

Emerging computational trends for nanoscale data analysis with nanoinformatics

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Abstract: Numerous key challenges in nanotechnology research specify a need for nanoinformatics that uses informatics practices to process and manage information on nanobiomolecules and nanomedicines in particular and nanomaterials in general. Nanoinformatics being a subset of materials informatics, allows discovery of hidden information and patterns in nanoscale data. Usually, nanomaterials datasets are small with considerably both large dimensionality and variance. Analysis of such nanoparticles datasets using existing big data analytics is a challenging and computationally intensive task. This study has been focused on survey of emerging databases and computational tools for the progress of nanotechnology research and exploring nanoinformatics that can be optimally used to address the challenges on nanolevel data analysis.

Keywords: Nanotechnology, nanoinformatics, computational tools, nanomedicine, nanomaterials, machine learning.

1. Introduction

Nanoinformatics deals with nanoscale information and aims to develop tools for its management and application in nanotechnology research [1]. The integration of nanobiotechnology, bioinformatics and computational material science with machine intelligence in nanoinformatics enables to study structure-function relation and properties of nanomaterials. Nanotechnology allows the handling of particle of scale ranging from 1 to 100 nanometers [2]. The behavior of such nanoparticles is subjected to molecular, atomic and ionic interactions and hence nanoparticles exhibits variable properties with the effect of quantum mechanics [3]. These effects alter the electrical, magnetic and optical properties of nanomaterials due to the random activities of the electrons. Informatics practices on material science enable the study of nanostructures and properties of these smart nanomaterials. Nanoinformatics is a subclass of informational materials science that allows uncover of significant information and patterns from the existing data. The