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as of 06-Feb-2019

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STEM Degrees: **STEM Participants:**

Major Goals: The PI's current ARO program (Grant: W911NF-14-1-0257) aims to develop microstructure-failure-strength relationships at mesoscales in lightweight metallic systems under dynamic loading conditions and bridge the gap between atomistic and continuum simulations. To achieve this goal, the PI's novel mesoscale modeling method called quasi-coarse-grained-dynamics (QCGD) is developed by the PI that extends the time and length scale capabilities of molecular dynamics (MD) simulations to the mesoscales. While these simulations allow the investigation of the evolution of temperature, pressure during deformation and failure, the investigation of the micromechanisms and the evolution of defects/damage, the interaction of defects/damage and the evolution of microstructure is still a challenge due to the massively large data sets generated in these simulations.

The current visualization capabilities available to the PI and the remote access of data (currently ~100 TB) on DoD archives limits the analysis of these snapshots to investigate the micromechanisms. The detailed analysis of this Big Data is the current bottleneck in the generation of the scaling relationships and the investigation of the mechanisms for nucleation, evolution and interactions of defect and damage structures that define the deformation and failure behavior of these lightweight metallic materials under dynamic loading conditions.

The requirements are the ability to directly visualize temporal evolution of microstructure comprising of snapshots generated using MD and QCGD simulations. Such a visualization is very demanding in terms of memory and processor requirements due to the large data sets comprising of trajectories of systems comprising of tens to hundreds of millions of atoms. The DURIP award provides the computational infrastructure needed to meet this challenge. The computational equipment comprises of two Dell 7920 workstations, ARIVIS Visualization software that is customized to the atomic scale and mesoscale datasets and a 3D visualization projector. ARIVIS visualization software also enables the rendering of the atom datasets in virtual reality environments allowing you to walk/fly through the datasets and enable statistical analysis of the size, distribution and fractions of defect/damage in the microstructures. The equipment will also enable significant enhancements in the research program on the mesoscale model of cold spray particle impacts funded by the US Army Research Laboratory (Grant: W911NF-15-2-0026).

Accomplishments: The 3D visualization is achieved by processing the atom trajectories into voxels that are rendered in VR environments. Such rendering reduces the data size and memory requirements to the order that allows the current hardware to visualizing large amounts of data (few hundred million atoms) and enables interactive analysis (slice, remove atoms, make atoms transparent, create objects, identify connectivity between objects etc. Two example videos are added to this report that demonstrate these capabilities. The vidoes are uploaded online on a Youtube channel for the group and are also being used to showcase computational capabilities to visitors, collaborators, undergraduate students as well as during various outreach events.

Video (a) shows the capabilities to visualize microstructure in VR environments that shows the snapshot of a single crystal Al system undergoing spall failure [1]. The atoms are colored as green (FCC), blue (disordered), orange (surface), yellow (faults). The video shows the capability to walk/fly through the structure to identify the distribution of defects and voids. The video shows the capability to fly through the distribution of voids and the analysis enables the identification of the interconnectivity of voids as well as the distribution of defects.

Video (b) shows the distribution of twinned regions in a polycrystalline Mg microstructure generated at high strain rates. Algorithms are designed to identify various types of twinned regions and identify connectivity of twinned regions across multiple grains [2]. Here, atoms are colored as magenta (compression twins), blue (disordered) and the bulk hcp atoms are removed.

This equipment is now being used to investigate the evolution of defects/twins during deformation and failure under shock loading conditions as well as during cold spray particle impact. The current simulations are aimed at developing analytical relationships for evolution and distribution of voids as well as deformation twins for varying loading conditions and microstructures generated using QCGD simulations. The approach allows the visualization of any aspect of the microstructure. 3D visualization of the data will be used to validate these descriptors and identify key mechanisms responsible for the predicted materials response.

Training Opportunities: The 3D visualization modules are now being used to train the graduate students Garvit Agarwal, Sergey Galitskiy, and Sumit Suresh who are funded on the two projects in addition to providing opportunities for undergraduate students. The software will also be made available for graduate students and undergraduate Seniors who are taking the PI’s class on classical atomic scale simulations in Materials Science and Engineering at UConn.

Results Dissemination: Publication of analyzed data in open-access journals in the field of materials science, applied physics and mechanical engineering will be the primary mode of data dissemination. In addition, a YouTube channel is created to share videos of 3D visualization of datasets. The algorithm data will also be retained on the secure server in the PIs research group and will be made accessible for download through links on the Group website. Computational data, analysis data and Electronic data will be archived on the secure sever hosted by UConn and will be available to share upon request.

