# ZENO: an efficient code for computing particle properties

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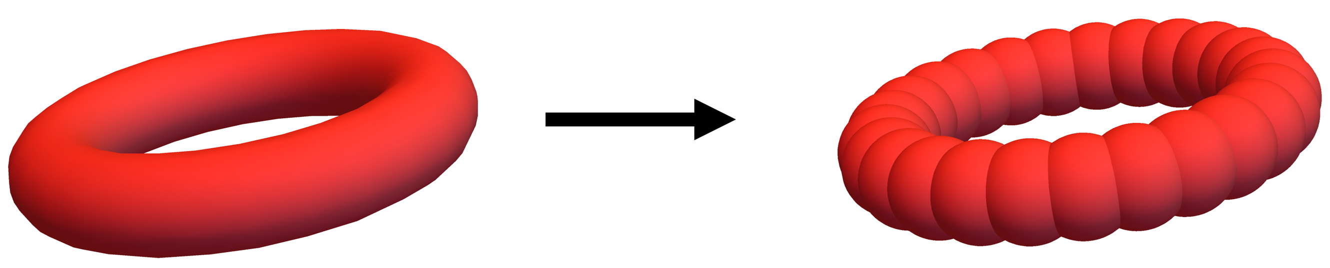
## 14 computed properties

Capacitance, electric polarizability tensor, eigenvalues of electric polarizability tensor, mean electric polarizability, intrinsic conductivity, volume, gyration tensor, capacitance of a sphere of the same radius, hydrodynamic radius, viscometric radius, intrinsic viscosity, intrinsic viscosity with mass units, friction coefficient, diffusion coefficient, and sedimentation coefficient

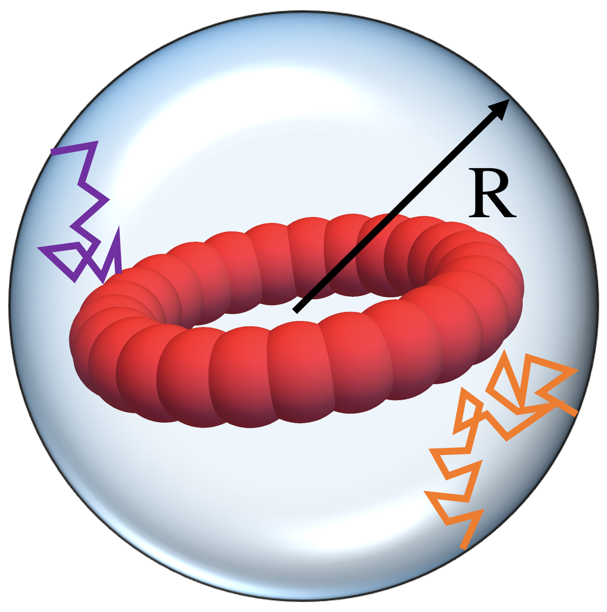
## Input

The object for which the properties are calculated must represented by a collection of spheres. For many objects including molecules, this is a straightforward procedure.



