

The IBA DataFurnace Information for Users

Contents

Hardware Required to Run DataFurnace.....	2
Current Version Installation.....	2
Automatic EBS.....	2
Manuals.....	2
Other Documents.....	2
DataFurnace Practical Course	3
Executable updates.....	3
Version History.....	4
WiNDF	4
NDF.....	5
NDF Manual	6
Examples	6
Licensing Information	7
New Users - Demonstration Code	7
Stopping Powers Used	7
Frequently Asked Questions	8
My new installation doesn't run!.....	8
You get the "can't find licence" message.....	8
My new installation doesn't run on an NT machine!!	8
I can run windf.exe and ndf.exe, but ndf ends with an "exit code 0" message.....	8
I get a "can't find windf.ini" error	8
Can you support my data format?.....	8
DataFurnace seems very difficult to use!	9
Other interesting links:	9
Fitting and Simulation Programs.....	9
High Resolution.....	9
Multiple Scattering.....	9
Non-Rutherford scattering (EBS)	10
IBA Services.....	10
IBA web sites.....	10
Contacts	10

Hardware Required to Run DataFurnace

DataFurnace runs under Windows, including Windows 95, 98, NT, 2000, XP, Windows7 and Windows8. It is computation intensive, so faster machines will be better! It is also space intensive, since it is optimised for speed, and it needs at least 200MB RAM disc space free. See [Specifications](#). Please (as ever) report bugs to us.

DataFurnace is not supported for Vista, but some users report that it runs on this operating system.

Current Version Installation

The latest published installation of DataFurnace (18 February 2014) is [DataFurnace-Setup](#) (WiNDF v9.3.68, NDF v9.6a; zip of EXE file, 17.5MB). Please download executable updates as they become available to replace these ones. This DataFurnace version also includes support for the automatic use of evaluated EBS ([SigmaCalc](#)) files.

We distribute ZBL 2000 stopping powers. You can download SRIM2013 from the [SRIM](#) website (we are not allowed to distribute this). SRIM is highly recommended. You can also supply your own stopping powers, NDF supports any we know of.

Automatic EBS

The new NDFv9.3f and above supports angle interpolated EBS (elastic backscattering) non-Rutherford cross-sections. These are valid for data evaluated over a range of angles. Essentially this means [SigmaCalc](#) data, although some other data can also be defined. You should download R33 files from Alexander Gurbich's [SigmaCalc](#) (see [NIMB 268, 2010, 1703-1710](#)) and create a matrix of angle resolved data files (using the matrix generator utility below) into c:\NDF\sigmacalc.

Here is the [MatrixGenerator](#) utility (v1.0.16, zipped executable, 33 kb, 10th February 2011) for you to create these files directly from SigmaCalc. If new parameters are put into SigmaCalc (for example, $^4\text{He}(\alpha,\alpha)^4\text{He}$ has a resonance at 3038 keV, not 3045 keV as from 2011) you will need to re-create the matrix.

Manuals

You can download the [NDF Manual](#) 9.6a (10 March 2014: PDF, 1.2 MB). Advanced users will need to refer to this.

You can download the [WiNDF v7.0 Manual](#) (1Mbyte illustrated PDF document). Users should initially need only this which is still useful even though it is written for support with NDF v8 and below. Please see the [DataFurnace Practical Course](#) (below) for more extensive, up-to-date and explicit help.

Other Documents

The capabilities of the code distributed in 1999 (v.7) are summarised briefly in the (unpublished) paper we presented at the [Dresden IBA-14 Conference](#) in July 1999 (500kB PDF). A [summary](#) was also presented then (this is not in the Proceedings: you can download it, 500kB PDF).

A full [DataFurnace Review](#) has been completed (September 2002). This is published as a Topical Review in [J.Phys.D 36 \(2003\) R97-R126](#) and considers many subtle details of IBA at length, including a careful description of Simulated Annealing, and a detailed discussion of the issue of ambiguity (using Butler's example presented at the Kingston IBA conference - [NIMB 45, 1990, 160-165](#)).

