

Advanced Data Processing using NMRPipe within VnmrJ 3.2 Software

Technical Overview

Introduction

Sophisticated data processing tools have co-evolved with the development of NMR applications for biomolecules from the earliest days of modern biomolecular NMR. New NMR experiments, such as multidimensional NMR, have spurred computer hardware and software development for the last three decades. Both commercial and academic groups recognized the needs of the NMR community and responded with products and tools for analyzing NMR data. One response was the development of NMRPipe by Frank Delaglio, first at NIH in association with the Ad Bax group, and then later at NMR Science. NMRPipe is the premier stand-alone processing software package used by most of the biomolecular NMR community. With VnmrJ 3.2, Agilent introduces the integration of NMRPipe into standard VnmrJ software. VnmrJ 3.2 provides complete implementation of the widely-used NMRPipe system, specially augmented for use with spectral data from Agilent spectrometers. For those users experienced with NMRPipe processing, all the familiar tools are available at the click of a button. For those not familiar with NMRPipe, the processing is handled by VnmrJ macros, with data display and plotting performed by the standard VnmrJ commands and parameters. This Technical Overview describes the capabilities of the new Agilent VnmrJ 3.2 software interface with NMRPipe, which was designed to meet the needs of both new and experienced users, and for routine automated and advanced data processing.



Agilent Technologies

Harnessing the power of NMRPipe

NMRPipe is a UNIX-based collection of programs and scripts for manipulating multidimensional NMR spectra. NMR structural biology uses a wide variety of methods, and is often practiced by those who might not be completely familiar with details of multidimensional signal processing. As a result, the VnmrJ 3.2 implementation of NMRPipe includes an emphasis on automation.

NMRPipe has become so widely employed for spectral processing of biomolecular NMR data that its use is noted in more than 50 % of the NMR structures accepted into the Protein Data Bank (PDB) since 2000. Application examples include sophisticated 3D and 4D data processing schemes, multidimensional peak analysis, extracting rates from various NMR relaxation and kinetics data, calculating residual dipolar couplings, and extracting restraints for structure calculations, to name only a few. The key features of NMRPipe are summarized in Table 1. VnmrJ 3.2 software provides users with an interface that enables both new and advanced users to access to the power of NMRPipe.

The NMRPipe interface

Figure 1 shows the interface for NMRPipe within VnmrJ 3.2. The **Process** folder now includes a page (NMRPipe) along with the other standard BioPack processing pages. All of the relevant operations are performed within the **Parameter Panel**. Experiment setup macros now include the automatic creation of variables needed by NMRPipe for automatic conversion of the VnmrJ data to NMRPipe format.

Parameter values are automatically set for each BioPack pulse sequence. The operator only needs to use a menu to select the **Experiment Type** (e.g. HNCO). The **dimension** parameter is

automatically set, but can be changed prior to processing. This parameter specifies the order of evolution, by nucleus. The parameter **BPpipetype** is displayed and can be modified by adding keywords from the menu or by simple editing.

Two checkboxes are provided for user input. One checkbox is for specifying the relevant region of the observe dimension to be used for processing the indirect dimensions, thereby reducing the amount of data to be processed and speeding up the total time of processing. The second checkbox is for specifying whether NMRdraw or VnmrJ is to be used for displaying the data.

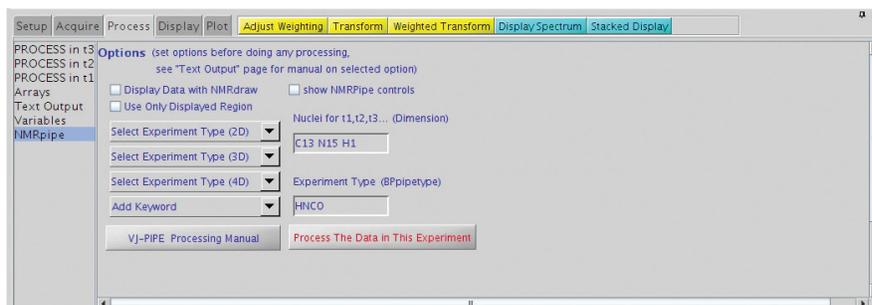


Figure 1. The NMRPipe interface panel. This is used for calling for automatic NMRPipe processing of data in the current experiment or workspace.

