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ARTICLE

Computational Calculations for the Advancement or Development of Technology

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Abstract

During the last couple of decades, exponential increase in the application of computers have been reported by the scientific community that includes personal computers, laptops, workstations and high-performance clusters. In addition to these applications, main purpose of improving the computational power of computers is technological development for the future applications. In order to develop new technologies, researchers are dependent either on experimental means or on computational efficiency and accuracy of computers. Due to high cost and time involved in experimental techniques, preliminary analysis in most of the cases are performed on computers. Computers have found its application in biomedical science, automotive research, aerospace and in diagnosing diseases. Aim of this article is to discuss the importance of computational power in developing technologies for different applications.

1.0 Introduction

Computers have become the essential or mandatory part of our daily life, and dependency is more critical in developed nations as compared to developing nations. In our daily life, we are dependent on computers, for running finance related calculations in banks, hospitals, communication (e.g. email, social networking sites), etc. But, in addition to these general applications, scientists are increasing the computational power of computers to use it as a tool to investigate, study or develop new technologies. **1-2**

In aerospace industry, experimental testing of big structures such as fuselage and wings is always considered as a cumbersome task. Computational based simulations are alternative means to study the structural strength of these giant structures.**3** During the last couple of decades, many software's have been developed by the engineers and researchers that can assist them in performing different types of analysis on such critical structures. Now the technique of simulating the performance of different components used in the aerospace area, is further extended to other industries such as the automobile-**4** and power sectors.**5** In addition to these areas, computational methods are in forefront to develop technologies for biomedical applications-**6**, energy storage for future automobiles-**7** and materials with superior properties.**8** Aim of this article is to review, different types of computational techniques that can be used by the researchers at different scales.

2.0 Computational Models

Experimental means of investigating the structural strength, thermal performance, aerodynamics of any structures is considered as expensive and time consuming. For experimental analysis a prototype is required, which in certain cases is not possible either due to huge size (airplane fuselage) or extremely small size, as of nano-graphene. Computer based technique to study these huge and extremely small structures are emerging as a viable alternative to expensive and time consuming experimental techniques.

Based on the computational scale (spatial and temporal), these models can be divided broadly under three areas. Continuum, atomistic and quantum based models for any structure or material. The three stages of modeling is explained with the help of Fig.1.

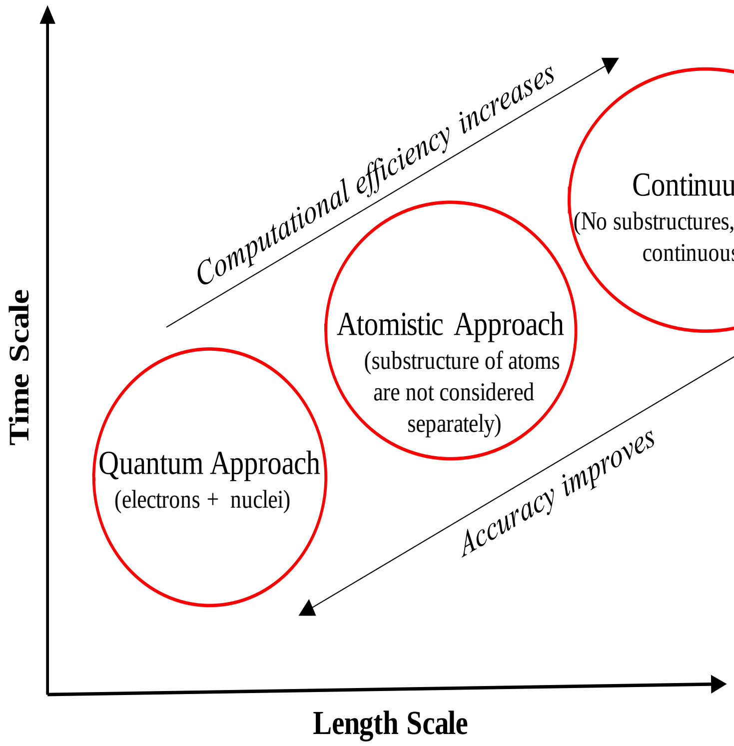

Fig.1 Different types of computational models

2.1 Continuum models

It can be inferred from Fig.1 that continuum based approach is least intensive as well as least accurate, when comparing with the other two types of approaches. Due to least computational cost, continuum approach is used for investigating the properties or behavior of any structure at macro-level. Continuum based models neglects the details of the material such as electronic states, nucleus, etc., which helps in improving the computational efficiency.

