**Geometric Network Science**

*Sitharam group’s research projects*

*By*

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“Network science” <http://en.wikipedia.org/wiki/Network_science> is currently a popular term referring to a body of techniques for extracting information and analyzing large networks of pairwise relationships between entities in our society, economy, engineered world or in nature. These networks could be explicit, say, atop the internet; or implicit, existing only in conceptual form. The goal could be design, management or control of network behavior.

The highly general network (aka graph) theory techniques use no further information about the entities (aka vertices) in the network, or their pairwise relationships (aka edges), except whether or not an edge exists between a given pair of vertices.

Consequently, graph theory techniques are typically widely applicable, but relatively weak. In other words, utilizing more information about the vertices and edges may restrict the scope of applications, but usually yields stronger techniques.

The primary research topic of the Sitharam group is the study of networks where the edges represent pairwise *geometric* relationships between the vertex entities. The accepted term for such a “geometric network science” is the *study of geometric constraint systems*.

FIGURE 1: Sitharam research group 2013: Jialong Cheng, Menghan Wang, Aysegul Ozkan, Meera Sitharam, Ruijin Wu

A description...

Geometric constraint sytems are immediately visible in some applications such as: (i) computer-aided mechanical and geometric modeling, design and manufacturing; (ii) robotics; gaming, virtual reality and user-interface design; and (iii) geometry-based educational software. Although less obvious, geometric constraint systems are the essential underlying structures in a variety of other applications, including (iv) molecular modeling and (v) machine learning. In fact, geometric constraint systems are fundamental abstract structures (vi) inherent in many longstanding open problems at the interface or confluence of geometry, algebra, graph theory and combinatorics and complexity theory. Hence the study of geometric constraint systems generates new structures and techniques of independent mathematical interest.

The Sitharam group works on *all* of the above-mentioned theory and applications of geometric constraint systems. Below we briefly discuss all of them.

In the past 3 years, besides Prof. Sitharam, group members have included 5 PhD students, a masters thesis student, an undergraduate research student, and a K-12 teacher. The group works both independently and in collaboration with mathematicians, molecular scientists, engineers

and education researchers, as well as other computer scientists. The group’s work extends from proving theorems to designing algorithms to writing opensource software to providing research experiences to K-12 teachers that they can translate into classroom use. The group’s research has been continuously supported for the past 20 years by grants from different divisions of the *National Science Foundation* sometimes jointly with the National Institute for General Medical Sciences (NIGMS), one of the National Institutes for Health that supports research on foundational principles. The group’s support also includes a gift from *SolidWorks,* a computer-aided design and manufacturing company. Recently, the group’s work is increasingly recognized by molecular scientists, improving its eligibility for grants directly from NIGMS.

A sketch of the group’s projects from the past 3 years follows. Publications and other details can be found at [http://www.cise.ufl.edu/~sitharam](http://www.cise.ufl.edu/)

**Viral and Molecular Assembly Modeling**

Supramolecular or macromolecular assembly is a remarkable phenomenon that occurs spontaneously and widely in nature and underlies many processes from assembly of viral capsids to the assembly of nanomaterials to intracellular mechanisms to the action of drugs. A molecular assembly configuration space refers to the set of configurations (positions and orientations) a collection of rigid molecules (or molecular parts) assume relative to each other in the presence of force fields, each of which is between a pair of atoms, situated in different molecules. The configuration space is typically high dimensional and geometrically intricate, yet it determines *configurational entropy*, an important ingredient of the free energy which in turn determines the preferred assembly configurations of the molecular collection. Predicting these preferred configurations or designing molecules that arrive at preferred assembly configurations, requires efficient and accurate free energy and configurational entropy computation, which is a notoriously difficult problem that computational molecular scientists (molecular biologists, chemists and physicists) have studied for decades. Established methods are generally based on full-blown molecular dynamics (MD) simulations or exhaustive Monte Carlo (MC) sampling of the configuration space. Both methods suffer from the dual curses of dimensionality and geometric intricacy of the configuration space.

By modeling the pairwise intermolecular atomic force fields as a geometric constraint system, the Sitharam group has leveraged a theory of stratification and parametrization of assembly configuration spaces of geometric constraint systems developed by the group [http://link.springer.com/article/10.1007%2Fs00454-009-9160-8#](http://link.springer.com/article/10.1007%2Fs00454-009-9160-8)

and designed an efficient algorithm for obtaining an *atlas*

of an assembly configuration space that captures the intricate geometry as interconnected regions of varying dimensions.