Table 1. Summary of NMRPipe features

| Feature | Application | Feature | Application |
|--|--|---|---|
| Conversion of Agilent Spectral Data | Agilent spectral data can be imported for use with NMRPipe automatically, without the need to manually adjust parameters | Extensive line-shape fitting functions | Precise and convenient spectral quantification, including direct fitting of pseudo-3D data, such as relaxation series or J-modulated series |
| Facilities to process, rephase and display multidimensional data | Sophisticated 3D and 4D data processing schemes using Maximum Entropy Reconstruction (MEM), Linear Prediction (LP), and Maximum Likelihood Frequency Maps (ML) | Analyze PDB | List H-bonds, secondary structure and turn classification, mass, volume, and surface area; add Hydrogen atoms to a protein PDB file via simulated annealing |
| Facilities to manipulate and visualize dipolar couplings | Calculating residual dipolar couplings, including restrained fitting and cross-validation of tensor parameters | Predict protein backbone angles based on backbone chemical shifts; simulate and display protein backbone chemical shifts based on protein structure | Extracting restraints for structure calculations; help validate assignments and structure |
| NMR Homology Search | Identify structurally homologous fragments based on chemical shifts and dipolar couplings | Automated 1D and 2D batch processing and series analysis | Screening and process control |

If VnmrJ is to be used for display, NMRPipe is used to process the data and the resulting data is used by VnmrJ to display projection planes and 2D slices in the standard BioPack/VnmrJ manner. Users familiar with VnmrJ 2D or 3D display will use the same panels, buttons, and menus they have used in the past.

Processing parameters are automatically relevant to the acquisition times in each dimension before processing begins. Phasing in indirect dimensions can be first performed using standard VnmrJ displays. The phasing parameters determined for each dimension are then used by NMRPipe. Referencing is automatic. Processing is performed by a simple click of the **Process The Data in This Experiment** button. Display of the processed data follows automatically.

Greater flexibility

More options are available for the user by clicking the **show NMRPipe controls** box in the interface, as shown in Figure 2. This adds expert tools for creating and editing conversion scripts and running specific types of NMRPipe processing. One can create, edit and run NMRpipe scripts by the click of a button. The text editor used for the script modifications can be chosen in the text editor entry, and actual shell script names are specified in the respective entries (Figure 2).

Figure 3 shows the results of using the **edit conversion script** button in the lower right-hand section of the screen. A previously created VnmrJ to NMRPipe conversion script, **fid.com**, is opened in a text editor, ready for modifications. Figure 4 shows the results generated by using the **edit 2D XY** processing script button under the edit NMRPipe processing scripts in current exp: header on the lower right-hand side of the screen. Once edited, the script can be executed by clicking the **run it** button, producing data such as that in Figure 5. Advanced displays such as **strip plots** are also selectable using the expert controls (Figure 6).

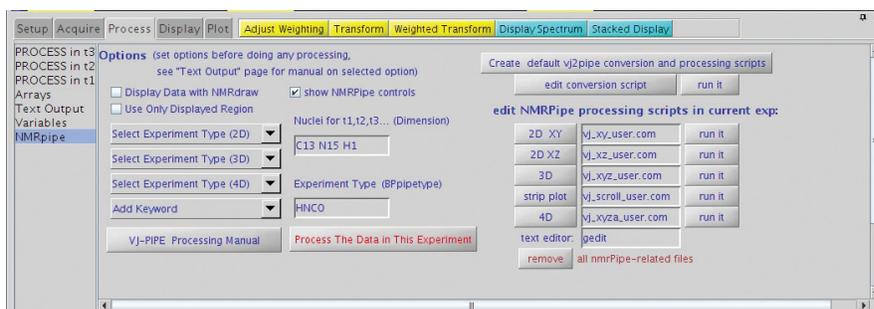


Figure 2. The expanded NMRPipe interface panel as used for advanced NMRPipe processing of data in the current experiment or workspace.