A summary of the [IAEA-sponsored intercomparison of IBA software](#) was presented in the Hyderabad IBA conference in 2007 by C.Jeynes, and published in 2008 (Barradas *et al*, [NIMB 266, 1338 -1342](#)). This shows that DataFurnace (with [SIMNRA](#)) is one of the two "new generation codes". Also at this conference a description of NDF version 9 (including PIXE) was presented by N.P.Barradas (Barradas & Jeynes, [NIMB 266, 2008, 1875-1879](#))

The [Pitfalls Chapter](#) (Jeynes & Barradas) in the new [MRS IBA Handbook](#) (published 2010) covers many important analytical topics, including the determination of the electronic gain (together with the effect of the

pulse height defect). These things are treated in authoritative detail in the important paper on [RBS at 1% traceable accuracy](#) by Jeynes, Barradas & Szilágyi (*Analytical Chemistry* 84, 2012, 6061-6069) a paper which establishes the state-of-the-art for RBS. This has been followed up by a very detailed paper by Colaux & Jeynes (*Analytical Methods* 6, 2014, 120-129)

The idea of [Total IBA](#) (the self-consistent treatment of multiple IBA techniques, particularly EBS+PIXE) was presented by C.Jeynes at the Brazil IBA conference in 2011, subsequently published in [NIMB 271, 2012, 107-118](#).

DataFurnace Practical Course

At the [Joint ICTP/IAEA Workshop: Advanced IBA Simulations](#) held in Trieste, Feb. 2009, a DataFurnace Practical Course was included. You can download materials from this course here:-

1. The DataFurnace [Practical](#) materials, including an overview and a detailed step-by-step approach to specific examples (ZIP file, 26.8MB). This zip includes a READ.ME file which explains the contents.
2. **Lecture 4** on the 2007 [IAEA-sponsored Intercomparison of IBA Software](#) (3.13MB PowerPoint file)
3. **Lecture 8** on overcoming the [ambiguity](#) of IBA particle spectra by using multiple techniques (4.77MB PowerPoint file)
4. **Lecture 12** on overcoming the ambiguity of IBA spectra by using [PIXE](#) (29.2MB PowerPoint file)
5. **Lecture 14** on [Pitfalls](#) in IBA (presentation based on the new [MRS IBA Handbook Pitfalls Chapter](#)) (2.01MB PowerPoint file)
6. **Lecture 16** on [Techniques Complementary to IBA](#) (12.2MB PowerPoint file), with useful [overview](#). This "covers" XRF, XRD, TEM, MEIS & LEIS, AES & XPS.
7. There is also a [Masterclass](#) on the advanced IBA analysis of a meteoric impact-glass fragment which includes RBS, EBS and PIXE, with the PIXE critical for determining the minor and trace elements, and including information extracted on the nanostructuring of the sample using resonant EBS (15.2MB PowerPoint file)

Executable updates

[WiNDF v.9.3.76 executable](#) (ZIP, 4th April 2014, 1.5 MB) Major change from v.9.3.60 (which was a major change from v9.3.47). Fix a large number of bugs including some extremely annoying ones. Supports NDFv9.6a (mostly). Change font in QED window (Courier is non-proportional so tables are read more easily); Poisson noise now works. Add "warnings" window which records all Warnings in the background without disturbing the user whether or not the "Warnings" flag is up. Fixes SimpleSim to run for SPX (NDF does not run correctly in rep-mode for the SPX setting).

Added [Glossary v.9.3.68](#) (18th February 2014; Menu item: first stab at better documentation; please download this 23kB RTF file and store in c:\NDF).

Molecules can be >132 characters (NDFv9.5e and above). Accepts pathnames with spaces for PCs running Windows7. PIXE M lines accepted (NDFv9.5f and above). Exit angle calculator in general geometry supplied. Supports the new SCREEN (electronic screening) command in NDF. Supports ERF and ERFC functions in Formulae. Simple Simulator is greatly improved and now supports (some further) modifications of the structure file. Support for NEC machine spectra. Add "P" button to "PlotStructure" window, to put profile on clipboard (to place straight in spreadsheet). Now supports batches with up to 360 samples, also supports the CROSS keyword (GEO file) for BI fitting of EBS cross-sections.

