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COMBINATORIAL AND ALGORITHMIC RIGIDITY: BEYOND TWO DIMENSIONS

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Final Technical Report

Results of the complete effort: December 2008 - December 2012

Distribution Statement A

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Our grant project *"Combinatorial and Algorithmic Rigidity: Beyond Two Dimensions"* was submitted in 2008, under the DARPA solicitation "Mathematical Challenges, BAA 07-68". It addressed *Mathematical Challenge Ten: Algorithmic Origami and Biology* and proposed "a line of attack on the central problem in three-dimensional rigidity theory: the combinatorial characterization of minimally rigid bar-and-joint frameworks". Appearing implicitly in James C. Maxwell's work from the 1860's, this problem is currently referred to as *Maxwell's problem.*

i. Accomplishments compared with the goals of the grant

The main tenet of the project was that "rigidity should be explored on a *wide array* of frameworks and structures with various blendings of combinatorial sparsity and geometrical constraints". Indeed, this principle guided our investigations throughout the grant effort and led to significant results and advances which exceed, in many respects, the explicit goals of the grant.

Regarding *theoretical foundations*, a prominent accomplishment is our **deformation theory of periodic frameworks** which established and developed new concepts and techniques for understanding periodic structures. By *relating finite and periodic frameworks* , we disclosed unsuspected connections and depth in Maxwell's problem and opened a new avenue of research. Equally important, in our estimate, are the applications of our deformation theory to displacive phase transitions in crystalline materials.

A second prominent theoretical and algorithmic accomplishment relates to **robot arms with revolute joints**. This line of investigation was directly motivated by protein backbone chains modeled as serial hinge structures. Again, our rigorous mathematical formulations led beyond the initial horizons and we were able to solve a whole string of fundamental problems in robotics, which had been open for more than forty years: characterization of extremal reaches and determination of the singularity locus and the workspace boundary. In addition, we devised a number of optimal algorithms and provided critical complexity analysis.

The topic of **algorithmic origami** was successfully engaged from the same perspective of hinge structures, more precisely as panel-and-hinge surfaces. We explored Lang's Universal Molecule Algorithm, clarified the conceptual setting of heuristic sections, obtained a first complete proof of correctness and improved the algorithmic analysis. In the process, our rigidity analysis uncovered important families of *non-foldable* designs. These results have implications for deployable structures and nano-origami materials.

All our theoretical endeavors and accomplishments occurred in steady dialogue with the gradual growth and refinement of the **rigidity analysis of proteins** integrated in the KINARI software (**KIN**ematics **A**nd **RI**gidity analysis).

This overview of our grant efforts shows that the project's established goals were met and that our anticipations about lines of approach and effective techniques were, on the whole, correct and fruitful. In fact, several of our reported accomplishments went far beyond initial expectations and opened new areas of discovery and development.

In the following paragraphs, we give a closer correspondence between our completed results and objectives listed in the milestone chart of the grant project.

1. Setting up the models: theoretical foundations. This milestone objective was instrumental and influential in several directions: periodic frameworks with their own diversity, ranging from bar-and-joint to mixed plate-and-bar articulations [6, 9, 14, 15, 11], volume frameworks [13], Delauney triangulations [1], linkages [19], hinge structures, either serial [4, 3, 5, 7, 12] or surface-like (origami) [17, 18, 39, 38, 35, 37, 16].

2. Developing proof techniques: Invariant theory Factoring out equivalences under the action of a given group of 'trivial' transformations was all-important for enumerative estimates and effective parametrizations. We used invariant theory perspectives to full advantage in [14, 2, 13]. Matroidal techniques are implicated in [15, 44]. Theorems of Maxwell-Laman type were obtained in [9, 15, 43].

3. Counting and Enumeration. As anticipated in the project, we relied on methods of algebraic-geometry for obtaining bounds on the number of realizations of various types of minimally rigid frameworks and for complexity analysis of robot arm workspaces [9, 13, 12].

4. Studies of configuration spaces. General properties of configuration spaces for periodic frameworks were determined in [6, 14]. We obtained precise descriptions for periodic structures of high significance in mineralogy, such as quartz, cristobalite and tridymite [10]. Previous insights into geometric deformation possibilities for these structures were limited to a few one-parameter illustrations, in spite of a long tradition of studies. Cyclic volume frameworks also lead to remarkable configuration spaces [13]. Geometric descriptions of singularities played an essential role in our solution of the workspace determination problem for robot arms [7].

