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relax and its applications for the study of internal and domain mobility in biomolecules

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The open source software relax (http://www.nmr-relax.com) is designed for molecular dynamics studies through the analysis of experimental NMR data. It is widely used for the Lipari-Szabo model-free analysis of relaxation data, implementing a new protocol which reverses the logic of previous studies and solves many of the problems faced in the past. The program is also used for exponential curve-fitting for determining the R_1 and R_2 rates, the steady-state NOE calculation, consistency testing of relaxation data, and reduced spectral density mapping. The current status of the project will be presented including:

- The new version of the graphical user interface (GUI), exposing more of the power and flexibility available within the prompt and scripting interfaces.
- The multi-processor framework used for speeding up model-free calculations by using the MPI protocol to run on multi-threaded or multi-processor machines or on clusters.
- The tight integration of relax and the Biological Magnetic Resonance Data Bank (BMRB). Data mining will be used to show the utility of model-free data deposition for understanding protein motions. The integration allows for very easy BMRB deposition of previously published data from relax, Modelfree4, Dasha, and Tensor2.
- Its extendibility to other NMR fields, for example the chemistry question of the determination of the absolute stereochemistry of flexible molecules.
- The study of domain motions using the N-state or ensemble model. The analysis of the conformational space of the sugar lactose will be used as a demonstration, applicable to larger molecules, whereby the inter-sugar (or inter-domain) motion was explored using RDC and PCS data.
- The development of the new frame order analysis of domain motions, using calmodulin bound to a target peptide as an example. This combines a new theory consisting of the 3D, rank-4 frame order tensor, used to describe how Brownian motion modules a rank-2 NMR interaction, together with modelling using isotropic and pseudo-elliptic cones and torsion angle restrictions.

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