[NDF v9.6a executable](#) (ZIP 10 March, revised from 17 Jan 2014, 1.5 MB) PIXE M-lines introduced. Foil thickness inhomogeneity introduced (not well handled in WDEPTH). Valentina Paneta's open-source implementation of [Gurbich's severe roughness algorithm](#) implemented. BI/MCMC of formula parameters introduced. Introduced inhomogeneous active layer thickness. Change pre-defined molecules (and relax conditions on molecules). Modify treatment of NDFPRF.ORD. Changes from v9.4e: ERF and ERFC functions available. Moliere, Universal, Lenz-Jensen and Bohr potential screening available. "Force" and PIXE error inputs

- see Manual (& bug fixes). [NDF Manual 9.6a](#) (10 March 2014: PDF, 1.2 MB); put this into c:/Program Files/WiNDF/Manual).

Extra [DLLs and PIXE files](#) are also needed from NDFv9.5f (unzip all these files into c:/ndf/). (These are now included in the v.68 Installation executable.)

The default position of WiNDF on your computer is c:\Program Files\windf\windf.exe. The default position of NDF on your computer is c:\ndf\ndf.exe.

Some previous executables can be found in the version history section.

We are upgrading DataFurnace frequently. Only the latest version is supported (both of NDF and WiNDF), so if you have problems please first see if they go away with the upgrade. We are leaving the previously released versions on the website so that you can downgrade if necessary (it happens!).

Please send bug reports to [Chris Jeynes](#).

Please see [FAQ](#) for problems.

(See Version History for release dates, sizes, and other information, including some bug information we are aware of).

Version History

WiNDF

[WiNDF v.9.3.76 executable](#) (ZIP, 4th April 2014, 1.5 MB) Fix many bugs. Poisson noise now works. Fixes SimpleSim to run for SPX (NDF does not run correctly in rep-mode for the SPX setting).

[WiNDF v.9.3.73 executable](#) (ZIP, 11th March 2014, 1.5 MB) Fix many bugs. Also v.74, 21st March. Also v.75, 1st April: Change font in QED window (Courier is non-proportional so tables are read more easily). Add "warnings" window which records all Warnings in the background without disturbing the user whether or not the "Warnings" flag is up.

[WiNDF v.9.3.72 executable](#) (ZIP, 7th March 2014, 1.5 MB) For SimpleSim, *.SPX, and charge linking implemented. Display button for *.SPX. Formatted batch file write.

[WiNDF v.9.3.70 executable](#) (ZIP, 28th February 2014, 1.5 MB) Fix many bugs.

[WiNDF v.9.3.68 executable](#) (ZIP, 18th February 2014, 1.5 MB) Implement Gurbich roughness and density variation. Support NDFv9.6a which implements recalculation with modified charge, gain & offset, and fitted molecules. Implement comment lines in GEO file. Fix many bugs, including in the simulator and auto-ranging in PlotSpectra and PlotFits.

[WiNDF v.9.3.60 executable](#) (ZIP, 13th August 2013, 1.4 MB) Fix many bugs. Supports NDFv9.5f (mostly). Molecules can be >132 characters (NDFv9.5e and above). Accepts pathnames with spaces for PCs running Windows7. PIXE M lines accepted (NDFv9.5f and above). Exit angle calculator in general geometry supplied.

[WiNDF v.9.3.47 executable](#) (ZIP, 11th December 2012, 1.4 MB) Fix many bugs. Supports NDFv9.5b (mostly).

[WiNDF v.9.3.42 executable](#) (ZIP, 10th October 2012, 2.7 MB) Major change. Added [Glossary](#) (Menu item: first stab at better documentation; please download this 11kB RTF file and store in c:\NDF). Supports the new SCREEN (electronic screening) command in NDF. Supports ERF and ERFC functions in Formulae. Simple Simulator is greatly improved and now supports (some further) modifications of the structure file. Support for NEC machine spectra. Add "P" button to "PlotStructure" window, to put profile on clipboard (to place straight in spreadsheet). Add "T" button to "TextResults" window, to put *.RES file Totals on clipboard (to place straight in spreadsheet). Fix a large number of bugs including some fatal ones. Now supports batches with up to 360 samples, also supports the CROSS keyword (GEO file) for BI fitting of EBS cross-sections.

