NAME

fdatap.h − NMRPipe Data and Header Definitions

DESCRIPTION

The NMRPipe parameter header array FDATA currently consists of 512 4-byte floating-point values which describe the spectral data. While all numerical values in this array are floating point, many represent parameters (such as size in points) which are integers. Some parts of the header contain packed ascii text.

There are currently three variations of spectral data in the NMRPipe format:

1. Single-File (1D and 2D): the data are recorded in a single binary file consisting of the header followed by the spectral intensities, stored in sequential order as 4-byte floats.

2. Multi-File (3D and 4D): the data are stored as a series of 2D file planes, each with its own complete header followed by the spectral intensities in sequential order.

3. Data Stream (1D-4D): the data are in the form of a pipeline stream, with a single header at the beginning followed by all of the spectral intensities in sequential order.

The header values can be manipulated directly, but this is not recommended. Instead, the functions getParm() and setParm() can be used to extract or set header values according to parameter codes and the dimension of interest (if any). See the source code distribution for examples of these functions.

The NMRPipe format was created to be compatible with an older format which pre-dates phase-sensitive NMR and multidimensional NMR. So, for historical reasons, there are some potentially confusing aspects regarding definition of dimension sizes, data types, and interleaving of real and imaginary data.

In the NMRPipe nomenclature, the dimensions are called the X-Axis, Y-Axis, Z-Axis, and A-Axis. The X−Axis refers to rows from the spectral data file or data stream; the Y−Axis refers to the next dimension etc. Some rules of thumb about the data format follow:

1. Complex data in the X-Axis is stored as separated 1D vectors of real and imaginary points (see below).

2. Complex data in the Y-Axis, Z-Axis, and A-Axis is stored as interleaved real and imaginary points.

3. The X-Axis size is recorded as complex points.

4. The Z-Axis and A-Axis sizes are recorded as total points real+imag.

5. If both the X-Axis and Y-Axis are complex, the Y-Axis size is reported as total points real+imag.

6. If the X-Axis is not complex but the Y-Axis is complex, the Y-axis size is reported as complex points.

7. TPPI data, and Bruker QSEQ mode data are treated as real data.

1D FORMAT

The NMRPipe 1D format consists of a header, followed by a list of real values, and optionally a list of corresponding imaginary values:

1D Real Format:
(512-point FDATA)

(N real points...)

1D Complex Format:
(512-point FDATA)
(N real points...)
(N imag points...)

2D HYPERCOMPLEX FORMAT;

The NMRPipe 2D Hypercomplex format consists of a header, followed by a series of complex vectors. The vectors are alternating real and imaginary in the indirect dimension (Y−Axis).

```
(direct dimension = t2, indirect dimension = t1):

(512-point FDATA)
(N t2=real points... for t1=1 Real)
(N t2=imag points... for t1=1 Real)
(N t2=real points... for t1=1 Imag)
(N t2=imag points... for t1=1 Imag)
(N t2=real points... for t1=2 Real)
(N t2=imag points... for t1=2 Real)
(N t2=real points... for t1=2 Imag)
(N t2=imag points... for t1=2 Imag)
... etc ...
(N t2=real points... for t1=M Real)
(N t2=imag points... for t1=M Real)
(N t2=real points... for t1=M Imag)
(N t2=imag points... for t1=M Imag)
```

3D AND 4D HYPERCOMPLEX FORMAT

The 3D hypercomplex format consists of a series of 2D hypercomplex planes above, which are alternating real and imaginary in the Z−Axis.

Likewise, the 4D hypercomplex format, consists of a series of 3D hypercomplex spectra above, which are alternating real and imaginary in the A−Axis.

DIMENSION−SPECIFIC PARAMETERS

The following are generalized integer codes for parameters which have a specific value for each dimension of the spectrum. In the codes given, NDPARM currently has a value of 1000. This assures that all of the generalize codes will be different that the actual parameter array location codes 0−511. For each ND code given here, there are four corresponding header locations for each of the for possible dimensions. For a complete list of all parameters, see the file **fdatap.h** in the source code distribution.

