

1133-92-229

**Ileana Streinu\*** ([istreinu@smith.edu](mailto:istreinu@smith.edu)), Smith College, Computer Science Department, 100 Green Street, Northampton, MA 01063, and **Mojtaba Nouri Bygi** ([mnouribygi@smith.edu](mailto:mnouribygi@smith.edu)), Smith College, Computer Science Department, 100 Green Street, Northampton, MA 01063.

*Efficient protein rigidity and flexibility analysis for large scale applications.* Preliminary report.

Pebble game rigidity analysis is an efficient method for extracting rigidity and flexibility information of biomolecules without performing costly molecular dynamics simulations. The algorithm works on a multi-graph associated to a mechanical model constructed from an arbitrary atom-bond network. Motivated by large scale protein flexibility and simulated unfolding applications, we have developed a faster and more robust variation tailored to the specificities of bio-polymers. We demonstrate this new 'backbone pebble game' as implemented in the new release of our software Kinari-2. (Received July 26, 2017)