2.2 *Atomistic models*

One stage higher in accuracy to continuum approach is referred to as atomistic approach, which is commonly known as classical mechanics based approach. In this stage, continuum structure of any material, fluid or chemical is viewed as a cluster of atoms. The spatial and temporal scale is limited to micrometers and nanoseconds. Due to miniaturization of technology, this computational technique is emerging in forefront among all the three approaches. Computers/electronics engineers are developing new processors to increase the spatial and temporal scale that can be modeled within this approach. Due to exceptional mechanical, thermal and electrical properties, nanomaterials such as carbon nanotubes and graphene are emerging as potential materials for the future applications.9 Superior properties of these materials can only be captured at the atomistic scale; hence, atomistic modeling is used for investigating the application of these materials as nanomembranes for desalination-10, energy storage devices-**11**, reinforcement for weak polymers-**12**, effects of radiation-**13**, etc.

2.3 *Quantum models*

The most accurate modelling technique on computers is quantum approach, which discretized the atoms further into electrons and nuclei. Due to classification of materials in substructures as electron and nuclei, the computer simulation is limited to few hundred atoms. Supercomputers are developed to perform quantum-based simulations. These simulations are highly accurate in predicting the properties, but on the other hand, highly computational intensive.**1**

3.0 Applications of different modeling approaches

As discussed above, continuum based computer models are used in aerospace and aircraft industries for performing different types of aerodynamics, structural and thermal analysis on engine components as well as on the structure of the airplane. In addition to these continuum approach is also used to simulate bridges (Fig.2), pipes (Fig.3), automobile components (Fig.4) and structures (Fig.5) as well.

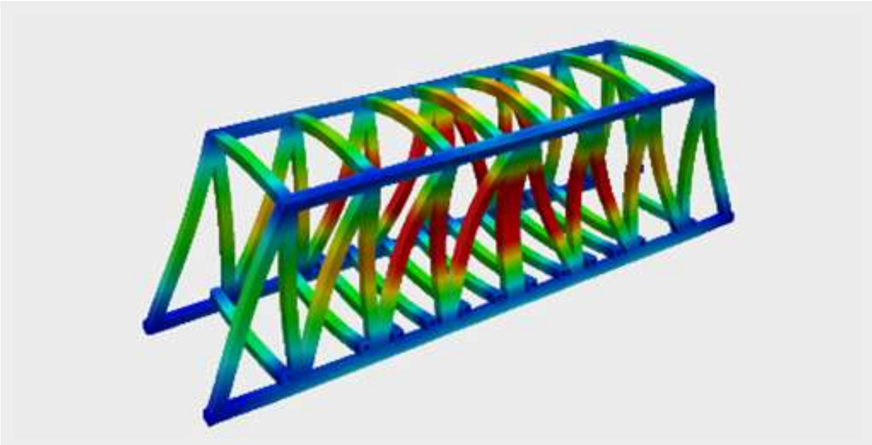

Fig.2 Structural analysis of bridge structure (red color in the online version of the paper referred to regions experience higher deformation) -**14**

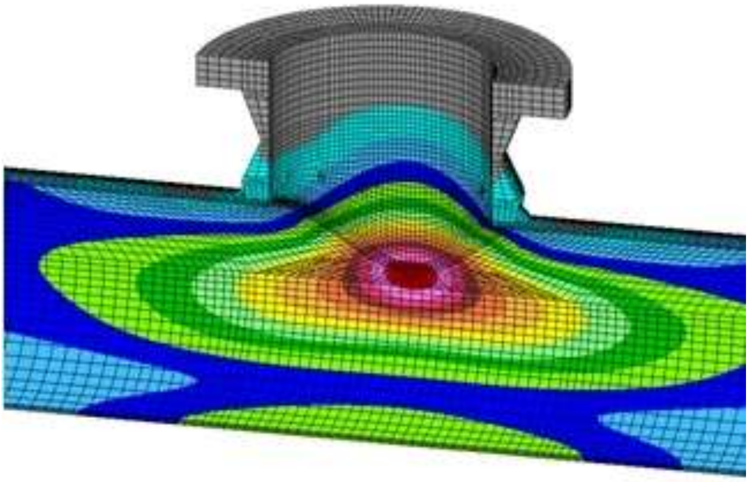

Fig.3 Structural analysis of pipe joint (red color in the online version of the paper referred to regions experience higher deformation) -**15**

