



Hamilton Institute

A view into the biomolecular world through the
computational lens: why and how we run
molecular simulations

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Abstract: One of the most active areas in biomedical research concerns the development of highly specific diagnostics tools and of more effective therapeutic strategies, leading to what is known as personalized medicine. The quest for the proteins, also known as biomarkers, central to the progression or the inhibition of specific malignancies is at the core of this field. In this seminar I will discuss how high performance computing (HPC)-based numerical simulations are advancing biomolecular research in terms allowing an atomistic level of detail into the structure-function relationships of complex biomolecular systems.

Venue: Seminar Room, Hamilton Institute, Rye Hall, NUI Maynooth

Time: 2.00pm - 3.00pm

Travel directions are available at www.hamilton.ie