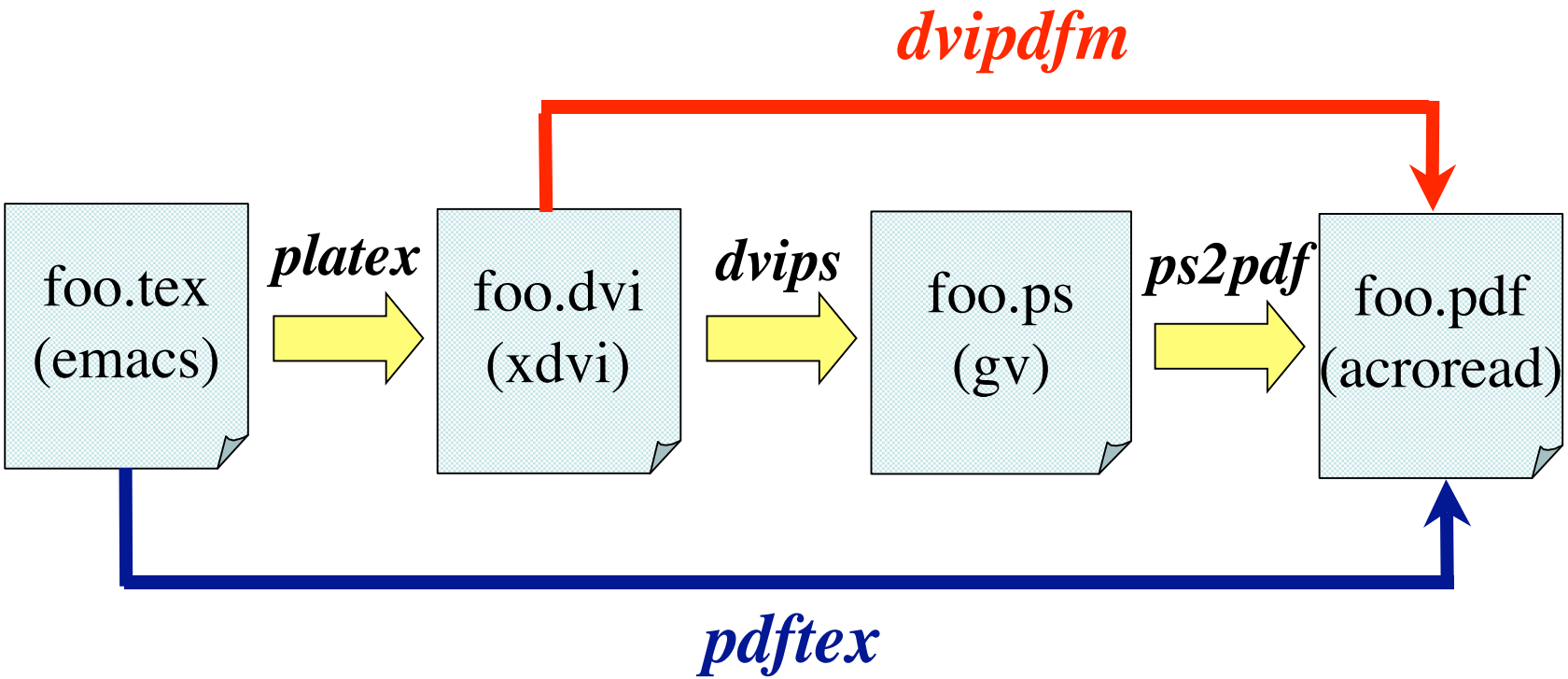
b) LaTeX –> HTML

TtH: No images for Eqn (using MathML) => fast !
but *Symbol Fonts (for Eqn) depend on Browsers.*

HEVEA : No images for Eqn, -nosymb option (–> *low quality*)

(NB: **LaTeX2HTML, TeX4ht** : *many images are needed*)

From LaTeX to PDF



Example of “LaTeX to PDF” (hyperref.sty)

```
\documentclass{article}
\usepackage[colorlinks]{hyperref}
\begin{document}
\section{}
        …
\hypertarget{tag}{displayed strings} % “label”
\hyperlink{tag}{displayed strings}    % “cite”
\href{URL}{displayed strings}         % URL
        …
\end{document}
```

For further details, see, for example,
http://www.tug.org/applications/hyperref/manual.html

Example of TtH (browsed with IE, not Mozilla!)