WiNDF v.9.3.32 executable (ZIP, 22nd December 2011, 1.3 MB) Fix a large number of bugs. The SimpleSimulator utility for rep-mode simulations now works reasonably well, although it is not yet quite stand-alone: the structure file cannot yet be changed with this tool. Roughness can be accessed, but inclusions as yet cannot. Includes Molodtsov & Gurbich pileup (NIMB 267, 2009, 3484–3487) implemented by Nuno Barradas (NDFv9.3e), and support for the spectral peaks & edges output by NDF (see NDF Manual section 8.3.2)

WiNDF v.9.3.31 executable (ZIP, 5th December 2011, 1.3 MB) Fix a large number of bugs. The SimpleSimulator now works reasonably well, although it is not yet quite stand-alone: the structure file cannot yet be changed with this tool. Roughness can be accessed, but inclusions as yet cannot.

WiNDF v.9.3.21 executable (ZIP, 7th June 2011, 1.25 MB) Fix a number of bugs in the Structure file editor. Add datatype #35. Fix various other small bugs. Introduce new SimpleSim utility for rep-mode simulations (this doesn't work yet, sorry). Fixed bugs in the AssociateAll button. Add "S" button to *.RES view window (the "QED" window) to read the current structure file onto the clipboard.

WiNDF v.9.3.14 executable (ZIP, 7th February 2011, 1.25 MB) Access to the spectral peaks & edges output by NDF (see NDF Manual section 8.3.2). This allows easy monitoring of pulser and surface signals over a dataset. Also fixed bug with display of partial spectra in plotfit window.

WiNDF v.9.3.13 executable (ZIP, 28th January 2011, 1.25 MB) Bug fixes. Implement Molodtsov & Gurbich pileup completely. Much easier access to GEO file variability. Access to ERD foil inhomogeneity.

WiNDF v.9.3.11 executable (ZIP, 21st December 2010, 1.17 MB) Bug fixes

WiNDF v.9.3.7 executable (ZIP, 10th December 2010, 1.17 MB) Bug fixes

WiNDF v.9.3.5 executable (ZIP, 19th October 2010, 1.17 MB) Bug fixes

WiNDF v.9.3.4 executable (ZIP, 7th September 2010, 1.17 MB) Bug fixes (many of them ...)

WiNDF v.9.3.1 executable (ZIP, 14th June 2010, 1.13 MB) Includes Molodtsov & Gurbich pileup (NIMB 267, 2009, 3484–3487) implemented by Nuno Barradas (NDFv9.3e)

WiNDF v.9.3.0 executable (ZIP, 10th June 2010, 1.13 MB) supports most features of NDF v.9.3c, including SIMS. Handling of partial fitted spectra has been improved and various bugs fixed.

WiNDF v.9.2.30 executable (ZIP, 3rd June 2010, 2.27 MB) supports most features of NDF v.9.3c

WiNDF v.9.2.28 executable (ZIP, 18th May 2010, 1.13 MB) supports most features of NDF v.9.3c

NDF

NDF v9.6a executable (ZIP 10th March, revised from 17 Jan 2014, 1.5 MB) PIXE M-lines introduced. Foil thickness inhomogeneity introduced (not well handled in WDEPTH). Valentina Paneta's open-source implementation of Gurbich's severe roughness algorithm implemented. BI/MCMC of formula parameters introduced.

NDF v9.5f executable (ZIP 15 July 2013, 1.4 MB) Introduced inhomogeneous active layer thickness. Change pre-defined molecules (and relax conditions on molecules). Modify treatment of NDFPRF.ORD

NDF v9.5b executable (ZIP 31st January 2013, 1.5 MB) READGEO directive introduced (not supported yet in WiNDF). NDFPRF.ORD introduced. Volume fraction of inclusions can now be fitted.

NDF v9.4h executable (ZIP 24 August 2012, 1.8MB) ERF and ERFC functions available. Moliere, Universal, Lenz-Jensen and Bohr potential screening available. "Force" and PIXE error inputs - see Manual (& bug fixes).