Fig.4 Structural analysis of connecting rod of a tractor -**16**

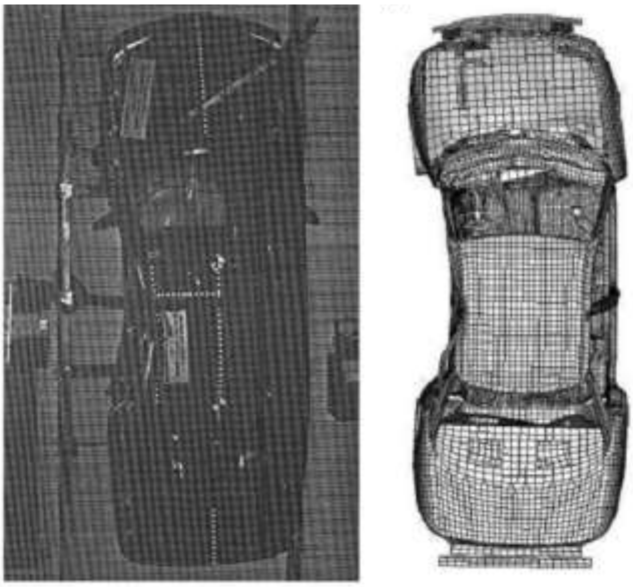

Fig.5 Real and simulated deformations of a car -**17**

Results obtained from continuum approach for the impact analysis of a car is shown in Fig.5. It can be inferred from the figure that the car is damaged from one side. Due to destructive nature of analysis, computer based simulations help in reducing the cost and time of the analysis as well, otherwise, many prototypes are required to perform experimental analysis. In addition to structural analysis, continuum based approaches are used by orthopaedic surgeons to test the shape and configuration of implants, before placing it within the body of a patient.**18**

In contrast to continuum, atomistic approach is used to model nanomaterials, localized effect of irradiation, diffusion of one material into the other and several other problems. Superior properties of nanomaterials (e.g. graphene, boron nitride nanosheet and BNNT, as illustrated in Fig.6) are derived from their atomistic structure, hence atomistic approach is more suitable for simulating the behaviour of such materials.**12**

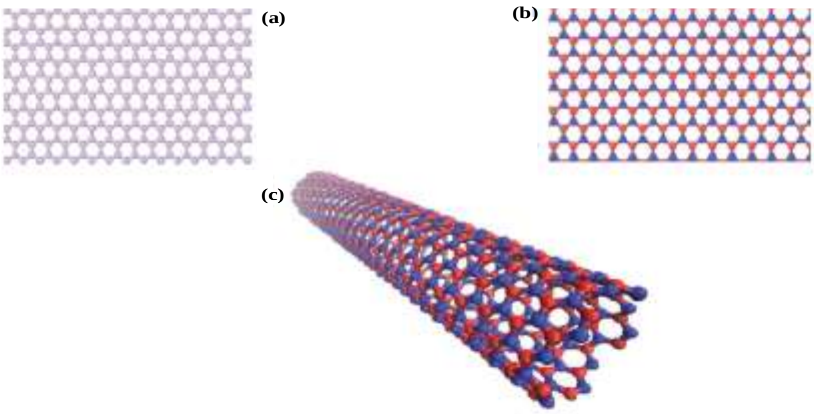

Fig.6 Atomic configurations of (a) graphene sheet (GS), (b) boron nitride nanosheet and (c) boron nitride nanotube (BNNT). Red and blue dots correspond to boron and nitrogen atoms, respectively.**12**

In terms of accuracy, atomistic approach is more accurate than continuum approach, but simulations are limited to few million atoms that corresponds to one micrometer region only. In addition to nanomaterials, problems related to irradiation damage, which is atomic level phenomenon is also studied with the help of atomistic approach as illustrated with the help of a schematic in Fig.7. Conducting experiments with irradiated samples is a challenging task, health hazards always deteriorates the efficiency and accuracy of experimental with such samples. In such a case computer base simulations are potential alternatives to study such systems.**13**One more example, where atomistic approach seems to be a better solution is desalination with the help of nanomembranes.19 In addition to structural applications, atomistic modeling is extensively used for investigating the effect of newly developed medicines on human cells.**20**

Even though quantum mechanics based approach is most accurate in all the three modeling approaches, but its application is very limited due to high computational time. Quantum based techniques are generally limited to studies that involved localized chemical reactions, configuring a stable configuration for a molecule.**21**

4.0 Conclusion

It can be concluded from this article that computers are not essential for our daily lives, but also for the development of new technologies. In some cases, experimental techniques are proved to be expensive as well as time consuming, hence, computer based techniques are emerging as potential alternatives to experimental characterization. Different types of modeling techniques have been developed by the researchers that have their own advantages and challenges.

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