Electric Probes in Magnetized and Flowing Plasmas

We simplify our treatment of the electrons by making the very standard assumption that the electron density is everywhere given by a Boltzmann factor for thermodynamic equilibrium,

$$n(\mathbf{r}) = n_\infty \exp\left(\frac{e\phi}{T_e}\right) \quad , \tag{1.1}$$

where T_e is the electron temperature and ϕ is the electric potential in the plasma, measured relative to its value at `infinity' (i.e., far from the perturbing effects of the probe), where the density is n_∞. This equation will be an excellent approximation for most cases because: (1) electrons move much faster than ions and so they readily reach thermal equilibrium; and (2) the case usually of most interest is where the electrons are being repelled, i.e., the probe potential, ϕ_p, is negative. (Discussion of this assumption is given, e.g., in [1].)

The total electric current emitted by the probe is

$$I = eA\,(\Gamma_e - \Gamma_i) \quad , \tag{1.2}$$

where A is the collection area, the ions are assumed singly charged, and Γ_e, Γ_i are the electron and ion flux densities to the probe. Generally, the ion flux variation with probe potential is minor provided the probe is much bigger than the Debye length. Therefore, writing $I_{si} = -eA\Gamma_i$ as the ion saturation current, the probe current characteristics is

$$(I - I_{si}) \quad \propto \quad \Gamma_e \quad \propto \quad \exp\left(\frac{e\phi_p}{T_e}\right) \quad , \tag{1.3}$$

(taken from **TtH page (http://hutchinson.belmont.ma.us/tth/)**)

Example of TtH (browsed with Mozilla (Netscape 7.0))

Electric Probes in Magnetized and Flowing Plasmas

We simplify our treatment of the electrons by making the very standard assumption that the electron density is everywhere given by a Boltzmann factor for thermodynamic equilibrium,

$$n(\mathbf{r}) = n_{\infty} \exp\left(\frac{e f}{T_e}\right) , \qquad (1.1)$$

where T_e is the electron temperature and f is the electric potential in the plasma, measured relative to its value at `infinity' (i.e., far from the perturbing effects of the probe), where the density is n_{∞}. This equation will be an excellent approximation for most cases because: (1) electrons move much faster than ions and so they readily reach thermal equilibrium; and (2) the case usually of most interest is where the electrons are being repelled, i.e., the probe potential, f_p, is negative. (Discussion of this assumption is given, e.g., in [1].)

The total electric current emitted by the probe is

$$I = eA\,(G_e - G_i) , \qquad (1.2)$$

where A is the collection area, the ions are assumed singly charged, and G_e, G_i are the electron and ion flux densities to the probe. Generally, the ion flux variation with probe potential is minor provided the probe is much bigger than the Debye length. Therefore, writing $I_{si} = -eAG_i$ as the ion saturation current, the probe current characteristics is

$$(I - I_{si}) \;\mu\; G_e \;\mu\; \exp\left(\frac{e f_p}{T_e}\right) , \qquad (1.3)$$

HTML for Mozilla should be different from that for IE !

(TtH can manage it, so two types of HTML would be necessary for IE and Mozilla)

Example of TtH (Infos/Theory/1WF.tex)

* For the generation of the density from wavefunctions, as well as for the application of the local part of the potential, one needs to be able to compute $\psi_{n\mathbf{k}}(\mathbf{r})$ or $u_{n\mathbf{k}}(\mathbf{r})$ for a 3D-mesh of **r**-points, extremely fast, from the values $c_{n\mathbf{k}}(\mathbf{G})$.

[note : spin up and spin down parts can be treated separately in this operation, so they do not need to be specified otherwise in this section 5.]