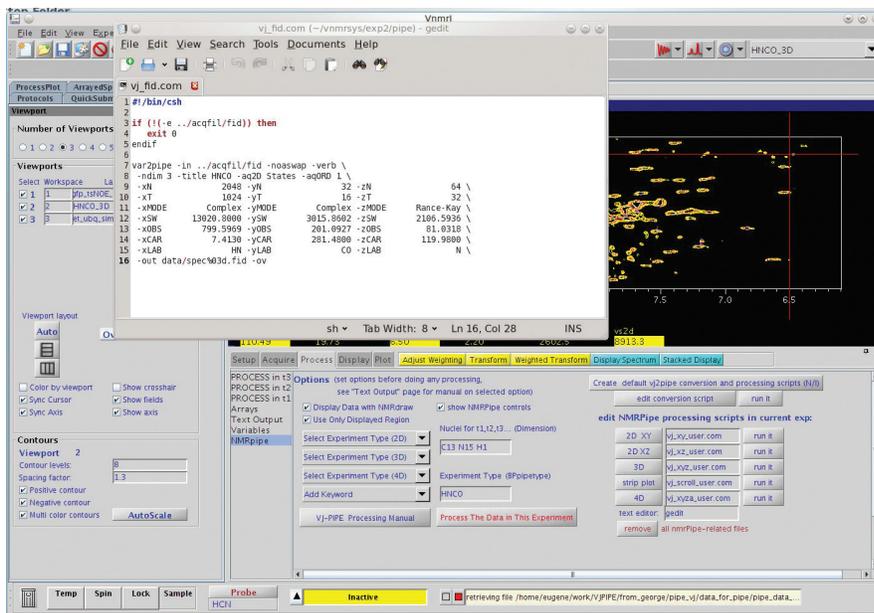


Figure 3. This popup appears when the **Edit Conversion Script** button is clicked.

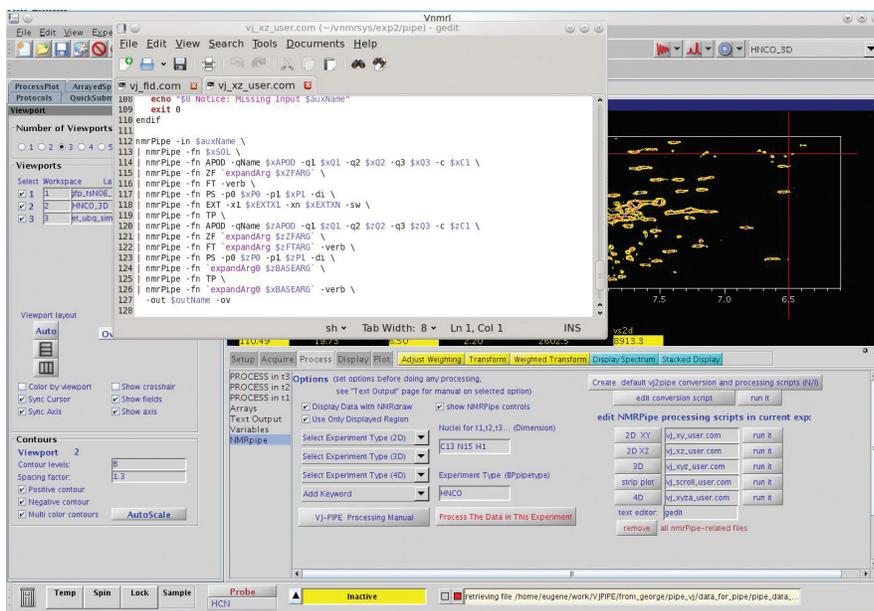


Figure 4. This popup appears when the **2D XY** button is used for editing the XY processing script.

