

NMRBox and VCell: Common Flexible Infrastructure Supporting Two Very Different Virtual Research Communities

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NMRbox is a shared computational platform for NMR which aims to simplify and integrate the dissemination, maintenance, support, and application of NMR data processing and analysis software packages. From the NMRbox perspective, the collection of myriad tools has enabled (1) development of meta-packages that utilize multiple tools to accomplish complex tasks that are beyond the scope of individual packages and (2) fosters critical comparison of different software packages that accomplish the same or similar tasks (e.g. comparing 11 different non-Fourier methods of spectrum analysis). BioMagResBank (BMRB) is the international repository for biological NMR data, and depositions have already enabled meta-analyses yielding novel insights into biomolecular structure and function based on chemical shifts (nuclear resonance frequencies). However depositions of other types of bioNMR data remain insufficient for meta-analysis. NMRbox utilizes the data model underlying BMRB as the organizing principle for annotating NMR data processing and analysis workflows, and consequently transparently facilitates and enriches BMRB depositions. VCell is a unique computational environment for modeling and simulation of cell biology that is deployed as a distributed application freely available over the Internet. VCell provides for “one-stop simulation shopping” whereby deterministic (compartmental ODE or reaction-diffusion-advection PDE), stochastic (several SSA solvers), spatial stochastic (reaction-diffusion with Smoldyn), hybrid deterministic/stochastic, and network-free agent based simulations can be easily created to study the same biological system/hypothesis. Model geometries may be derived from idealized analytical expressions or from experimental 2D or 3D microscope images and support for membrane flux, lateral membrane diffusion and electrophysiology is included. Inexperienced modelers can enter reactions and pathways in a biology-based interface and VCell automatically creates the mathematical system of equations according to the all possible formulations listed above. Models and simulations can be accessed from anywhere and can be shared among collaborators or made publicly available through the VCell database. NMRBox and VCell are supported by a common HPC infrastructure that exploits modern virtualization, distributed, and cloud computing technologies to provide high availability as well as software persistence, using customized, flexible, and evolving solutions for the respective projects and research communities. Both NMRBox and VCell lower the barrier to entry by non-experts in a number of ways: first, by solving the problem of software discovery and installation; second, by providing GUI “wrappers” that hide the complicated syntax utilized by many packages and solvers; and third, by seamlessly handling data conversions and import/export operations required for interoperability within the respective software platforms or with other external tools.

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