EXPRESS

R.L. Vold and Gina L. Hoatson
Department of Applied Science
College of William and Mary
Williamsburg VA 23187-8795

This is a pre-release version of EXPRESS. Use the program with caution and at your own risk! Please do not acknowledge its use in print, other than something like "MATLAB program provided by R.L. Vold and Gina L. Hoatson, private communication", please let us know if you plan to do this. Also, please do NOT pass this code on to other laboratories.

The hope is that by trying this code out, you will help us to uncover bugs, clumsy features, and other aspects that could/should be improved. Please keep us informed of any progress/problems, via e-mail to rlvold@wm.edu or call 757-221-1518.

SYSTEM REQUIREMENTS

This program requires MATLAB version 7; it will not run under MATLAB 6 or earlier. It is coded in MATLAB Release r2007a and r2007b (the latest version for MAC OSX as of 8/1/2007). EXPRESS will probably run under MATLAB 7.3, but the latest version is highly recommended. It does not use any of MATLAB's optional toolboxes.

We usually run the code on a Mac powerpc (dual processor G5) and also on a MacIntel Powerbook Pro, both with 1G memory. It will run with less, but at least 1G is recommended if you are going to do multi-site jump simulations with MAS/OMAS. Our implementation of Floquet methods for these problems leads to very large matrices…

The code has been tested under MATLAB for Windows XP, and works without modification on this platform. You may have to resize some of the screens if you have a tiny display... we have not tried the code under Windows Vista, and have no intention of doing so.

INSTALLATION

Installation is simple; just put the express folder wherever you keep new programs, and add appropriate entries to the MATLAB path. Full instructions for doing this are illustrated in the powerpoint tutorial, learning_curve.ppt.

DOCUMENTATION

The files EXPRESS.doc and EXPRESS.pdf (for those with an aversion to MS WORD) contain a discussion of the formulae and algorithms used by express, including a detailed description of units and tensor conventions. The program itself is supposed to be self-documenting. Hovering the mouse over most buttons displays a brief comment

about their function. More extensive help for each button can be obtained by pushing the "HELP" button. This disables all the other buttons and if you click on any of them, an explanatory message should appear in the main text window. Releasing the HELP button restores the interface to active status. Occasionally, messages may appear in the MATLAB command window. For the most part, these can be ignored.

All the source code for EXPRESS is kept in the express.beta/source folder; feel free to examine it to see what the program is doing. Before modifying this code, it is a good idea to make a backup copy. If you make substantial changes that result in improved simulations, we would greatly appreciate hearing about them and will try to include them, with appropriate acknowledgement, in future releases.

LICENSEING

Please feel free to run this code on as many machines with as many users as you wish. There is nothing in the code to prevent this. However, do refrain from passing the code on to other research groups. We plan to fix bugs and add features periodically, and new users should not have to put up with bugs from old releases… also, any commercial (aka, for-profit) use of this program is strictly prohibited under terms of the GNU public license, see http://www.gnu.org/copyleft/gpl.html.

RUNNING EXPRESS

When first invoked from the MATLAB command line, EXPRESS displays a welcome message in the main display window and a set of default parameters in the appropriate places. The default parameter set is a twelve site simulation of a deuterated methyl group, that undergoes three-fold hops about an axis that itself jumps among four orientations within a narrow cone. The default experiment is a static quadrupole echo line shape, with just enough powder orientations to outline the line shape. We recommend playing with the powder increment number to see what effect this has on the cpu time. This is especially useful if you select 2H OMAS; magic angle spinning line shapes tend to be time consuming (especially for slow spinning speeds, where there are lots of side bands and the matrices are HUGE). The powerpoint tutorial, learning_curve.ppt, provides useful information about how to use the somewhat daunting variety of simulation options.

Several EXPRESS simulations can be run concurrently on a single computer (given enough memory) by invoking separate MATLAB sessions. It is not possible with the present release to run more than one EXPRESS from a single MATLAB session. The express.beta/examples folder includes several directories that contain MATLAB figure files (*.fig). These were generated from within express, using the SAVE option, and are best viewed through EXPRESS using the LOAD button. After such an operation, all the usual buttons are active and the file can be edited as desired for a related simulation. In addition, the folder express.beta/scripts includes instructions and examples for re-running simulations outside the EXPRESS gui, stepping through parameter ranges.