Computational Geometry in MEMS and Nano Design

MAE 294 – Computational Geometry for Design and Manufacturing

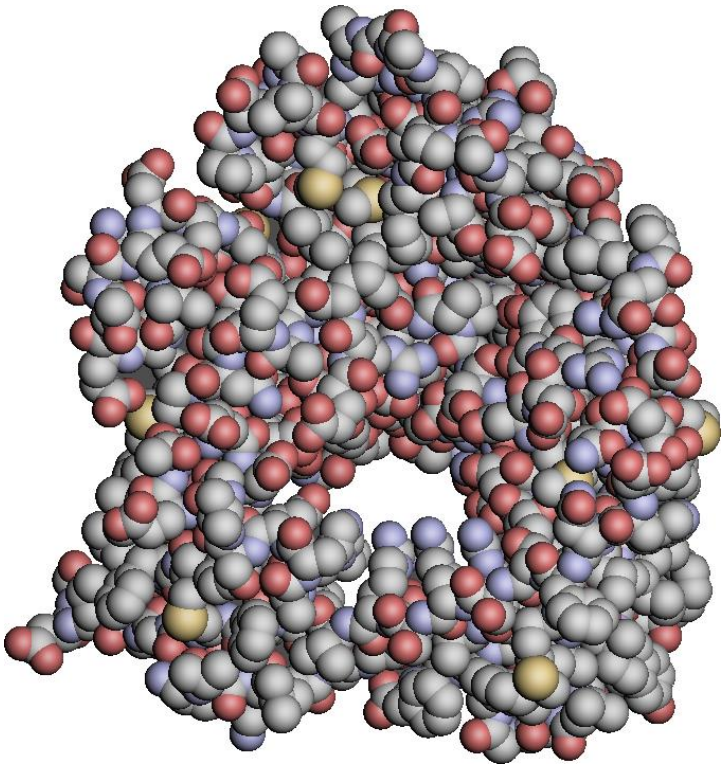

Figure 1: Computational Modeling of Poring molecule (Wiki, 2006).

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1 List of Acronyms

Symbols	*Descriptions*
CAD	Computer Aided Design
CAGD	Computer Aided Geometric Design
CAM	Computer Aided Manufacturing
CCG	Combinatorial Computational Geometry
CG	Computational Geometry
MEMS	MicroElectroMechanical Systems
NCG	Numerical Computational Geometry
NURBS	Non-Uniform Rational B-Spline
SCC-DFBT	Self Consistent Charge-Density Functional Tight Binding
STL	StereoLitography
SWCNT	Single Wall Carbon NanoTubes

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3 INTRODUCTION

In recent years, the technological leaps in the field of computer hardware, visualization, and software have made computational geometry (CG) crucial to many fields from science, engineering, biology, and even the entertainment industries (Amenta, et al.). Computational geometry now extends throughout many field of science and engineering fields through its strong implication in modeling and visualization using Computer Aided Design (CAD) (Amenta, et al.). Many scientific field have been revolutionized due to the success in computational geometry along with improvement in computer aided design in may field for modeling.

In this research, we will go over the importance of computational geometry and its revolutionary impact in many fields of science in MEMS and nanotechnology designs. This research will explore the various applications computational geometry brings forth for MEMS and nanotechnology from the biological side to the computational modeling side.

Computational geometry plays an important role in the design of geodesic polyarenes in nanotechnology to graphic design for Micro-Electro-Mechanical Systems (MEMS). Using computational geometry to design geodesic polyarene are just some examples of what computational geometry design are capable of (Trzaskowski, Adamowicz, Beck, Muralidharan, & Deymier, 2014).

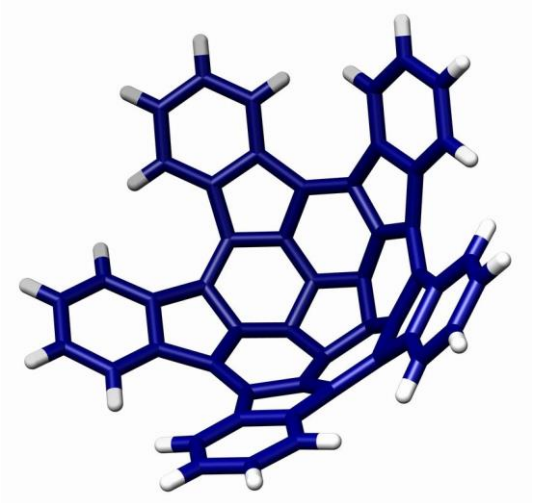

Figure 2: Geodesic Polyarene example: crystal structure of Pentaindenocorannulene (Wiki, 2007).