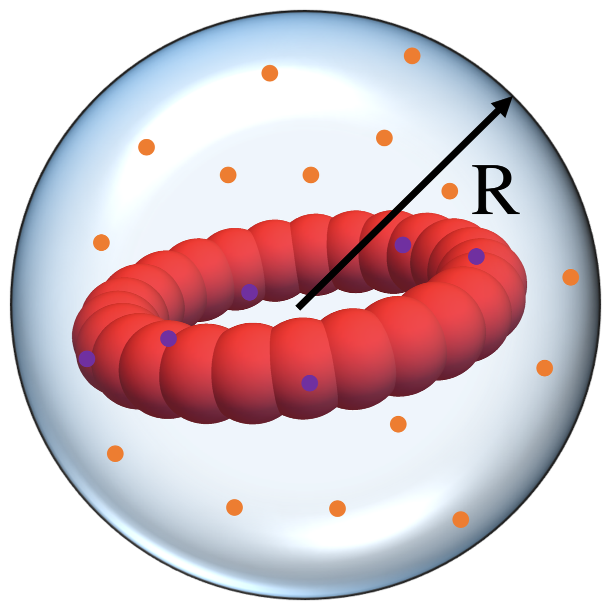
## Algorithms

The ZENO code is composed of two types of calculations: exterior and interior. The exterior calculation is used to determine electrical properties and, by invoking an electrostatic-hydrodynamic analogy, to estimate hydrodynamic properties. The interior calculation is used to determine properties such as the volume.




The exterior calculation involves solving Laplace's equation using an method called walk on spheres. Specifically random walks are generated starting at the launch sphere. The capacitance is then determined using the fraction of walks that hit the object over the total number of walks multiplied by the launch sphere radius.

The interior calculation uses a Monte Carlo method to determine properties such as the volume and radius of gyration. In the case of the volume, points are generated within the launch sphere. The volume is then estimated by taking the fraction of points inside the object over the total number of points multiplied by the launch sphere volume.



