

SEMINARI I DEPARTAMENTIT TË MATEMATIKËS “Math UP Seminar”

Kemi kënaqësinë t'ju njoftojmë se ligjërata e radhës në kuadër të Seminarit të Departamentit të Matematikës në FSHMN ka folës:

Dr. Carl Christian

Orari: 12 shtator 2024, 13:00—14:00

Titulli: The need for accuracy and smoothness in numerical simulations

Abstract

We consider the problem of estimating the error when solving a system of differential algebraic equations. Richardson extrapolation is a classical technique that can be used to judge when computational errors are irrelevant and estimate the discretization error. We have simulated molecular dynamics with constraints using the GROMACS library and found that the output is not always amenable to Richardson extrapolation. We derive and illustrate Richardson extrapolation using a variety of numerical experiments. We identify two necessary conditions that are not always satisfied by the GROMACS library. In reality, we address the fundamental question: How accurate do we have to be when conducting numerical simulations?