NDF v9.4e executable (ZIP 17 January 2012, 1.8 MB) Major changes from v9.3c (see NDF manual). Not-back-compatible changes to stopping power treatment. Molecular stopping powers supported in a much more general way. Also spectral peaks and edges are output. Evaluated non-Rutherford (EBS) cross-sections

(see [SigmaCalc on the IAEA site](#)) interpolation by angle, handled transparently. This starts to make EBS as easy as RBS to use. Gamma roughness (see Manual). Formula works for molecules. NDP now also working properly. Livetime now input (not real time) as first number in data file (real time can be second number).

[NDF v9.4d executable](#) (ZIP 29 November 2011, 1.8 MB) Gamma roughness now works properly. Formula works for molecules. NDP now also working. Livetime now input (not real time) as first number in data file (real time can be second number).

[NDF v9.4a executable](#) (ZIP 14 June 2011, 1.7 MB) Gamma roughness introduced, IDF outputs, point-by-point for NRA (iff no energy inversion!)

[NDF v9.3f executable](#) (ZIP 14 January 2011, 3.2 MB) this executable works with demo licences! Major changes. SigmaCalc interpolation handled transparently. Not back-compatible changes to stopping power treatment. Molecular stopping powers supported in a much more general way. See Manual. Also spectral peaks and edges are output. Bugs in MG PUP fixed. This executable does not work with demo licences (sorry)!

NDF v9.3c executable (ZIP 3 June 2010, 1.2 MB) this has (small) syntax changes from v.9.2d. WiNDF will not support the old versions of NDFv9. This executable does not work with demo licences (sorry)!

NDF v9.2d executable (ZIP 22 October 2009, 1.1 MB) this is the first published version of NDF v.9

[NDF Manual](#)

[NDF Manual 9.6a](#) (10th March, revised from 10 Jan 2014: PDF, 1.2 MB).

NDF Manual 9.5f (15 July 2013: PDF, 1.1 MB).

[NDF Manual 9.5b](#) (31 January 2013: PDF, 1.1 MB).

[NDF Manual 9.4h](#) (24 August 2012: PDF, 639 kB, zipped to 579 kB)

[NDF Manual 9.4d](#) (11 November 2011: PDF, 974 kB, zipped to 228 kB)

NDF Manual 9.4a (14 June 2011: PDF, 631 kB)

NDF Manual 9.3i (9 May 2011: PDF, 623 kB)

[NDF Manual 9.3f](#) (14 January 2011: PDF, 623 kB).

NDF Manual 9.3a (12 March 2010: PDF, 600 kB).

NDF Manual 9.2c (2 December 2008: PDF, 690 kB). This is the first distributed Manual for NDF v.9

[Examples](#)

You can download the Examples that are referred to in the WiNDF Manual (see below):

[Example 1.](#) (Au/Ni/SiO₂/Si calibration sample, double detector, RBS): zipped to 192 kbyte

Example 2. (High dose implants, double detector, RBS, 12 samples): zipped to 192 kbytes

[Example 3.](#) (Ion exchanged polymers, single detector, RBS, 20 samples): zipped to 540 kbytes

[Example 4.](#) (TaNiC films on Si, H EBS/RBS, 16 samples): zipped to 367 kbytes

[Example 5.](#) (CN_x:H films, He RBS/ERD, 2 detectors, 21 samples): zipped to 1042 kbytes

[Example 6.](#) (Deuterated polymer films, 3He NRA/RBS & 4He RBS/ERD, 3 detectors, 11 samples): zipped to 766 kbytes

[Example 7.](#) (Optical multilayer - zirconia & silica on glass, He RBS, two incident angles, with error bars): zipped to 300 kbytes

Example 8. (High accuracy RBS, IRMM Geel Sb certified sample, 2 detectors): zipped to 204 kbytes

Licensing Information

The IBA DataFurnace is licensed software by N.P.Barradas, C.Jeynes & R.P.Webb with the copyright held by the University of Surrey.