NDSIZE (1+NDPARM)

Number of points in the given dimension. For the X−Axis, this is given in complex points. For the Y−Axis, this is given in total points real+imag if both the X−Axis and Y−Axis are complex, and in complex points otherwise. For the Z−Axis and A−Axis, this is given in total points real+imag.

NDAPOD (2+NDPARM)

Current time-domain size. In the case of time-domain data, this is the current number of valid

complex time−domain points in the data. In the case of frequency−domain data, this is the number of valid complex time−domain points which would be available if the data was inverse transformed.

NDSW (3+NDPARM)
Full Sweep Width Hz.

NDORIG (4+NDPARM)
Axis origin (location of last point in the data) in Hz.

NDOBS (5+NDPARM)
Spectral observe frequency in MHz.

NDFTFLAG (6+NDPARM)
Fourier transform flag;
0 = Time Domain
1 = Frequency Domain

NDQUADFLAG (7+NDPARM)
Quadtrature Mode Flag; describes the data type of the dimension;
0 = Complex (States, States−TPPI)
1 = Real (Bruker QSEQ, TPPI)
2 = Bruker Pseudocomplex (Obsolete handling for QSEQ)

NDUNITS (8+NDPARM)
Axis Units Code; currently unused.
1 = Seconds
2 = Hz
3 = PPM
4 = Points

NDLABEL (9+NDPARM)
8-character Axis Label.

NDP0 (11+NDPARM)
Zero Order Phase, Degrees.

NDP1 (12+NDPARM)
First Order Phase, Degrees.

NDCAR (13+NDPARM)
Carrier Position, PPM.

NDCENTER (14+NDPARM)
Point Location of Zero Frequency.

NDAQSIGN (15+NDPARM)
Sign adjustment needed for forward FT:
0 = No Sign Adjustment
1 = Real Sign Alternation
2 = Complex Sign Alternation
16 = Negate Imaginaries
17 = Real Sign Alternation, Negate
18 = Complex Sign Alternation, Negate Imaginaries

NDAPODCODE (16+NDPARM)
Window function used. Current values are:
0 = NA No Window Used
1 = SP Adjustable Sine Bell
2 = EM Exponential Multiply
3 = GM Lorentz−to−Gauss

4 = TM Trapezoid
5 = ZE Zero Range
6 = TRI Triangle Window

NDAPODQ1 (17+NDPARM)
Window parameter Q1.

NDAPODQ2 (18+NDPARM)
Window parameter Q2.

NDAPODQ3 (19+NDPARM)
Window parameter Q3.

NDC1 (20+NDPARM)
First point scale - 1.0

NDZF (21+NDPARM)
Negative of Zero Fill Size.

NDX1 (22+NDPARM)
Extract region origin, if any, in points.

NDXN (23+NDPARM)
Extract region endpoint, if any, in points.

NDOFFPPM (24+NDPARM)
Additional PPM offset, used by assignment software.

NDFTSIZE (25+NDPARM)
Size of data when a forward Fourier transform was last performed.

NDTDSIZE (26+NDPARM)
Original time-domain size in complex points.

ORIGINAL 2D PARAMETERS

FDMAGIC 0
Should be zero in valid NMRPipe data.

FDFLTFORMAT 1
Constant defining floating point format; see **CONSTANTS** below.

FDFLTORDER 2
Constant defining byte order; see **CONSTANTS** below.

FDSIZE 99
Number of points in current dimension, complex points.

FDREALSIZE 97
Number of valid time-domain points (obsolete).

FDSPECNUM 219
Number of complex 1D slices in 2D file plane.

