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Simulation for Innovation - Atoms to Aircraft

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***Abstract* – The Coupling Molecular Dynamics and FEA yield models that link fundamental material processes at an atomic level with the continuum field responses at higher length scales. There has been a need to make a connection between the two inherently different simulation frameworks which are effectively independent. The numerous ways to make this connection require that the finite element mesh to be refined to atomic resolution, simulations to be carried out at 0 K and restrict modelling to two-dimensional material domains. This paper provides an insight and reviews the existing methods to achieve coupling and the drawbacks of the same which paves way for an efficient method to address the issue by taking into account the advantages of the same.**

***Keywords* – Nano Scale Simulation, Finite Element Method.**

I. Introduction

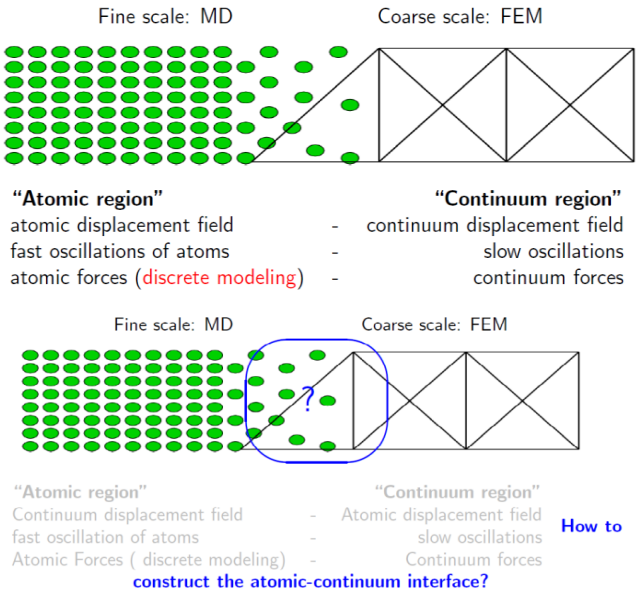
The market for nano materials and nano mechanics is on a boom and has opened up the ways for engineers to search and find valuable solutions to problems which are widely prevalent today. Coupling Molecular Dynamics with FEA is one of the problems for which the solution has to be found because of the various advantages like the development of physics-based 'bottom-up' multistate analyses that can aid in understanding the evolution of failure mechanisms across length scales. However FEA at an atomic level cannot be done throughout as it eats up a lot of time and effort of an engineer. In coupling atomistic and continuum material representations, the continuity of material properties must be maintained while transitioning from individual atoms interacting through nonlocal forces to the local stress-strain field formalism of continuum mechanics. There has been a large amount of research which has been done and is still being carried out which has yielded ways through which this problem can be addressed. A common feature of many of these approaches for coupling atomistic and continuum representations is the refinement of the finite element (FE) mesh to atomic length scales to link the kinematics of the FE nodes to that of the discrete atoms along an interface. In this paper a critical review of the existing methods has been done and the need for a new and efficient way which bridges the gap prevailing has been emphasized.

II. Motivation & Need

The computational issue occurs in cases like crack propagation and dislocation formation where there arises a need to do atomic level simulation only in critical areas and normal FEA in the less critical areas. Since Atomistic modelling and Integration of the complete area take up a long time, there is a need to reduce the computational cost of simulations, the time and effort put into it. In order to bridge these gaps there is a need to link the two independent frameworks of Molecular Dynamics and FEA. It is thus necessary to first understand, evaluate and find gaps in the existing methods of coupling so that either the best possible method is chosen or a new method can be developed which addresses the problem of developing a seamless link between the frameworks.

III. Challenge

- In the current world, there has been a lot of research going on both in the fields of Molecular Dynamics (Fine Scale) and FEM (Coarse scale), but the challenge lies in constructing the atomic continuum interface which not only reduces the computational cost but also the sensitivity of the local stress to the local atomic environment will lead to its expanded use in understanding materials behaviour at the atom level.