You can see the standard terms of the IBA DataFurnace Licence by downloading a [specimen Licence Document](#) (PDF, 49 kB). Please notice that the licence is very non-restrictive: it is the accelerator that is named and all your academics, students and collaborators are encouraged to use the code. We expect you to make multiple copies. We are keen to give licensed users every help, including supporting your data formats.

Please contact [Chris Jeynes](#) if you wish to have a licence, and also if you wish to have a trial of the code (see [New Users](#)).

New Users - Demonstration Code

If you wish to become a licensed user please see "[Licensing Information](#)". Please look at the [specifications of the DataFurnace code](#).

You can download the [DataFurnace installation](#). If you have a DataFurnace version prior to v9 you need to replace it with this installation. Please ask [Chris Jeynes](#) for a demonstration licence. You can run the full up to date code under this demonstration licence. Use of the code assumes you agree to the [licence terms](#).

Please overwrite the existing licence file (the pathname is probably c:\ndf\licence9.dat) with the demo licence. Please also update the executables (c:\ndf\ndf.exe and c:\program files\windf\windf.exe [with the current version](#)). Please note that the [Barradas stopping powers](#) for Si are in [pscoef.dat](#) which should replace the installation data (c:\ndf\pscoef.dat: this file is public domain TRIM88 data). If you have an existing installation and it doesn't work then you are probably better off uninstalling it (note, uninstall does not yet remove the c:\ndf directory) and using the new installation.

When using DataFurnace we assume that you have all your data in separate data directories: don't use the program directories for the data! Note that the windf.ini file is just a file of defaults kept in your last used data directory, and that when ndf.exe finishes without crashing it shows "exit code 0"!

Please also see [FAQ](#).

Stopping Powers Used

(And corrections for Si and SiO₂) (*THIS SECTION HAS BEEN MADE LARGELY OBSOLETE BY SRIM2003*)

We distribute the public domain TRIM88 data with the code. Note that Ziegler's [SRIM2001](#) has markedly different stopping powers from the TRIM88 values that we use, and that ICRU is also developing new values. DataFurnace supports other stopping powers including SRIM2000, the heavy ion stopping powers by Helmut Paul (Paul & Schinner, NIMB 179, 2001, 299 & NIMB 195, 2002, 166), and the [stopping power predictor](#) code by Tessica Weijers et al (NIMB 215, 2004, 35). Please see the NDF Manual.

For much better (2% uncertainty) stopping powers of 4He in Si please put this file with [corrected 4He stopping powers for Si](#) into c:\ndf\ (or the equivalent on your machine), overwriting the pscoef.dat file that is there already. This data for He on Si is by Barradas et al [Accurate determination of the stopping power of 4He in Si using Bayesian inference, NIMB 194 (2002) 15], following Konac et al 1998 (the "KKKNS" stopping power measurements by Kalbitzer's group presented at the Lisbon IBA conference: NIMB 136-138 (1998) 159-165) confirmed by Lennard et al NIMB 152 (1999) 370-376 and Bianconi et al NIMB 161-163 (2000) 293-296 Please note: these values for He in Si are 2% higher than the KKKNS values, as justified further in Boudreault et al [[Accurate RBS measurement of ion implant doses in silicon](#), Surf.Interface Anal. 33 (2002) 478]. To use the KKKNS values choose a multiplier of 0.98 for the Si stopping in the WiNDF geometry file editor.

For much better stopping powers of 4He in SiO₂, Nuno Barradas has parameterised the data of Pascual-Izarra et al (NIMB 196, 2002, 209-214). These data are confirmed at about 2% by Lennard et al (NIMB 215, 2004, 297) also see Boudreault et al (to be submitted to NIMB shortly). Please use this file according to the instructions for using molecular stopping powers in the NDF Manual and note the following extra Warning:

WARNING: NDF will change the a1-a8 coefficients of the ZBL90 parameterisation; hence, this will only work if you use those stopping powers (e.g. MSTAR stopping values will not be affected). Also, this means that the stopping of any ion in the given target element will be affected; hence, you should only do this for single ion experiments. Also, if you have more than one experiment at different geometries, you should put all the stopping corrections in the same GEO file, and only in that one. Which means if you have the readstop sio2 sio2.1 line in one geo, that is enough! And if you have measured the same sample with Li as well, the stopping of Li in SiO₂, which is calculated actually from the same a1-a8 params (with something extra), will also change.

