# *PDFgetN*: a user-friendly program to extract the total scattering structure factor and the pair distribution function from neutron powder diffraction data

**P. F. Peterson, M. Gutmann, Th. Proffen and S. J. L. Billinge**

# computer program abstracts

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## 1. The crystallographic problem

The total scattering structure factor, $S(Q)$, and the atomic pair-distribution function (PDF) are usually obtained from powder diffraction data employing either neutrons or X-rays (Billinge & Thorpe, 1998). Many steps have to be performed to convert the measured diffraction data to $S(Q)$ data, which are Fourier transformed to obtain the real-space PDF (Billinge & Thorpe, 1998). A weakness of current analysis programs is that the parameters used to obtain a particular $S(Q)$ are not saved automatically, making it difficult to reproduce a particular $S(Q)$ from raw data. Also, many existing neutron PDF data analysis programs do not propagate random errors. This is becoming more important as $S(Q)$ and PDF data are increasingly being modeled using regression.

## 2. Method of solution

PDFgetN is a user-friendly program with a graphical user interface for obtaining $S(Q)$ values. The final $S(Q)$ and PDF data are contained in multiple-column ASCII files with the processing parameters appended to them. They can be automatically reloaded into PDFgetN for further analysis. The file format is compatible with the PDF modeling programs PDFFIT and DISCUS (Proffen & Billinge, 1999; Proffen & Neder, 1997), but the flexible format means that $S(Q)$ and PDF data can be easily exported to other packages. The data analysis programs that are called by PDFgetN are derived from the GLASS package (D. L. Price, internal report) and have been described by Billinge (1993).

## 3. Software environment

The current version of PDFgetN is 1.3 and is written in Perl 5.0 using the Perl/Tk 800 module. Programs that are called by PDFgetN are written in Fortran 77. The source code is distributed and thus the aforementioned compilers are needed during installation. While the Fortran 77 compiler as well as Perl 5.0 are usually included in Linux and Unix, Perl/Tk 800 has to be downloaded from the Internet, but is freely available. The installation of KUPLOT is recommended and will enable graphical display by PDFgetN, but is not essential.

## 4. Hardware environment

PDFgetN has been successfully used on a DEC-ALPHA computer with Digital Unix installed, as well as on PCs running Red Hat Linux 6.0; PDFgetN should run on all Unix platforms. PDFgetN and its underlying programs and sample data need less than 15 Mbytes of disk space for installation on a hard drive. There are no special hardware requirements.

## 5. Program specification

PDFgetN allows flexible data analysis, for example including background scaling, different choices for smoothing algorithms and a master file in which additional parameters can be edited.

## 6. Documentation and availability

A user manual is provided with the distributions and on the Web. This includes tutorials, using sample data from various diffractometers.

PDFgetN and KUPLOT are available by contacting the authors (e-mail: billinge@pa.msu.edu). Additional information is available on the PDFgetN homepage at http://www.pa.msu.edu/cmp/billinge-group/programs/PDFgetN.

## References

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