Figure 2: EASAL generates Atlas of molecular assembly landscapes

A description...

Aysegul Ozkan, a PhD student in the Sitharam group developed an opensource software EASAL implementing these algorithms <http://www.proceedings.com/10931.html> (page 233) and <http://arxiv.org/abs/1203.3811>, with help from James Pence, an undergraduate researcher in the group and Ruijin Wu, a co-advised PhD student. EASAL is currently being tested by a computational chemist (Maria Kurnikova of CMU) and physicist (Miranda Holmes-Cerfon, NYU) interested in using EASAL in conjunction with traditional methods for configurational entropy and free-energy computations.

EASAL’s predictions of crucial intermolecular interactions that drive assembly of viral capsids <http://dl.acm.org/citation.cfm?id=2383061> have been validated by a structural biology collaborator Mavis Agbandje-Mckenna at UF.

Another aspect of entropy that plays a crucial role in the case of symmetric macromolecular assemblies such as the icosahedral viral capsid assembly is the notion of

combinatorial entropy that indicates the number of different pathways of subassembly formations that lead to successful assemblies. In collaboration with Mathematicians Miklos Bona and Andy Vince at UF, the Sitharam group has given a method to explicitly count a simplified type of assembly pathways for symmetric macromolecular assemblies <http://www.ncbi.nlm.nih.gov/pubmed/21174231>

**Computer-aided Geometric and Mechanical Modeling and Robotics**

Instead of specifying parts, assemblies and mechanisms as explicit drawings to scale, ideally, one would like to simply declare various crucial geometric constraints that should hold within and between parts, and automate the actual drafting of the part, assembly or mechanism. In addition, we would like software to visualize or answer queries about the configuration or motion space of a mechanism that has been specified as a geometric constraint system. Despite the passage of 3 decades since the introduction of the concept of geometric constraint systems into the computer-aided mechanical design community, CAD systems are only able to handle a very small percentage of such

tasks even for 2dimensional parts, mechanisms and assemblies.

The Sitharam group introduced and gave efficient algorithms for so-called Decomposition-Recombination planning for geometric constraint systems arising in CAD. The group then developed an opensource software called FRONTIER for geometric constraint decomposition about a decade ago (still maintained on Sourceforge). More recently, the group added efficient recombination algorithms to FRONTIER, <http://dl.acm.org/citation.cfm?id=1746833>

which incorporated semi-numeric polynomial system solving <http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.152.9251>, collaborating with the and Peters group here at CISE.

The Sitharam group’s later work on a grant provided by SolidWorks together with Mathematician Neil White, of UF, and Computer scientists Audrey Lee-StJohn and Ileana Streinu of Mt. Holyoke, Smith and UMass, provided the first formal treatment of many of the geometric constraints that are useful in mechanical computer aided design <http://www.sciencedirect.com/science/article/pii/S0925772112000235>

Current PhD student Menghan Wang in the Sitharam group has developed efficient algorithms and opensource software called CayMos to represent and visualize the movement of mechanisms specified using geometric constraints, employing a new theoretical technique called Cayley analysis of linkage configuration spaces, also developed by the group (see below). In a paper accepted to the 2013 SIAM-ACM Solid and Physical Modeling conferences, which was characterized by one of the anonymous reviewers as “destined to become a classic in the analysis of mechanisms,” Menghan uses CayMos to analyze and find unusual properties and motions of common mechanisms such as the well-known and amusing Strandbeest. The paper will also be published in the CAD journal. CayMos is web-enabled and can be found at <http://www.cise.ufl.edu/~menghan/caymos>

FIGURE 3: CayMos’ Cayley analysis of Theo Jansen’s Strandbeest

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**Combinatorial geometry, algebra and complexity theory**

A senior PhD student Jialong Cheng from the Sitharam group has made progress on a 150 year open problem posed by James Clerk Maxwell in 1874 concerning a characterization of when a 3D bar-linkage (in effect a distance constraint system) is rigid. The goal is a characterization that is purely combinatorial, i.e., independent of the actual lengths of the bars in the linkage (distance values in the constraint system), yielding a graph algorithm for determining 3D rigidity. The question was completely answered for 2D in 1970 and has since given rise to an entire area of Mathematics called

Combinatorial rigidity theory. Jialong shows that either he has found a much sought-after combinatorial characterization of rigidity of 3D distance constraint systems, or he has disproven another longstanding conjecture about a purely combinatorial abstract rigidity notion.