Computational Geometry is a branch of computational science and mathematics devoted to the study of algorithms that can be stated in terms of geometry. Once understanding the history, we will focus our review on molecular modeling in structural nano-toxicology, geodesic dome, and geodesic polyarenes.

4 BACKGROUND, HISTORY, PRINCIPLE, AND CURRENT PRACTICE

Computational geometry is a devoted mathematics and computer science field that focus on study of algorithms in terms of geometry to solve geometrical problems. Algorithms created for the computational geometry calculations and results can vary from days, hours, or seconds. Therefore, the importance of making an efficient algorithms is crucial to computer scientists and mathematician in the field of computational geometry.

Computational geometry is continuously pushed onward by two main field of focus, that is computer graphics, and computer aided design and manufacturing (CAD/CAM). The boundary of this field is continuously being pushed forward due to computer graphics and CAD reliance on computational geometry algorithms to create models and graphics for visualization (Amenta, et al.).

There are various applications for computational geometry varying from robotics applications for motion planning and visibility issues to computer visualization and biological modeling all are just part of the large picture of what computational geometry is capable of (Amenta, et al.).

Computational geometry includes computer aided engineering (CAE) that generate meshes and perform engineering numerical calculations. From here, computational geometry can be broken into the following branches:

- Combinatorial computational geometry (CCG)
- Numerical computational geometry (NCG)

Twenty years ago, the field of computational geometry was set to create analytical and computational tools to build geometric computing (Amenta, et al.). The idea of computational geometry twenty years ago was to create the necessary tools for computer programmers to face the problem of geometric problems. There are two ways computational geometry have been helping the field of science. One way is to have applications feed computational geometry with practical problems (Amenta, et al.). Another way is to use computational geometry to use algorithms and mathematic tools to provide us with sound and good predictions (Amenta, et al.).

4.1 *Combinatorial Computational Geometry (CCG)*

CCG deals with geometrical objects as individual or discrete entities in its algorithms. This method originally dates back to 1975 by Shamos and Preparata. Another name for CCG is algorithmic geometry.

For computer scientists and mathematicians their main goal in the CCG field is to develop efficient algorithms and data structures for designing, calculating, and solving problems. These problems are usually given in terms of points, segments, polygons, etc. with predefined properties.

The idea in CCG is to create the necessary algorithms and data structures to manipulate the necessary points, vectors, etc. to obtain the solution to the problem in the most efficient methods.

4.2 *Numerical Computational Geometry (NCG)*

This field tries to model real world objects in forms that are suitable for computer graphics or computer computations in CAD/CAM software. This field sometime goes by the name of Computer Aided Geometric Design (CAGD) because of the development of descriptive geometry for the modeling of the real world objects with computer graphics (Amenta, et al.). NCG main purpose is to perform curve and surface modeling and representation (Amenta, et al.).

To perform these modeling computational geometry require parametric curves and parametric surfaces using Bezier curves, spline curves, and Non-Uniform Rational B-Spine (NURBS).

In this research topic, we will try to focus on NCG or CAGD for the MEMS and nanotechnology. Many computational geometry design for MEMS and nanotechnology turns out to be classical in nature and require computer graphics or CAD to create virtual models. Some of these models and design comes from mathematical visualizations. We will explore some geodesic polyarenes and biomolecules design from computational geometry (Trzaskowski, Adamowicz, Beck, Muralidharan, & Deymier, 2014).

5 ADVANTAGES OF USING COMPUTATIONAL GEOMETRY

Computational geometry has made it possible for the field of MEMS and nanotechnology to continue to grow. With the development of computational geometry in the recent century along with computer hardware and software graphics design, the visualization of MEMS and Nano molecules becomes possible giving scientists and the general public of what these structures entails in its features.

Without computational geometry, the double helix cannot be created in such vivid detail and colors. When computational geometry is integrated into the biomedical field, creating double helix with the necessary structural integrity becomes possible. Computational geometry basically breathe life into DNA, molecules, and organisms modeling and break the boundary that was not possible with just vivid drawing models.