5. Protein chains and hinge structures. All our discoveries about robot arms with revolute joints and origami folding were guided by this milestone objective. The definitive theoretical and algorithmic results obtained on extremal reaches and workspace boundaries [3, 5, 8, 7, 12] are now apt to be integrated with related components of protein structure determination or validation procedures. The steady growth of capabilities in the KINARI software for rigidity analysis of proteins is documented in a series of contributions, which include profiling, benchmarking and validation efforts on up to 10,000 protein structures from the Protein Data Bank (PDB) [22, 23, 24, 25, 26, 27, 30, 31, 32, 33, 40].

6. Rigid clusters and flexibility. Algorithms for finding rigid clusters and flexibility parameters (such as degrees of freedom and of redundancy) have been devised for very general classes of sparsity in [41, 42, 28, 34]. New obstructions to the accurate calculation of 3D bar-and-joint rigid clusters have been identified in [19].

The development of KINARI [24] led to new mathematical problems motivated by the mechanical modeling of biological macro-molecules for which the rigidity and flexibility analysis can be accurately and efficiently performed [26, 20, 27].

We summarize in tabular form the results of our grant efforts which we deem of *breakthrough* or *new departure* character and indicate related new directions.

TOPICS AND KEY PAPERS	DEFINITIVE RESULTS	NEW DIRECTIONS
Robot arms with revolute joints: panel-and-hinge chains [3, 5, 8, 7, 12]	**extremal reaches:** complete characterization and polynomial time algorithms **workspace boundary determination:** exact description and complexity analysis	singular configurations for the general body-and-hinge case; criteria for recognizing the workspace boundary among singular points; robot arm design
Periodic frameworks: bar-and-joint, body-and-bar, mixed plate-and-bar; [6, 9, 10, 14, 15]	**fundamental concepts and deformation theory:** characterizations of minimal rigidity , crystallographic symmetry, flexibility and deformation spaces	ultrarigidity, geometric auxetics, liftings: from quotient graphs to periodic graphs
Frameworks related to various **groups**: volume frameworks, symplectic frameworks. [13, 39]	**sparsity** in the finite and periodic context; **bounds** for possible realizations **singularities**	a general principle on *periodicity and sparsity*
Origami [17, 18]	**rigid origami** as panel-and-hinge surfaces	foldability and connected components
Rigidity analysis for proteins and KINARI software [24, 32]	KINARI web-server and library http://kinari.cs.umass.edu	extension to nucleic acids, viruses and crystalline materials

ii. Established goals

All established goals were met.

iii. Other pertinent information

For further dissemination of our results, we have presented tutorials on robot arms and rigidity analysis for proteins and biological molecules [36, 40, 25] at international conferences and gave video-taped talks at mathematical meetings [11, 38]. In addition, PI Streinu has been interviewed for the NSF-funded documentary on bio-mathematics, *Darwin's Extra sense* http://www.math.dartmouth.edu/publicity/general/extrasense/.

We also (co-)organized annual workshops on rigidity theory and applications in computational biology http://linkage.cs.umass.edu/barbados/, http://biophysics.asu.edu/workshops/2008_GeomSimTech/, two conferences on

Rigidity Theory, at the Fields Institute of Mathematics in Toronto (Oct. 2011) and at the Banff International research Station (July 2012) and a 2 day Colloquium, "100 Years of Crystallography" at Rider University. We served on the program committee of several competitive conferences in computational geometry (SoCG'13), discrete mathematics and algorithms (SODA'11 and ESA'11), computational biology (ICCABS'12, ISBRA'12, CSBW'12 at IEEE-BIBM'12).

Educational efforts included the training of two post-docs and 5 graduate students, three of whom [45, 29, 21] have defended their PhD theses.

PI Streinu's mathematical work on the Carpenter's Rule Problem (which can be viewed as an abstract model for a 2-dimensional "protein" backbone) was rewarded in 2010 with the Robbins Prize of the American Mathematical Society. The Robbins Prize is given every three years for a paper that reports on novel research in algebra, combinatorics, or discrete mathematics. The full citation and additional information can be found at http://www.ams.org/ams/prizebooklet-2010.pdf. In November 2012, PI Streinu became a Fellow of the American Mathematical Society.

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