

Prof. Fabio Nobile Institute of Mathematics - CSQI

SEMINAR OF NUMERICAL ANALYSIS

WEDNESDAY 18 OCTOBER 2017 - ROOM CM 1 120 - 16:15

Prof. Andres SZEPESSY (KTH Royal Intitute of Technologie, Sweden) will present a seminar entitled:

Quantum particle dynamics approximated by molecular dynamics »

Abstract:

I will first show how Irvine and Zwanzig derived the fundamental conservation laws of continuum fluid dynamics from quantum mechanics and then modify it to include approximation by ab initio molecular dynamics.

A motivation for the molecular dynamics derivation is e.g. to have a computational method to determine the stress tensor and the heat flux, for any temperature, and estimate the accuracy.