Frequently Asked Questions

My new installation doesn't run!

You get the "error with licence, refer to Surrey" message.

Have you copied the licence file that Chris Jeynes sent you to c:\ndf (or wherever you put it), remembering to change the name to "license9.ndf" (you should overwrite the existing file). Have you copied the up-to-date executables (windf.exe and ndf.exe) from this website overwriting the existing files?

Have you rebooted after installation? Did you run the Windows install program to completion (don't just copy files!)?

You get the "can't find licence" message.

The autoexec.bat file should include the lines (to complete the installation you have to have the right to modify the autoexec.bat file - you have to be Administrator on Windows NT systems for example):

```
SET PATH+%PATH%;c:\ndf (or whatever your pathname is!)  
SET PATHNDF=c:\ndf
```

Remember you have to reboot after changing autoexec.bat. There may also be an entry in Registry. This entry is not essential, but is an item in HKEY_CURRENT_USER\Software\WiNDF\App and should contain two entries: filepath set to c:\(where ever the last file used was...) path set to c:\ndf (where ever ndf actually is....)

My new installation doesn't run on an NT machine!!

NDF is very greedy for space, and in NT you can manipulate the swap page size. It may well be that the swap page size needs increasing. Please see how to do this in Setting up NT for NDF. This has been a problem for v7.6b and above.

I can run windf.exe and ndf.exe, but ndf ends with an "exit code 0" message

Don't worry about this: "exit 0" means that it has run correctly, probably (that is, with zero errors!) But do look at the NDF output because it tries to tell you if it has found errors, and these cases will also give the "exit 0" message. An "exit code 1" message means that NDF has crashed - there is an untrapped error. We have tried to avoid these untrapped errors, but there are still some left (sorry).

I get a "can't find windf.ini" error

Don't worry about this, it is just the defaults for the displays etc which WiNDF tries to remember for you. We do our best not to frustrate the users, but don't always succeed...

Can you support my data format?

Yes, we have a policy of supporting the data formats of our licensed users so that they are able to take maximum advantage of the high volume data handling capability of DataFurnace.

DataFurnace seems very difficult to use!

Remember, you are used to a simulation program. These are very simple creatures! DataFurnace is a whole new way of thinking about the data. The machine now does the simulations (very many of them, until the data is fitted) and your job is to set the parameters of the data space in which it looks for solutions. First you have to get the geometry file right (beam energy, keV/ch, scattering angle etc). Remember that you have to put in the collected charge too, and NDF is very fussy about this - it is much stupider than you are and will believe what you tell it, even if it is wrong ... NDF will generally give you a solution, and quite often completely stupid solutions can be good fits, so beware! Assuming you have all these basic things right you then have to fight the real ambiguity of the data. We have provided a series of tools to help you persuade NDF not to consider various sorts of solutions, which objectively might be perfectly valid.

DataFurnace is a tool for real analysts to handle large numbers of spectra from real samples with speed, delicacy and accuracy. We have provided very considerable flexibility because we needed it to treat the variety of samples presented to us. If you want to do something and can't see how, please ask! Probably we have done it already. If not we are eager to extend the code to handle more cases, so we may change the code for you!

Other interesting links:

Fitting and Simulation Programs

Application of Yves Serruys' PERM code. This is a fitting program for RBS data.

Leo Kuzmin's [BEAM EXPERT](#) site. Beam Expert is also a fitting program for RBS/NRA and channelling data.

The SQUEAKIE program from the Garching group (Borgersen, Behrisch & Scherzer, Appl.Phys.A27, 1982, 183-195) uses matrix inversion maths to fit RBS spectra only if the partial elemental spectra are separated. This has a number of problems which are discussed at length in the [Topical Review](#) (Jeynes et al, J.Phys.D 36, 2003, R97-R126), briefly: errors in the stopping powers gives inconsistent results, and the surface is not treated correctly.

The ERD analysis program from Subhash Gujrathi's group at Montreal (Oxorn et al, NIM B45, 1990, 166-170) fits ToF-ERD spectra using the fact that the ToF recoil spectra are usually well mass resolved.