- For example, if you could consider the example of an aircraft failure, very few people think where first the failure happened which actually happens due to a crack at an atomic level near one of the rivet holes out of thousands of them. But, carrying out an analysis at an atomic level for the entire aircraft is not possible because of the large amount of cost, time and effort involved in it. Whereas analysis at a coarse scale is also not applicable since it doesn't answer the question of analysing at an atomic level. There exists a need wherein if a simulation tool is capable to carry out analysis at both length scales, so that the real cause of the problem could be found and answered at an atomic level.
- Another example of an aircraft material undergoing brittleness due to humidity and snowfall issues can also be

considered. The reason of this issue can be addressed through the simulation of water or snowfall or temperature variations on the aircraft by carrying out an analysis at the atomic level and the continuum level by using a single tool.

- There is also a larger computational demand and the finite time problem remains more or less unsolved.
- The application of the single simulation tool also can be found in fracture mechanics wherein crack regions can be resolved using Molecular Mechanics (MM) simulation. MM region must follow crack or must be chosen sufficiently large. But the cracks donot behave the way we want them to.

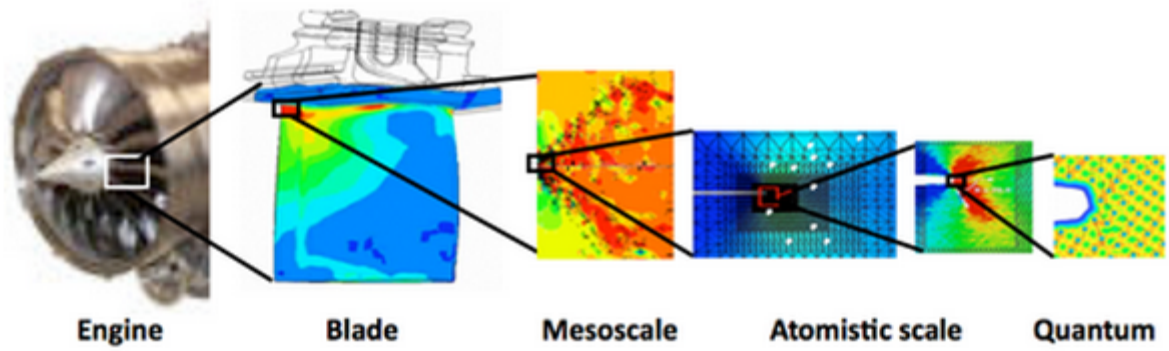
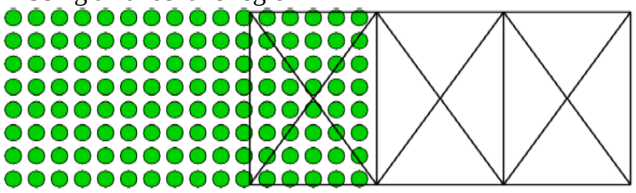


Fig.1. Multiscale modelling of fracture

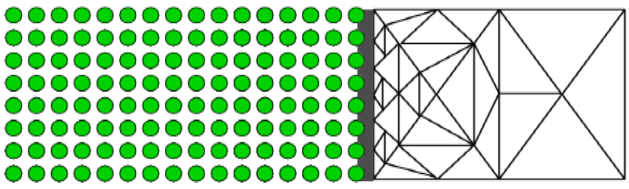
IV. Literature Review

To answer the above stated challenge, a lot of methods have come up over a period of time which has their own advantages and disadvantages however, al the existing methods can be broadly classified into three types based on the way the transition takes place between the atomic and the continuum regions. They are,

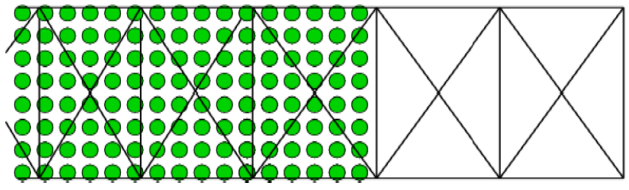
- Using a handshake region



- Small transition zone



- Coexistence of MD and FEM



A brief review of several representative coupling procedures follows to illustrate the current state-of-the-art.

a) Finite Element – Atomistic (FEAt) coupling procedure.

It was an early effort made by Gumbsch and Beltz to solve crack problems. It combined an embedded MD system with a finite element domain which comes under the third category of the broad classification.

b) Coarse Grained Molecular Dynamics (CGMD).

This is a generalized formulation of conventional FEM, which allows FEM nodes to be considered as coarse-grained MD "atoms". This can be considered as a handshake transition.

c) Coupling of Length Scales (CLS) method.

