

Editor February 1, 2020

Acta Materialia

Dear Editor,

I attach herewith a manuscript entitled “Five Degree-of-Freedom Property Interpolation of Arbitrary Grain Boundaries via Voronoi Fundamental Zone Octonion Framework,” by Sterling G. Baird, Eric R. Homer, David T. Fullwood, and myself. We would like to submit this paper to your consideration for publication in Acta Materialia.

In this work, we present a new method for computing distances between grain boundaries based on recent work by Francis, et al. who introduced the concept of grain boundary octonions, and attain computational runtimes orders of magnitude faster than the original octonion distance computations. Scaled Euclidean distances in a Voronoi Fundamental Zone approximate the original octonion metric with reasonable enough accuracy to produce accurate interpolations for large datasets, and the ability to use Euclidean distances allows us to leverage many existing code packages. We also develop a unique barycentric interpolation approach based on matrix transformations and hyperdimensional triangulation which can be applied for specialized applications. We test our method on 50,000 grain boundaries using a validation function and apply the framework to a large Fe simulation dataset, attaining higher accuracy than prior work using the same dataset. The structure-property models produced using this framework can be applied to grain growth simulations and other grain boundary engineering applications and accommodate the increasing availability of large experimental and computational datasets via high-throughput methods.

We, hereby, certify that this manuscript has not been previously published nor is it under consideration for publication elsewhere. It has been approved by all co-authors and any relevant authorities at the locations where the work was performed. Below are the names and contact information for five suitable reviewers:

Dr. Adam Morawiec

Dr. David J. Srolovitz

Dr. David L. Olmsted

Dr. Marc De Graef

Dr. Gregory S. Rohrer (Carnegie Mellon University): [gr20@andrew.cmu.edu](mailto:gr20@andrew.cmu.edu)

Dr. Jeffrey M. Rickman (Lehigh University): [jmr6@lehigh.edu](mailto:jmr6@lehigh.edu)

Dr. Elizabeth A. Holm (Carnegie Mellon University): [eaholm@andrew.cmu.edu](mailto:eaholm@andrew.cmu.edu)

Dr. Brian L. DeCost (NIST): [brian.decost@nist.gov](mailto:brian.decost@nist.gov)

Dr. Francesca Tavazza (NIST): [francesca.tavazza@nist.gov](mailto:francesca.tavazza@nist.gov)

We are looking forward to a review of this paper. Please advise if you require anything to proceed.

Sincerely,

Oliver Johnson

Assistant Professor

Department of Mechanical Engineering  
Brigham Young University

(801) 422-0972  
[ojohnson@byu.edu](mailto:ojohnson@byu.edu)