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 Mansfield, 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

NIST Operating Unit	Information Technology Laboratory, Software and Systems Division
Category	Monte Carlo random walks
Targeted Users	Physical scientists
Operating Systems	Linux, Mac
Programming Language	`C++11`
Inputs/Outputs	Computes physical properties from geometry as described in the documentation in detail
Documentation	https://doi.org/10.18434/T48W2J
Accessibility	N/A
Disclaimer	https://www.nist.gov/director/licensing

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 truths 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

[1] Juba D, Keyrouz W, Mascagni M, Brady M (2016) Acceleration and parallelization of ZENO/Walk-on-Spheres. *Procedia Computer Science* 80:269–278. https://doi.org/10.1016/j.procs.2016.05.319
[2] Mansfield M, Douglas J (2008) Improved path integration method for estimating the intrinsic viscosity of arbitrarily shaped particles. *Physical Review E* 78(4):046712. https://doi.org/10.1103/PhysRevE.78.046712
[3] Mansfield M, Douglas J, Garboczi E (2001) Intrinsic viscosity and the electrical polarizability of arbitrarily shaped objects. *Physical Review E* 64(6):061401. https://doi.org/10.1103/PhysRevE.64.061401

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