Two of the group’s previous results led up to the above result: one of them settled another longstanding question that has remained open since Maxwell. Both earlier results were well-received in two of three invited talks the group gave at a Fields institute workshop in October 2011 <http://www.fields.utoronto.ca/audio/11-12/wksp_rigidity/sitharam/>

and <http://www.fields.utoronto.ca/audio/11-12/wksp_rigidity/cheng/>

One of these papers gives systematic constructions of so-called “nucleation-free” graphs that are highly flexible and yet counter-intuively have pairs of vertices that maintain a fixed distance (implied non-edges). This is an obstacle in obtaining combinatorial characterizations of 3D rigidity. An earlier version appeared as a conference paper with Ileana Streinu of UMass in the Canadian Conference in Computational Geometry in 2009.

The last of the 3 invited talks the Sitharam group gave at a Fields Institute Workshop in October 2011 <http://www.fields.utoronto.ca/audio/11-12/wksp_rigidity/wang/>

concerned fundamental mathematical results concerning when so-called Cayley configuration spaces of distance constraint systems (linkages) in 2D have low complexity, i.e., the boundaries of these spaces can be described using simple ruler and compass construction. Such algebraic questions date back to the time of Galois.

This work is a continuation of recent papers by a former PhD student from the group, Heping Gao and recently graduated masters student Ugandhar on efficient parametrizations of Cayley configuration spaces <http://arxiv.org/find/all/1/au:+wang_menghan/0/1/0/all/0/1>

**Machine Learning and Cognitive Architectures**

Machine learning is an area sparse in mathematical proofs or guarantees of quality and efficiency. Recently an entire workshop at the NSF Center for Intractability in Princeton in Aug. 2012 was titled “Provable bounds for Machine learning” <http://intractability.princeton.edu/blog/2012/07/workshop-on-provable-bounds-in-machine-learning-august-1-2-2012/>. In contrast, Computational learning theory has proofs, but simplistic models .

The group’s recent PhD graduate Mohamad Tarifi's goal was to bring about a marriage of the two, using core geometric constraint techniques. His 2012 PhD dissertation succeeded in giving provable bounds for Dictionary Learning by using rigidity theory for a new type of incidence-based geometric constraint system. In addition, his dissertation included a new brain-inspired model of hierarchical machine learning using dimension reduction for the solutions of geometric constraint systems. A paper with him (and co-advisor Jeff Ho) on formalizing

a model of hierarchical machine has appeared in the proceedings of BICA

(Biologically inspired Cognitive Architectures) 2011.

<http://bicasociety.org/2011/>

**Geometry-based CS education**

Geometric constraint systems provide a natural entry into computational thinking and coding, both for K-12 teachers and students, since the same structures that are intuitively and physically constructed and handled are also formally and algorithmically constructed and manipulated on a geometry-based user interface using both algebra and geometry.

The algorithmic problems that arise in implementing the back-ends of such user-interfaces are at the cutting edge of geometric constraint solving research.

The Sitharam group’s current NSF grant from the Division of Mathematical Sciences contains a “Research Experiences for Teachers (RET)” supplement. Having been exposed to the group’s research, local K-12 teacher Eric Lenasbunt (MisterE the “mystery”) has found robust and inexpensive ways to get higher elementary and middle grade students to make and appreciate theunusual and counterintuitive 3D linkagessuch as nucleation-free linkages with implied non-edges described above. Additionally, having observed its enthusiastic reception at a weekly Math-CS circle that the Sitharam group has run in a local school for the past 6 years, MisterE is now an enthusiastic proponent for teaching children to write geometry programs and geometry-based game-like apps in the Scratch programming language. This success has led to a larger RET grant proposal that would involve 13 local K-12 teachers.

The above ideas have additionally resulted in a collaboration between the Sitharam group and two faculty members in the College of Education at UF, Albert Ritzhaupt and Pasha Antonenko, to propose to NSF a Massively Open Online Course for educating in-service K-12 teachers in Computer Science so that they can meet the CSTA standards for teaching high school Advanced Placement CS classes. A slight modification of the same idea shows promise for one or two GenEd level UF courses, both for attracting UF undergrads into CS to meet the demand for CS graduates and for ensuring that potentially all UF grads acquire the 21st century’s essential skill (coding)..