Chapter 4
Accelerated Discovery and Design of Nano-Material Applications in Nuclear Power by Using High Performance Scientific Computing

Liviu Popa-Simil
Los Alamos Academy of Science, USA

ABSTRACT

The accelerated development of nano-sciences and nano-material systems and technologies is made possible through the use of High Performance Scientific Computing (HPSC). HPSC exploration ranges from nano-clusters to nano-material behavior at mezzo-scale and specific macro-scale products. These novel nano-materials and nano-technologies developed using HPSC can be applied to improve nuclear devices' safety and performance. This chapter explores the use of HPSC.

INTRODUCTION

This chapter includes the following topics of interest:

1. Defining basic concepts of nano-materials and technologies while examining different perspectives of HPSC usage to clarify various fundamental aspects of physics and material science;
2. Providing a synthesis of existing approaches and solutions to the actual material simulation problems;
3. Investigating the potential of HPSC to develop bottom-up, large-scale simulations from pico-scale up to micro-scale products;
4. Highlighting the issues with existing approaches, specifically focused on the existence of various HPSC solutions from local to distributed systems; and
5. Investigating the potential integration opportunities of multi-scale, multi-dimension

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concepts and their applicability on various HPSC architectures.

SUMMARY OF NANO-MATERIALS, NANO-TECHNOLOGIES, AND ASSOCIATED PHYSICS AND ENGINEERING CAPABLE OF IMPROVING NUCLEAR POWER PERFORMANCE

We will introduce the reader to:

- Actual nuclear power applications with respect to fission, fusion, isotopic power, and annihilation sources, including related performance and problems;
- The concept of harmony among process, method, instrument, and environment as a fundamental explanation of the multi-scale, multi-dimension approach in modern nuclear applications;
- Physics processes in material structures from nano- to micro- and mezzo-scale and various related approaches;
- A brief presentation of models and actual computer simulation tools and their limitations; and
- Basic terminology used in this field.

Who First Defined Nano-Technology?

(Sandhu A., 2006) The term "nano-technology" was first defined by Norio Taniguchi of Tokyo Science University in 1974. (Taniguchi, 1974)

Where are We Using Nano-Technology?

- Medicine
  - Cell imaging
  - Cancer therapy—contact agents
  - Drug delivery vehicles
- Catalysis
  - Fuel cells
  - Catalytic converters
  - Photo-catalytic devices
- Cosmetics
  - Sunscreen
- Textiles
  - Water- and stain-repellent materials
  - Wrinkle-free materials
  - Invisibility coat—military
- Optics
  - Scratch-resistant coatings
- Foods
  - Anti-microbial packaging
- Vehicle manufacturing
  - Hard coatings for wear resistance
- Electronics
  - Quantum dots
  - Semiconductors
- Nuclear materials and applications
  - Direct energy conversion
  - Enhanced separation in transmutation
  - Self-repairing materials
  - Radiation guides and shielding

What Exactly is Nano-Technology?

Nano, is a submultiple of a unit having the meaning of one bilionth of that unit (meter → nano-meter; second →nano-second, etc.). At the scale of an atomic cluster of a few unit cells are at the size of one nanometer, and the experince shows that at this size conventional ideas of structure-property relationships no longer hold in the form they were previously known.

Why the emphasis on nano-technology? Nano-materials exhibit properties that we might be able to exploit to our advantage; for example, hard materials become 'super' hard if apropriately manufactured.

High performance materials are essential for many applications. For example, "Without Damascus steel it would be impossible to make Damascus swords." (Sanderson, 2006)