Online Flow-Based Numerical Simulations

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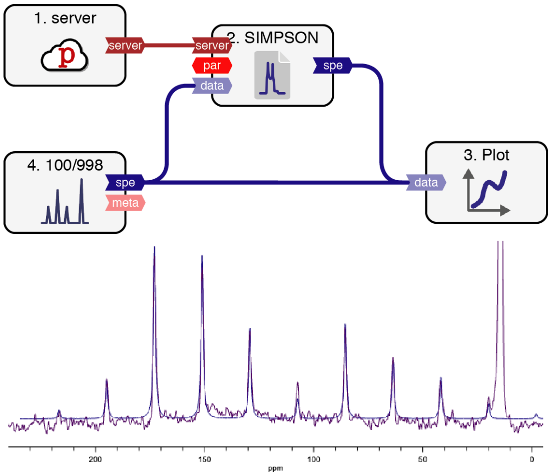
In the past two decades, numerous software tools have been developed to expand the range of simulations or the ease of interacting with a graphical user interface. The most frequently used software packages include DMFit (1), SIMPSON (2,3), SpinEvolution (4), SpinDynamica (5), and SPINACH (6). Of these, DMFit distinguishes itself by having a graphical user interface, while the other programs use more advanced inputs. In addition to these general-purpose software packages, many tools exist to perform dedicated simulations or visualisation of e.g. spectra for teaching (7), dynamics (8) or rapid simulation of protein NMR spectra (9). A general challenge with such community-developed programs is maintaining them on various computer platforms, even after the person who did the actual programming gets a new job…

A common feature of almost all NMR simulations is that they are part of a larger work flow that requires input and output of spectra and other parameters, data processing, establishing various models for the nuclear spin interaction simulations, and visualization of results. For example, to extract nuclear spin interaction parameters from experimental spectra, relevant regions must be selected, the appropriate models must be chosen, and the parameters optimised. In some cases, it is desirable to perform optimisations of multiple spectra simulaneously, e.g. to exploit different magnetic field dependencies of different interactions.

We present a flow-based programming (FBP) design to setup such simulations named EasyNMR, see https://easy.pastis.dk. This web-based solution gives a unique modularity and flexibility to setup *any* simulation. A central feature of the present FBP setup is access to an online server to perform e.g. SIMPSON (2,3) and SIMMOL (10) simulations but not limited to these two programs, so these may be performed on any device (e.g. laptop, mobile device, tablet) without any installation. In addition to the flexibility for the user, this is also of great advantage for the developer who only needs to maintain the software for a single computer architecture. We have tested the new FBP concept in courses and summer schools with up to 50 participants and experienced that all students were able to participate from their own devices, while when relying on conventional user-installed software programs, there will always be some 10-15 % of the students for whom the software installation fails. Flows are easy to share and are small and compact, since it is possible to store spectra on a server, so no large datasets need be sent around. In addition, users may easily contribute their own simulation models to EasyNMR with very little effort. The versatility of EasyNMR will be demonstrated by simulations of pulse sequences, lineshape patterns and rheo-NMR applications.



Flow-based programming example using EasyNMR. This flow reads an experimental spectrum (100/998) and inputs this to a SIMPSON simulation in order to determine the CSA parameters. The SIMPSON object is connected to the server and outputs to the Plot object. The resulting plot is shown below.

References

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