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Technology Transfer: Nothing to Report

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Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

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Project Contribution:
International Collaboration:
International Travel:

National Academy Member: N
Other Collaborators:

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Participant: Sumit Suresh
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

FINAL REPORT

DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

GRANT # W911NF-17-1-0191

3D VISUALIZATION EQUIPMENT FOR BIG DATA ANALYSIS OF MICROSTRUCTURAL EVOLUTION UNDER DYNAMIC LOADING CONDITIONS

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Proposed period of performance: April 19, 2017 – July 18, 2018

OBJECTIVES

The PI's current **ARO program** (**Grant: W911NF-14-1-0257**) aims to develop microstructure-failure-strength relationships at mesoscales in lightweight metallic systems under dynamic loading conditions and bridge the gap between atomistic and continuum simulations. To achieve this goal, the PI's novel mesoscale modeling method called quasi-coarse-grained-dynamics (QCGD) is developed by the PI that extends the time and length scale capabilities of molecular dynamics (MD) simulations to the mesoscales. While these simulations allow the investigation of the evolution of temperature, pressure during deformation and failure, the investigation of the micromechanisms and the evolution of defects/damage, the interaction of defects/damage and the evolution of microstructure is still a challenge due to the massively large data sets generated in these simulations.

The current visualization capabilities available to the PI and the remote access of data (currently ~100 TB) on DoD archives limits the analysis of these snapshots to investigate the micromechanisms. **The detailed analysis of this Big Data is the current bottleneck in the generation of the scaling relationships and the investigation of the mechanisms for nucleation, evolution and interactions of defect and damage structures that define the deformation and failure behavior of these lightweight metallic materials under dynamic loading conditions.**

The requirements are the ability to directly visualize temporal evolution of microstructure comprising of snapshots generated using MD and QCGD simulations. Such a visualization is very demanding in terms of memory and processor requirements due to the large data sets comprising of trajectories of systems comprising of tens to hundreds of millions of atoms. **The DURIP award provides the computational infrastructure needed to meet this challenge.** The computational equipment comprises of two Dell 7920 workstations, ARIVIS Visualization software that is customized to the atomic scale and mesoscale datasets and a 3D visualization projector. ARIVIS visualization software also enables the rendering of the atom datasets in virtual reality environments allowing you to walk/fly through the datasets and enable statistical analysis of the size, distribution and fractions of defect/damage in the microstructures. **The equipment will also enable significant enhancements in the research program on the mesoscale model of cold spray particle impacts funded by the US Army Research Laboratory (Grant: W911NF-15-2-0026).**

BACKGROUND

The current capabilities in any computational group is limited to the post-processing of data using software and visualization methods that are limited by our instincts as well as the 2D images rendered by the visualization methods. The current simulation sizes in the PI's group using MD/QCGD simulations comprises of systems that are greater than 100 Million atoms or Representative Atoms. The amount of data generated from these simulations (currently ~100 TB) on UCONN and DoD archives limits the analysis and identification of the micromechanisms that render the observed behavior. As a result, current efforts use machine learning algorithms such as neural networks, support vector machines, kernel ridge regressions, etc. to identify correlations. While these post-processing methods provide insights, the ability to visualize these correlations was missing. The new DURIP equipment discussed above provides the opportunity to use 3D interactive visualization and virtual reality (VR) to analyze this "Big Data" that is the current bottleneck in the understanding of the links between the atomic scale structures and the response of materials in various environments. The processing of data is now being done on the HPC servers that reduces the requirement to download terabytes of data onto to local storage drives and saves time required for post-processing of data sets.

EQUIPMENT

DURIP funding provided was used to purchase the following equipment that develops the capability to visualize "Big data" of microstructural evolution generated from molecular dynamics (atomic scale) and quasi-coarse-grained dynamics (mesoscale) simulations for projects funded by the US Army Research Office (ARO Grant: W911NF-14-1-0257) and US Army Research Laboratory (ARL Grant: W911NF-15-2-0026). The equipment, as shown below in Figure 1, comprises of:

a) **DELL 7920 Precision Tower** which includes Dual Intel Xeon Gold 6146 Twelve-Core 3.2 GHz processors, 256 GB 2666 MHz DDR4 RAM, GeForce GTX 1080 Ti 11GB GDDr5X Graphics Card, 1 TB PCIe NVMe Class 50 Solid State Drive and Two 2 TB PCIe NVMe Class 40 Solid State Drive drives. This workstation will be used for microstructure/defect visualization and analysis of evolution during shock loading of Al, Mg and Ti systems for the PI's current research funded by the US Army Research Office (Grant: W911NF-14-1-0257).

b) **DELL 7920 Precision Tower** which includes Dual Intel Xeon Gold 6146 Twelve-Core 3.2 GHz processors, 256 GB 2666 MHz DDR4 RAM, GeForce GTX 1080 Ti 11GB GDDr5X Graphics Card, 1 TB PCIe NVMe Class 50 Solid State Drive and Two 2 TB PCIe NVMe Class 40 Solid State Drive drives. This workstation will be used for microstructure/defect visualization and analysis of evolution during impact of Al6061 Al particles for the PI's current research funded by the US Army Research Laboratory (Grant: W911NF-15-2-0026).

c) **Arivis InViewR and Arivis Vision4D** (Base, Analysis, and Coloc): Novel 3D visualization software that is customized for immersing yourself in microstructural data using virtual reality to extract structural relationships not accessible by standard 2D or 3D viewing applications.

d) An EPSON 5040UBe 3D Projector that will render the visualization analysis as discussed in (a) and (b).