Here the nodes in a finite element model representing the continuum region are directly connected to the atoms in an atomistic region forming an interface of "pad" atoms. The region of "pad" atoms, used in this and other atomistic-continuum coupling methods, serves to minimize surface tension effects on the atoms in the atomistic system but also introduces a constraint due to the elasticity of the interface region. The constraining effect of this region is generally considered insignificant and is ignored. This method explains the coexistence of MD and FEM.

d) Quasicontinuum (QC) method.

This method reviewed by Miller and Tadmor, is formally based on an entirely atomistic description of the material domain. However, for computational efficiency, regions are identified in which discrete atoms may be grouped to form a local continuum.

e) Bridging Method.

Xiao and Belytschko developed this method and is based on an overlay approach in which MD and FEM representations are superposed in an interface region. This method allows interpolated FEM nodal displacements to be associated with atomic displacements in the bridging domain making it come under the third type.

f) Coupled Atomistic/Dislocation Dynamics (CADD) method.

Done by Shilkrot, this method is specifically designed to simulate, identify and pass dislocations between atomistic and continuum domains. The method was originally limited to 0 K simulations; but has been recently extended

to include finite temperature effects in the MD system by linking the MD to a quasistatic FEM domain through a thermal damping region.

g) Embedded Statistical Coupling Method (ESCM).

In this method, approaches that relate atoms and FE nodes in a one-to-one manner, or through a form of interpolation, will be referred to as direct coupling (DC) approaches. While DC approaches are straightforward, the fundamental difficulty in their development lies in the inherent differences between the atomistic and continuum computational models. This approach also is based on the coexistence of MD and FEM.

h) A parallel multiscale simulation toolbox(MACI)

This method introduced by Dorian Krause and Konstantin Fackeldey and Rolf Krause is a thin yet capable interface designed for efficient coupling between molecular dynamics (MD) and finite elements (FE) codes which addresses on modularity, performance and parallelization using Common Component Architecture (CCA) but clearly coupling is done using a handshake region focussing on reusing existing, established molecular dynamics and finite element implementations, such as TREMOLO, LAMMPS and UG.

i) Multi-Physics Molecular Dynamics Finite Element Method (MDFEM)

This method brought forth by Andr´e A.R. Wilmesy, Silvestre T. Pinho exactly embeds the equilibrium equations of Molecular Dynamics (MD) within the computationally more favourable Finite Element Method (FEM) and can implement any force field because constitutive relations are explicitly uncoupled from the geometrical element topologies. The method is proved by using it in investigating the effects of defects on the constitutive responses and fracture behaviour of CNT, was chosen as a reference to demonstrate the equivalence of the proposed MDFEM and MD in a highly non-linear environment up to, and including, bond failure by Belytschko et al. The proposed MDFEM matches MD results for CNT with defects at a reduced computational cost.

V. Conclusion

In recent years there has been significant progress made in modelling molecular dynamics which lead to better understanding of crack growth and fastener modelling but unless these nano scale simulation techniques are coupled with commercially available finite element codes the application will not be fruitful. Towards that current papers reviewed existing methods of coupling with molecular dynamic and finite element modelling. Still a universally accepted model is need of the hour.

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Author's Profile

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Convener - Engineering Innovation Initiative within Engineering at Infotech Enterprises.Ravi has 10 years of experience in the field of nuclear and aerospace engineering. He received M.tech from IIT Mumbai and B. E from Osmania University. Ravi is part of Infotech since 2012 has been instrumental in building and mentoring aero stress analysis team as stress analysis recruitment focal. He has been convener for Aero Structures Innovation council and successfully imbibed the culture of innovation across PDU. He initiated quarterly Innovation challenges based on themes for better service delivery. Under his leadership numerous first of its kind, proprietary tools and methods of analysis are built. He has guided students for their M.tech/B.tech projects.

Prior to Infotech he worked with Atomic Energy Regulatory Board India as scientist. He has been permanent invitee to Advisory Committee on Nuclear Safety (ACNS-AERB), Co-Coordinator for Sponsored research project in establishing innovative R&D collaborations with IIT Patna, IIT Guwahati, IIT Mumbai, IIT Hyderabad, IGCAR Kalpakkam, BARC, and NPCIL. He is instrumental in framing Regulatory safety Codes, Guides, Manuals for Indian nuclear reactors. He has worked closely with United States Nuclear Regulatory Commission (USNRC), International Atomic Energy Agency (IAEA)

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