MathSys MSc Project Proposal - 2021

It's all in the Void

a general-purpose algorithm to find regions of empty space in complex networks

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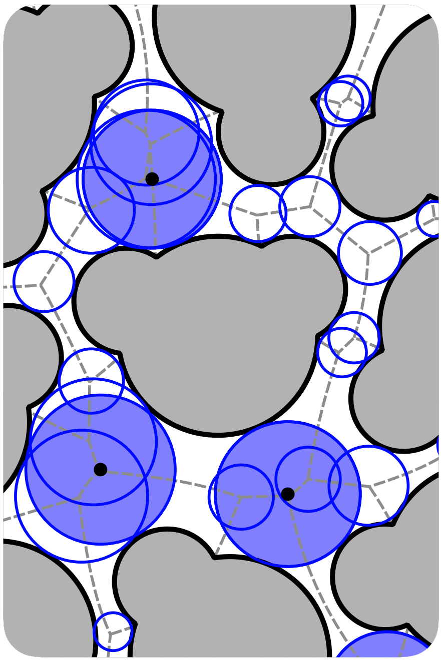
Background and Significance

Complex networks are ubiquitous objects [1]. Systems as diverse as molecular liquids such as water and 3D meshes for game design do share the same underlying structure: complex, often sparse graphs. Some networks are dynamical objects (i.e. they change in time), some others are meta-networks (where e.g. the nodes of the graph themselves are networks of their own, see the figure on the right depicting water at the molecular level). One feature that characterizes the vast majority of these networks is the fact that there exist regions of empty space in between the different nodes. Crucially, empty space matters. For instance, statistical mechanics provides a simple relation between the empty space in networks and the energy price you have to pay to insert a new node into them [2] – something the pharmaceutical companies care about in the form of the so-called solvation of drug-like molecules in liquids. In this respect, the issue that has been crippling the field for decades is the fact that regions of empty space are almost always assumed to be spherical [3]. This is hardly the case for complex dynamical networks – hence our recent efforts to craft a unified, general-purpose algorithm that will allow us to characterize empty regions of any shape and size in complex networks.



Project Outline and Objectives

This project seeks to develop a computational framework to characterize regions of empty space in complex dynamical networks. In particular, we will be building on the existing body of work (and computer code) that we have amassed within the SossoGroup to: (1.) develop the Svoid code (want access? Ask and you shall be given!) so as to account for dynamical networks. (2.) crash test this novel implementation on molecular liquids of increasing complexity.

Programme of work

Weeks	**Tasks**
1-2	Introduction to the basics of empty space: Voronoi/Delaunay tessellation and Apollonius problem.
3-6	Implementation of the methodology. Bespoke guidance (Dr. Berk Onat, Warwick Eng.) will be provided.
7-8	Crash test of the framework on molecular liquids of increasing complexity.
11-12	Future perspectives. Preparation of written report and oral presentation.

Skills to be learned

The student will get familiar with the basics of scientific computing: the Linux terminal, scientific programming (Python/Fortran/C++) and visualization software (VMD). In addition, by the end of the project the student will have acquired a solid knowledge base in the context of 3D topology and complex networks, both of which are of great relevance in the context of fields as diverse as drug discovery and game design.

References [1] S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, and D. Hwang, Phys. Rep. **424**, 175 (2006). [2] G. Hummer, S. Garde, A. E. Garcia, A. Pohorille, and L. R. Pratt, Proc. Natl. Acad. Sci. **93**, 8951 (1996). [3] G. C. Sosso, S. Caravati, G. Rotskoff, S. Vaikuntanathan, and A. Hassanali, J. Phys. Chem. A **121**, 370 (2017).