ZENO: Software for calculating hydrodynamic, electrical, and shape properties of polymer and particle suspensions

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1. Summary

The ZENO software tool computes material, solution, and suspension properties for a specified particle shape or molecular structure using path-integral and Monte Carlo methods. These properties include: capacitance, electric polarizability tensor, intrinsic conductivity, volume, gyration tensor, hydrodynamic radius, intrinsic viscosity, friction coefficient, diffusion coefficient, sedimentation coefficient, and related quantities.

The development of the current version (version 5) of the code was motivated by the need to modernize the code base and to significantly speed-up the computation. ZENO up to version 3.x was written in Fortran 77. These versions were developed by Dr. Marc Mansfeld, Dr. Jack Douglas, and coworkers; the code can be downloaded from https://web.stevens.edu/zeno/. For version 4, we ported the code to Fortran 2008. For version 5, we rewrote ZENO in C++. This new version takes advantage of parallelism and spatial data structures to deliver up to four orders of magnitude speed-up compared to the Fortran versions when run on an eight-node cluster [1].
2. Software Specifications

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3. Methods for Validation

The software has been subjected to multiple validation tests, the details of which are given in the documentation. The tests consisted of examining aspects of the statistical distributions of the software outputs as compared to ground truth values. The algorithms in ZENO have also been extensively tested previously [2, 3].

For some test cases, the ground truth could be generated analytically. For other, more complex, test cases, analytic ground truth did not exist; in these cases, surrogate ground truth values were generated by increasing the sample size by at least four orders of magnitude. While only the analytic ground truth tests demonstrated the accuracy of the code, all the tests gave information about the rates of convergence that could be expected with different geometries.

4. References


About the authors: Derek Juba and Walid Keyrouz are computer scientists in the Software and Systems Division at NIST. Their interests include scientific computing and high performance computing. Debra Audus is a chemical engineer in the Materials Science and Engineering Division at NIST. Her interests include the use of simulations, theory, and data to probe polymeric and colloidal systems. Michael Mascagni is with the Departments of Computer Science, Mathematics, and Scientific Computing at Florida State University and has a faculty appointment in the Applied and Computational Mathematics Division at NIST. His interests are in computational science, Monte Carlo methods, random number generation, and the application of these in biology, chemistry, and materials science. Jack Douglas is a Fellow in the Materials Science and Engineering Division at NIST. His interests include the physics of condensed matter; polymeric and glass-forming materials in particular. The National Institute of Standards and Technology is an agency of the U.S. Department of Commerce.