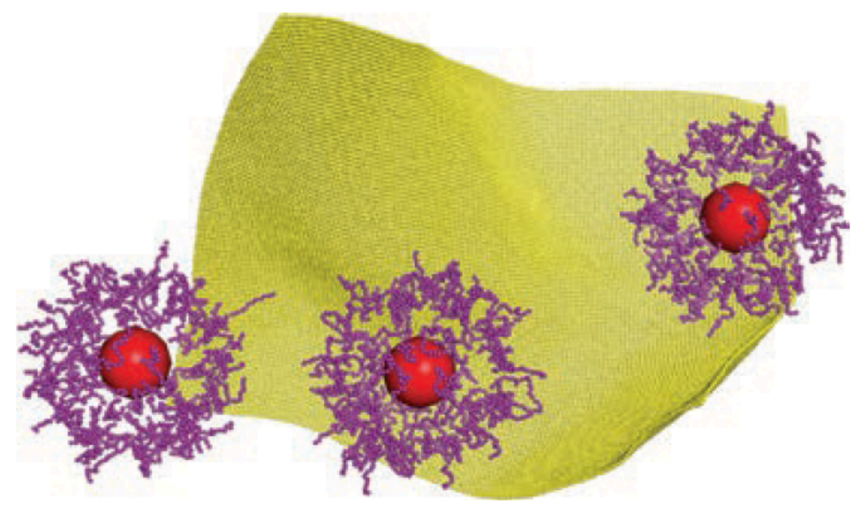

## Acquiring the code

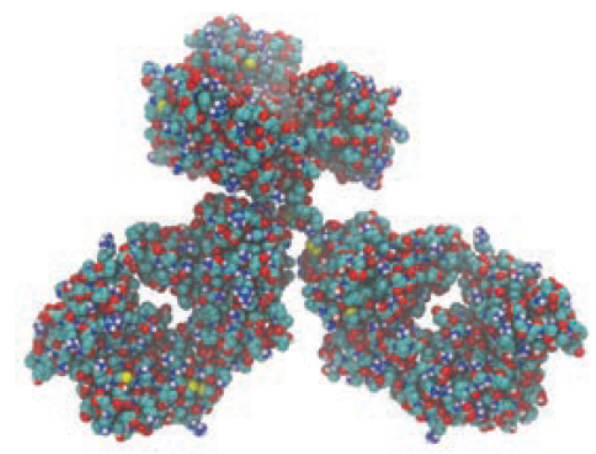
https://github.com/usnistgov/ZENO

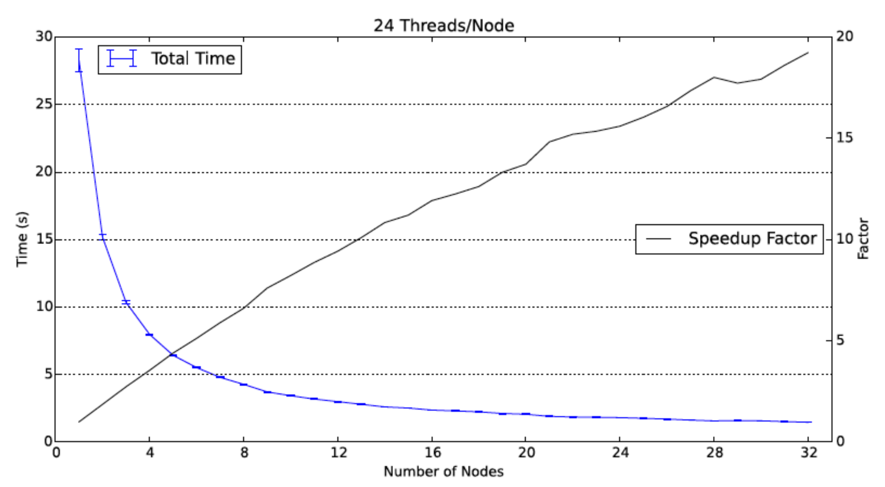
## Efficiency

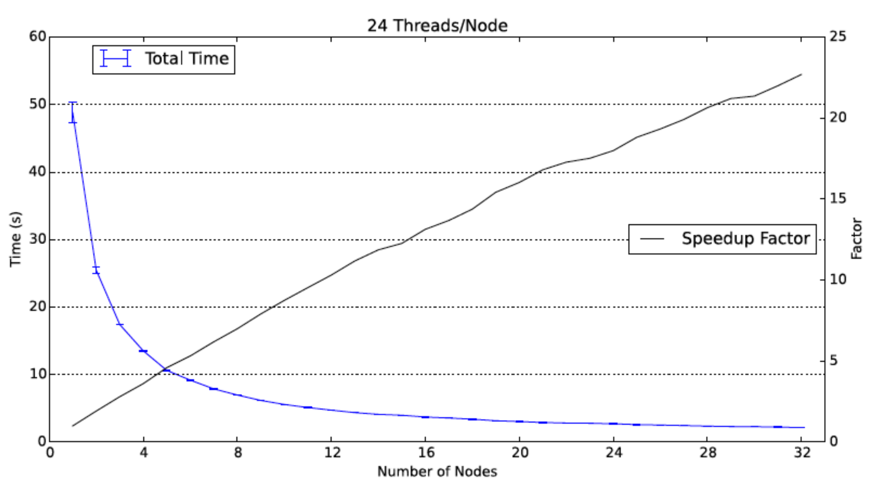
The code exhibits up to 4 orders of magnitude speed up when run on 8 nodes with 24 threads each compared to a previous, serial version (Fortran 2008). Please see D. Juba, W. Keyrouz, M. Mascagni, and M. Brady, "Acceleration and parallelization of ZENO/Walk-on-Spheres," *Procedia Computer Science*, **80**, 269-278 (2016) for further details.

| | *Gold Nanoparticle* | | | *Protein 1IGY* | | |
|---|---|---|---|---|---|---|
| | Time (s) | Speedup | Cumul. | Time (s) | Speedup | Cumul. |
| Fortran 2008 | 8240 ± 110 | 1× | 1× | 3710 ± 6 | 1× | 1× |
| C++/Linear | 3970 ± 4 | 2.08× | 2.08× | 2090 ± 2 | 1.77× | 1.77× |
| C++ | 42.0 ± 0.1 | 94.5× | 196× | 71.5 ± 0.1 | 29.3× | 52.0× |
| C++ 24 T | 3.27 ± 0.11 | 12.9× | 2520× | 5.42 ± 0.29 | 13.2× | 685× |
| C++ 24 T, 8 N | 0.797 ± 0.026 | 4.10× | 10300× | 1.14 ± 0.10 | 4.78× | 3270× |







