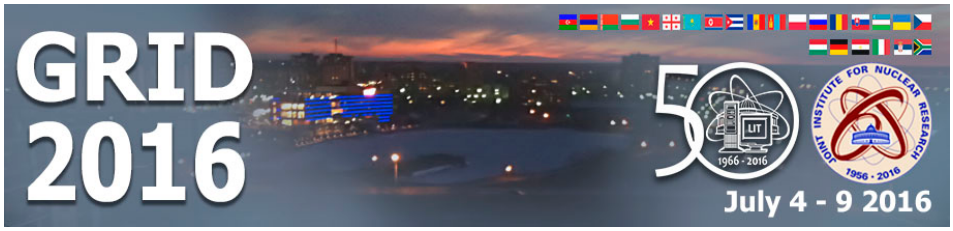

Contribution ID: **84** Type: **Sectional reports**

Design of nanomechanical sensors based on graphene nanoribbons in a distributed computing system

Thursday, 7 July 2016 14:30 (15 minutes)

Software tools for ab initio modeling of nanoscale resonators were implemented within the GRIDIFIN infrastructure, improving the yield of the computational workload. The distributed computing system was used for the investigation of elongated edge-passivated graphene nanoribbons with one open end and one fixed end, by means of density functional calculations. Their oscillatory behavior was studied through molecular dynamics simulations, as a function of key parameters like nanoribbon length, initial structural deformation and amplitude. Several practical utilizations are envisioned for such nanostructures, such as high-frequency oscillators or ultra-sensible acceleration detectors.
The scaling of the MPI application with the number of cores was studied and the results were used for defining the optimal number of cores in the subclusters on which separate instances of the code were distributely ran. The study was also used as an in-house benchmark of the grid system.

Primary authors: Dr VISAN, Camelia Mihaela (Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)); Dr NEMNES, George Alexandru (Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)); Dr VASILE, Ionut Traian (Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)); Dr DULEA, Mihnea Alexandru (Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)); Dr MITRAN, Tudor Luca (Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH))

Presenter: Dr VISAN, Camelia Mihaela (Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH))

Session Classification: 4. Scientific, Industry and Business Applications in Distributed Computing System

Track Classification: 4. Scientific, industry and business applications in distributed computing systems