FITTEIA

"Model fitting experimental results is a particular problem in the context of numerical analysis and numerical function fitting. Experienced users with software skills can program their own code and/or modify/adapt existing code or use open-source numerical libraries to obtain software packages that can be used to tackle the model fitting of non-linear functions to experimental data sets including frequency, temperature, etc., dependences and a reasonable number of model fitting parameters. The conventional approach has been to develop code and use graphical interfaces that, unavoidably, will be linked or are specific to a particular operating system (e.g. MS Windows, Unix, MacOS, Linux). The question of portability of the software immediately becomes an issue that is difficult to resolve. In the case of solutions based on proprietary software, the possibility of sharing one model fitting solution lies in having access to the software and/or the licence to install the required supporting software. The possibility of having a model fitting platform that does not require the installation of local software or the purchase of a software licence and, in addition, that can be accessed from any operating system represents an interesting solution to the problems mentioned above.

http://fitteia.org represents an effort in this direction. Examples of relaxation model fits to actual experimental results of recently published concerning the molecular dynamics in liquid crystals, magnetic ionic liquids, and polymers, are presented using the online platform. The software package is written in C, PERL, and HTML. It implements a n-dimensions least squares method and uses the MINUT routine, from CERN library, as the core minimization engine. The GUI interface accessible by any web browser [1]. Presently the models library includes relaxation models for molecular rotations, translational self-diffusion, RMTD, cross-relaxation, order director fluctuations in nematic and smectic LC phases, Rouse model, paramagnetic relaxation, etc., and can be easily extended.

[1] P.J. Sebastião, "The art of model fitting to experimental results", Eur. J. Phys. 35, 15017 (2014)"