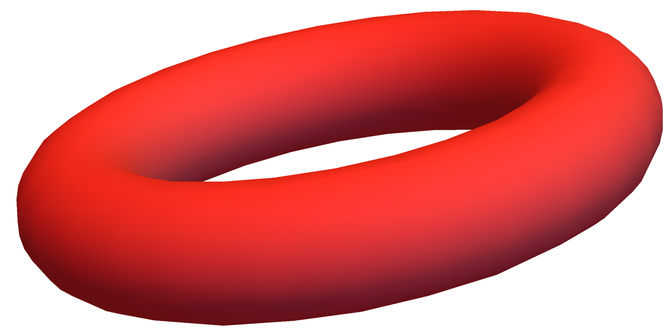




## Validation

Direct comparison to analytic results yielded relative expanded uncertainties of less than 0.06% for 1e7 walks and 1e7 samples. Uncertainties are higher for more complicated structures, but still less than 0.25%. Please see documentation at the ZENO github site for details.

Table 3: **Torus with a minor radius of 1 and major radius of 4**

| Property | Ground Truth | Units | Mean | Difference | Rel. Diff. | Std. Dev. | Std. Uncert. | Expand Uncert. | Rel. Exp. Uncert. |
|---|---|---|---|---|---|---|---|---|---|
| | | | **number of walks = 1e7; number of interior samples = 1e7** | | | | | | |
| $C$ | 3.72768 | L | 3.72771 | 3e-5 | 0.001 % | 1.11e-3 | 1.6e-4 | 3.2e-4 | 0.008 % |
| Eigenvalue of $\alpha$ | 156.53 | $L^3$ | 156.48 | 5e-2 | 0.035 % | 2.9e-1 | 4e-2 | 8e-2 | 0.053 % |
| Eigenvalue of $\alpha$ | 972.21 | $L^3$ | 970.89 | 1.3e0 | 0.136 % | 1.3e0 | 1.9e-1 | 3.8e-1 | 0.039 % |
| Eigenvalue of $\alpha$ | 972.21 | $L^3$ | 973.54 | 1.3e0 | 0.137 % | 1.1e0 | 1.6e-1 | 3.2e-1 | 0.033 % |
| $\langle\alpha\rangle$ | 700.31 | $L^3$ | 700.30 | 7e-3 | 0.001 % | 6.8e-1 | 1e-1 | 1.9e-1 | 0.028 % |
| $R_h$ | 3.72768 | L | 3.72771 | 3e-5 | 0.001 % | 1.11e-3 | 1.6e-4 | 3.2e-4 | 0.008 % |
| $V$ | 78.956835 | $L^3$ | 78.913530 | 4.33e-2 | 0.055 % | 1.19e-1 | 1.69e-2 | 3.40e-2 | 0.043 % |
| $C_0$ | 2.66134 | L | 2.66085 | 4.9e-4 | 0.018 % | 1.34e-3 | 1.9e-4 | 3.8e-4 | 0.014 % |
| Eigenvalue of **S** | 0.250000 | $L^2$ | 0.249928 | 7.2e-5 | 0.029 % | 3.87e-4 | 5.5e-5 | 1.10e-4 | 0.044 % |
| Eigenvalue of **S** | 8.375000 | $L^2$ | 8.363658 | 1.13e-2 | 0.135 % | 5.68e-3 | 8.03e-4 | 1.61e-3 | 0.019 % |
| Eigenvalue of **S** | 8.375000 | $L^2$ | 8.385071 | 1.01e-2 | 0.120 % | 6.28e-3 | 8.88e-4 | 1.79e-3 | 0.021 % |
| $[\sigma]$ | 8.8696 | | 8.8743 | 4.7e-3 | 0.053 % | 1.61e-2 | 2.3e-3 | 4.6e-3 | 0.052 % |



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