Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **2749** Type: **Invited Speaker / Conférencier(ère) invité(e)**

Computer simulations of biological membrane models: lateral structure and lipid-protein interactions

Thursday 6 June 2019 13:15 (30 minutes)

Biological membranes have a complex composition with hundreds of different lipids and a high protein concentration. The nature of the lateral structure of membranes is hotly debated as experiments reach increasingly higher spatial and temporal resolution and simulations increasingly larger time and length scales. Coarse-grained simulations with the Martini model have enabled a significant jump in time and length scale for detailed simulations, and currently can reach of the order of 100 microseconds on systems of ca. 100 x 100 nm size on relatively available computers. We are particularly interested the interactions between lipids and membrane proteins. The local environment around membrane proteins is uniquely shaped by the protein surface, resulting in a local composition and membrane properties that differ significantly from the average properties of the lipids that make up the membrane model. This may play an important role in shaping the lateral structure of biological membranes. This type of simulation also enables detailed studies on more specific interactions.

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Session Classification: R2-2 Membrane Biophysics Joint Session Part II (DPMB/DCMMP/BSC) | Session conjointe sur la biophysique des membranes II (DPMB/DPMCM/SBC)

Track Classification: Physics in Medicine and Biology / Physique en médecine et en biologie (DPMB-DPMB)