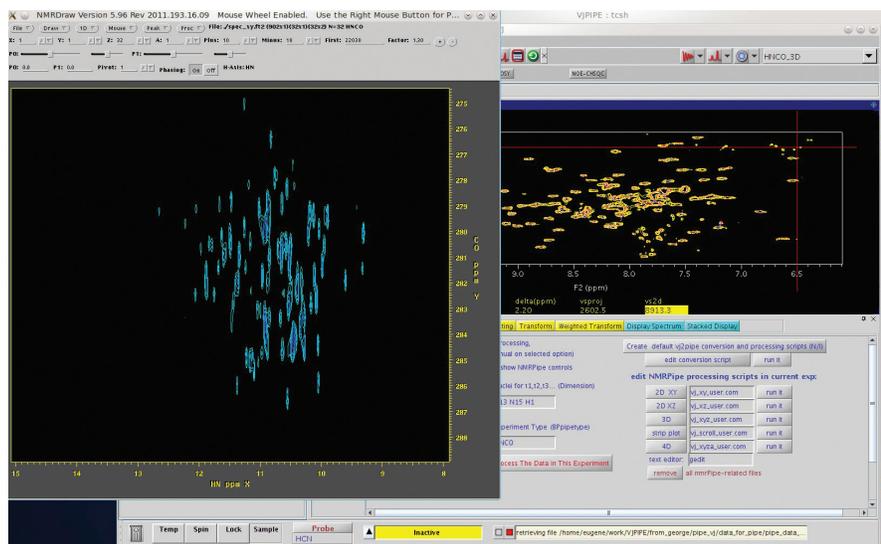


Figure 5. Using the **run it** button for the **2D XY** case calls NMRPipe for processing and then uses NMRdraw to display the processed data.

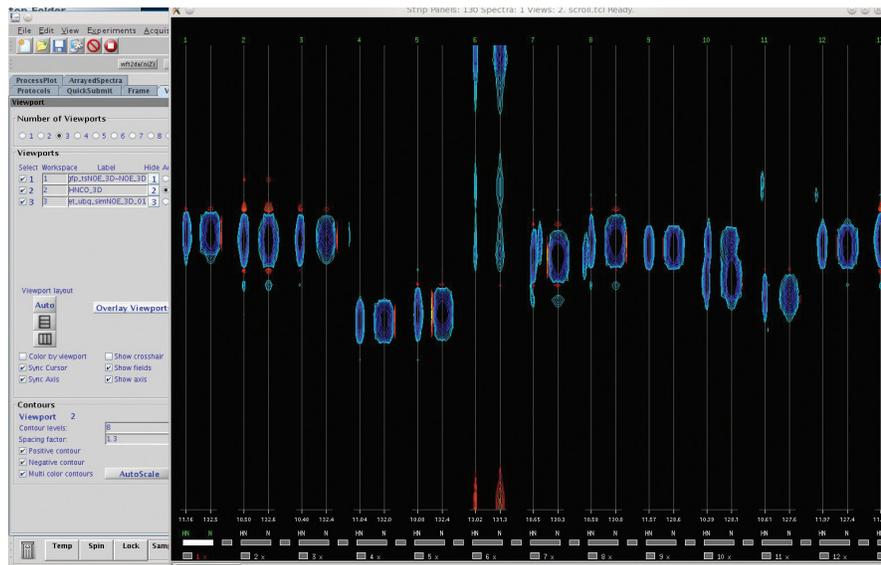


Figure 6. Example of Strip Displays produced by NMRPipe processing.

Conclusions

The power of NMRPipe is now available to VnmrJ software users following its integration into VnmrJ 3.2. Now the biomolecular NMR community can benefit from not only the full-featured, integrated VnmrJ processing software that has full support for advanced processing, display, and plotting of multidimensional NMR data, but also the most widely used advanced NMR processing software package. NMRPipe now provides a means for processing 4D NMR data acquired on Agilent NMR spectrometers, as well as many other leading edge capabilities.

References

1. NMRPipe: a Comprehensive Software System for Multidimensional NMR Applications, <http://www.nmrscience.com/nmrpipe.html>.
2. NMRPipe Spectral Processing and Analysis System Tutorial I: Introduction to Processing with NMRPipe, <http://spin.niddk.nih.gov/NMRPipe/doc1/>.

www.agilent.com/chem/nmr

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