FDQUADFLAG 106
This value is a function of both the X−Axis and Y−Axis data types. A value of zero means the X−Axis vectors should be treated as complex for purposes of reading data.
0 = Complex (States, States−TPPI)
1 = Real (Bruker QSEQ, TPPI)
2 = Bruker Pseudocomplex (Obsolete handling for QSEQ)

FD2DPHASE 256
Describes the type of 2D file plane.
0 = Magnitude Mode
1 = TPPI

2 = States or States–TPPI
3 = Image

DATA ORDER PARAMETERS

These parameters define the number of dimensions and their order in the data; a newly-converted FID has dimension order (2 1 3 4). These dimension codes are a hold-over from the oldest 2D NMR definitions, where the directly-acquired dimension was always t2, and the indirect dimension was t1.

FDTRANSPOSED 221
0 = Not Transposed
1 = Transposed

FDDIMCOUNT 9
Number of dimensions in the complete spectrum.

FDDIMORDER1 24
Dimension stored in X-Axis.

FDDIMORDER2 25
Dimension stored in Y-Axis.

FDDIMORDER3 26
Dimension stored in Z-Axis.

FDDIMORDER4 27
Dimension stored in A-Axis.

PIPELINE PARAMETERS

The following parameters describe the data when it is in a multidimensional data stream format (FDPIPEFLAG != 0):

FDPIPEFLAG 57
Dimension code of data stream. Non-standard.

FDPIPECOUNT 75
Number of functions in pipeline. Non-standard.

FDSLICECOUNT 443
Number of 1D slices in stream. Non-standard.

FDFILECOUNT 442
Number of files in complete data.

PARALLEL PARAMETERS

The following definitions are used for data streams which are subsets of the complete data, as for parallel processing:

FDFIRSTPLANE 77
First Z-Plane in subset. Non-standard.

FDLASTPLANE 78
Last Z-Plane in subset. Non-standard.

FDPARTITION 65
Slice count for client-server mode. Non-standard.

FDPLANELOC 14
Location of this plane; currently unused.

DISPLAY SCALE

The following define max and min data values, previously used for contour level setting:

FDMAX 247
Max value in real part of data.

FDMIN 248
Min value in real part of data.

FDSCALEFLAG 250
1 if the max and min values (FDMAX and FDMIN) in the header are accurate.

FDDISPMAX 251
Max value, used for display generation.

FDDISPMIN 252
Min value, used for display generation.

OTHER PARAMETERS

Locations reserved for User customization:

FDUSER1 70
User Parameter 1.

FDUSER2 71
User Parameter 2.

FDUSER3 72
User Parameter 3.

FDUSER4 73
User Parameter 4.

FDUSER5 74
User Parameter 5.

Defines date and time when data was converted:

FDMONTH 294
Month, 1–12.

FDDAY 295
Day, 1–31.

FDYEAR 296
Year (with century, e.g. 1998, 2003, etc).

FDHOURS 283
Hour, 0–23.

FDMINS 284
Minute, 0–59.

FDSECS 285
Seconds, 0–60.

MISCELLANEOUS PARAMETERS

FDMCFLAG 135
1 if a Magnitude Calculation was performed.

FDNOISE 153
Used to store an RMS noise estimate.

FDRANK 180
Estimate of matrix rank; Non-standard.

FDTEMPERATURE 157
Temperature, degrees C.

FD2DVIRGIN 399
0 if the data have never been accessed, and the header never checked or adjusted.

FDTAU 199
A Time value (for spectral series).

TEXT PARAMETERS

FDSRCNAME 286
Source file, 16 characters.

FDUSERNAME 290
Username, 16 characters.

FDOPERNAME 464
Operator name, 32 characters.

FDTITLE 297
Title, 60 characters.

FDCOMMENT 312
Comments, 160 characters.

CONSTANTS

FDATASIZE 512
Length of header in 4-byte float values.

FDIEEECONS 0xeeeeeeee
Indicates IEEE floating point format.

FDVAXCONS 0x11111111
Indicates DEC VAX floating point format; currently unsupported by NMRPipe.

FDORDERCONS 2.345
Constant used to determine byte-order.

SEE ALSO

fdatap.c, fdatap.h, showhdr.c