* The FFT algorithm starts from values of a function

$$z\,(j_1,j_2,j_3) \quad \text{for} \quad j_1=0\cdots(N_1-1),j_2=0\cdots(N_2-1),j_3=0\cdots(N_3-1)$$

and compute fast the transformed

$$\tilde{z}\,(l_1,l_2,l_3) \quad \text{for} \quad l_1=0\cdots(N_1-1),l_2=0\cdots(N_2-1),l_3=0\cdots(N_3-1)$$

with

$$\tilde{z}\,(l_1,l_2,l_3)=\sum_{j_1,j_2,j_3} z(j_1,j_2,j_3)e^{i2\pi([(j_1l_1)/(N_1)]+[(j_2l_2)/(N_2)]+[(j_3l_3)/(N_3)])}$$

* We want, on a FFT grid, the values of $u_{\mathbf{k}}(\mathbf{r})$ for

$$r^{red}{}_1 = \frac{0}{N_1},\frac{1}{N_1},\cdots\frac{N_1-1}{N_1}\left(=\frac{l_1}{N_1}\right)$$

$$r^{red}{}_2 = \frac{0}{N_2},\frac{1}{N_1},\cdots\frac{N_2-1}{N_2}\left(=\frac{l_2}{N_2}\right)$$

$$r^{red}{}_3 = \frac{0}{N_3},\frac{1}{N_3},\cdots\frac{N_3-1}{N_3}\left(=\frac{l_3}{N_3}\right)$$

(the choice of N_1,N_2,N_3 is not discussed here.)

Example of HEVEA (Infos/Theory/1WF.tex) -nosymb option for any browsers

1em * For the generation of the density from wavefunctions, as well as for the application of the local part of the potential, one needs to be able to compute psi$_{nk}(r)$ or $u_{nk}(r)$ for a 3D-mesh of r-points, extremely fast, from the values $c_{nk}(G)$.

[note : spin up and spin down parts can be treated separately in this operation, so they do not need to be specified otherwise in this section 5.]

1em * The FFT algorithm starts from values of a function

$$z(j_1,j_2,j_3) \quad \text{for} \quad j_1=0\cdots(N_1\text{-}1),j_2=0\cdots(N_2\text{-}1),j_3=0\cdots(N_3\text{-}1)$$

and compute fast the transformed

$$z(l_1,l_2,l_3) \quad \text{for} \quad l_1=0\cdots(N_1\text{-}1),l_2=0\cdots(N_2\text{-}1),l_3=0\cdots(N_3\text{-}1)$$

with

$$z(l_1,l_2,l_3)=\sum_{j_1,j_2,j_3} z(j_1,j_2,j_3)\, e^{i2\pi\left(\frac{j_1 l_1}{N_1}+\frac{j_2 l_2}{N_2}+\frac{j_3 l_3}{N_3}\right)}$$

1em * We want, on a FFT grid, the values of $u_k(r)$ for

$$r_1^{red}=\frac{0}{N_1},\frac{1}{N_1},\cdots\frac{N_1\text{-}1}{N_1}\left(=\frac{l_1}{N_1}\right)$$

$$r_2^{red}=\frac{0}{N_2},\frac{1}{N_1},\cdots\frac{N_2\text{-}1}{N_2}\left(=\frac{l_2}{N_2}\right)$$

$$r_3^{red}=\frac{0}{N_3},\frac{1}{N_3},\cdots\frac{N_3\text{-}1}{N_3}\left(=\frac{l_3}{N_3}\right)$$

(the choice of N_1,N_2,N_3 is not discussed here.)

HEVEA page (http://pauillac.inria.fr/~maranget/hevea/)

Future Plan (Open Discussion)

3) Anything else ?

- ***Techexplorer*** (IBM) : Browser plug-in for LaTeX documents
  This is not for equations in "source codes"
  All browsers accept the Plug-in or not ? (needs benchmark)
- Other possibilities may be available …

LaTeX–>PDF may be one solution (for browsing/printout)
at present, especially for Math equations, although
hyperlinkability may be somewhat lost … ***How do you think ?***

In any case,

Don't depend too much on the specification of ***one*** tool.
(Specifications will change !)

"Plan to throw one away; you will, anyhow"
(by Eric S. Raymond, "The Cathedral and the Bazaar")

Summary

- "***Robodoc*** & ***src2tex***" style (for browsing and printout.)
- LaTeX files –> PDF/HTML (linked with Source HTML)

  NB: How to call(link) local files from PDF ?

  Problem of symbol fonts for Browsers ?

Still, ***the search for tools should continue !***

The present style appears sufficiently *general*,
so possible further modification of the coding_rules
would be acceptable (if needed in future).

"*How to visualize Math equations with Browsers?* "

PDF, HTML (MathML) ?

Good Refs. "The LaTeX Web Companion", M. Goossens et al. (Addison-Wesley)

TtH page (esp. http://hutchinson.belmont.ma.us/tth/webmath.html)