Figure 1: Two Dell 7920 Precision workstations showing the VR headsets and the ARIVIS InViewR and Vision 4D Software.

CURRENT CAPABILITIES

The 3D visualization is achieved by processing the atom trajectories into voxels that are rendered in VR environments. Such rendering reduces the data size and memory requirements to the order that allows the current hardware to visualizing large amounts of data (few hundred million atoms) and enables interactive analysis (slice, remove atoms, make atoms transparent, create objects, identify connectivity between objects etc. Two example videos are added to this report that demonstrate these capabilities. The vidoes are uploaded online on a Youtube channel for the group and are also being used to showcase computational capabilities to visitors, collaborators, undergraduate students as well as during various outreach events.

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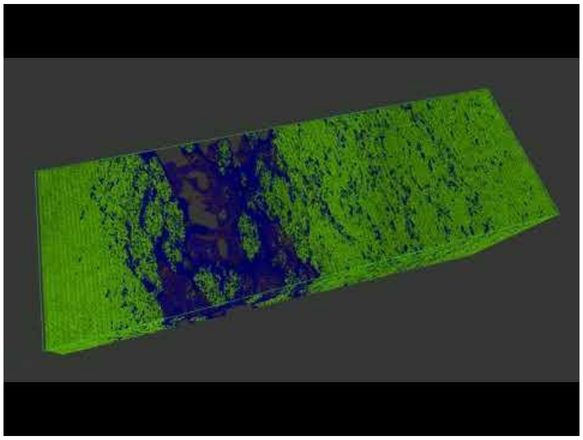
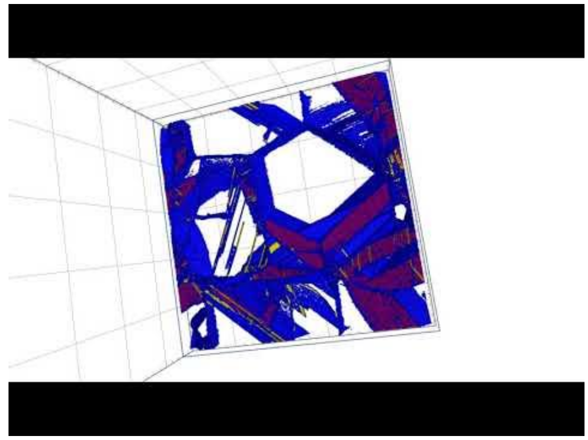


(a)



(b)

Videos: (a) Distribution of defects and voids during spall failure of single crystal Al predicted using molecular dynamics simulations [1]; (b) 3D Visualization of Nanocrystalline Mg Deformed Microstructure predicted using molecular dynamics simulations [3]. Click on videos to play on YouTube. The uploaded videos play in YouTube when clicked on the images.

TRAINING

The 3D visualization modules are now being used to train the graduate students Garvit Agarwal, Sergey Galitskiy, and Sumit Suresh who are funded on the two projects in addition to providing opportunities for undergraduate students. The software will also be made available for graduate students and undergraduate Seniors who are taking the PI's class on classical atomic scale simulations in Materials Science and Engineering at UConn.

DISSEMINATION

Publication of analyzed data in open-access journals in the field of materials science, applied physics and mechanical engineering will be the primary mode of data dissemination. In addition, a YouTube channel is created to share videos of 3D visualization of datasets. The algorithm data will also be retained on the secure server in the PIs research group and will be made accessible for download through links on the Group website. Computational data, analysis data and Electronic data will be archived on the secure sever hosted by UConn and will be available to share upon request.

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[1] G. Agarwal, A. M. Dongare, Defect and damage evolution during spallation of single crystal Al: Comparison between molecular dynamics and quasi-coarse-grained dynamics simulations, *Computational Materials Science* **145**, 68 (2018).

[2] G. Agarwal, A. M. Dongare, Damage Evolution and Mechanics during Spall Failure of Polycrystalline Al at the Mesoscales, *Acta Mater*, (in preparation for submission).

[3] G. Agarwal, A. M. Dongare, Microstructural Evolution and Deformation Twinning in Polycrystalline Mg Microstructures at the Mesoscales, *Journal of Mechanics and Physics of Solids*, (in preparation for submission).