I don't know of any other true global fitting programs (many simulation programs have facilities for local fitting)

There are many simulation programs which can be found on the IBIS or SigmaBase websites

The [RUMP](#) package at Cornell, maintained by Michael Thompson, dates from the 1980s and was very popular

[SIMNRA](#) by Matej Mayer is a state-of-the-art simulation program (with some fitting facilities). NDF and SIMNRA are recognised as the two "New Generation" codes (see the [IAEA-sponsored intercomparison of IBA software](#)).

High Resolution

For high resolution work [Szilágyi's DEPTH code](#) is indispensable. It calculates the energy resolution function with depth allowing NDF to convolute it into the spectral calculation during the fit as a sort of "custom straggle" function.

Multiple Scattering

There is an interesting new website on [Multiple Scattering](#) which is well worth looking at, including further information on the paper: *Small angle multiple scattering of fast ions, physics, stochastic theory and numerical calculations* by Amsel, Battistig & L'Hoir (NIM B201, 2003, 325-388)

Non-Rutherford scattering (EBS)

For non-Rutherford elastic backscattering (EBS) the [paper describing the SigmaCalc program](#) (PDF document: 156kbytes) of [Alexander Gurbich](#) is invaluable. The [SigmaCalc](#) website is now live, please use it.

Evaluated cross-section measurements are extrapolated to different scattering angles and are described in Gurbich's paper for the [IAEA Report of the Advisory Group Meeting on Long Term Needs For Nuclear Data Development](#) (Vienna, 28 November - 1 December 2000: INDC(NDS)-423 (2001) IAEA, Vienna p. 51) (PDF document: 119kbytes). The 2 week IAEA Workshop on Nuclear Data for Materials Analysis (May 2003) is also informative. The Report of the IAEA Technical Meeting on the Database of Evaluated Cross-sections for IBA Applications (October 2003) is also very informative. The CRP (coordinated research project) that IAEA set up as a result of these meetings were presented at the Athens ECAART (2010) and published as [NIMB 269, 2011, 2972-2978](#).

The IAEA Nuclear Data Service has recommended merging the SigmaBase and Gurbich's NRABase, resulting in the [Ion Beam Analysis Nuclear Data Library \(IBANDL\)](#), prepared by Alexander Gurbich, the Liaison Officer between the IBA community and the IAEA. These experimental data are mostly for elastic (non-Rutherford) cross-sections, although they also include some (and an increasing quantity of) NRA data. They are in R33 format, a recommended format accepted by NDF.

IBA Services

For IBA services (including depth profiling and microbeam applications) please see the [University of Surrey Ion Beam Centre](#) site.

For IBA on polymers you can go to [Richard Thompson](#) at [Durham University Department of Chemistry](#)

For microbeam hardware: [Oxford Microbeams Ltd.](#)

IBA web sites

[Surrey Ion Beam Centre IBA page](#)

[Jim Ziegler's IBA website](#). Latest documentation for ion stopping database.

The [Hotstop Project](#) by Carlos Pascual-Izarra is a fascinating exercise which uses simulated annealing to extract stopping power curves (or, as he points out to be consistent with ICRU terminology, stopping force curves) from RBS data, and then uses Bayesian inference to obtain confidence intervals to the curves obtained.

The [Ion Beam Information System](#) maintained by Edit Szilágyi and others in Budapest

The [Ion Beam Analysis Nuclear Data Library](#), (IBANDL) maintained by the IAEA

The [Q-value calculator](#) from Lund is also useful, as is of course qtool from Los Alamos, and the nuclide charts from Brookhaven.

The [IAEA Accelerator Knowledge Portal](#). A database of MV accelerators in the world community-driven portal to events, codes, online resources, documents and collaboration workspaces for the MV accelerators community.

Contacts

Dr. Nuno P. Barradas	nunoni@ctn.ist.utl.pt	+35 1 2199 46150
Dr. Chris Jeynes	c.jeynes@surrey.ac.uk	+44 (0)1483 689829
Prof. Roger P. Webb	r.webb@surrey.ac.uk	+44 (0)1483 689830