Before computational geometry comes into play molecules models sometime are either drawn or taken from X-ray imaging. An example of this would be the DNA double helix that was imaged using X-rays (Watson, 1980). Now with computational modeling complex representation of the DNA model could be achieve with computer graphics through NCG. An example of a computer graphical representation is shown in Figure 3. With more advanced technical representation such as this, better instructional education can be achieved due to easier communication of model imagery rather than just description.

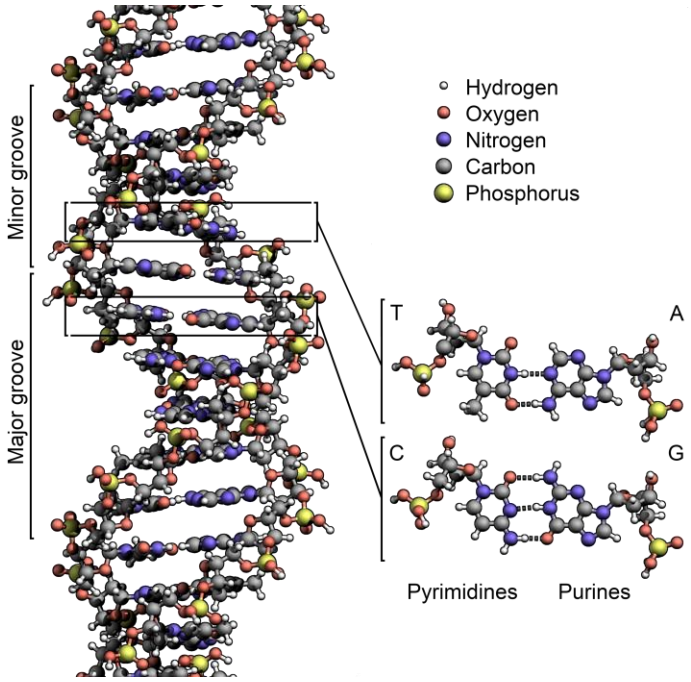

Figure 3: DNA CG model (Zephyris, 2011).

6 CURRENT PRACTICE AND RESEARCH TRENDS

So after understanding the role of computational geometry providing the necessary tools for MEMS and nanotechnology with molecular models and designs what are other research trends?

During this turn of the century computational geometry have solve basic geometric problems and asymptotic complexity such as convex hulls, triangulations, Voronoi diagrams, and optimization (Amenta, et al.). Now in field of computational geometry new sub-areas are being explored for algorithms design such as randomization and de-randomization. Other practices in computational geometry include using multidimensional searching, triangulation, geometric sampling, etc (Amenta, et al.).

During the great advances of the human genome project, computational geometry plays a huge role in this nano-size decoding. Computational geometry can deal with spatial structures of proteins and macromolecules (Amenta, et al.). Computational geometry will continue to deal with the spatial structures of proteins and macromolecules as there are many to be explored.

A few problems that computational geometry currently face with for this nano size field in biology are:

- Spatial structure of proteins
- Drug design

The new trend in computational geometry is to improve existing structure-based computational molecular modeling for the nano-size molecules. By doing this better biomedical knowledge can be gain through modeling and structure testing. Other trends in computational geometry field include creating tools to understand and predict interactions between nanomaterials and nano-biosystems. This would require computational analysis of structural principles behind interactions of molecules and nanomaterials (Yanamala, Kagan, & Shvedova, 2013).

In this article though, we will focus our review on molecular modeling in structural nano-toxicology, geodesic dome, and study of geodesic polyarenes.

7 COMPUTATIONAL GEOMETRY FOR MEMS AND NANO APPLICATIONS

In the field of MEMS and nanotechnology there are many applications needing computational geometry or computational approaches to model, simulate, or solve situation that cannot be ideally achieve. Computational geometry and simulation uses theoretical calculation and assumptions to predict simulation results from models. As we will learn that computational geometry plays a huge role in the nano-size world of biomolecules. Nanoparticles interactions with biomolecules at interfaces are some example in which computational geometry with its advance surface recognition and analysis becomes useful in helping identify receptors. Other uses computational geometry to design geodesic domes for other purposes. All this are results that can be achieve with computational geometry.

7.1 *Molecular and Nano Modeling with Computational Geometry (1st article)*

With the emergence of nanotechnology as the key player in science and technology, many applications could be explored. With the help of computational geometry, modeling and understanding the structure of these nanomaterials could be made easier. Modeling these molecules requires NURBS at times, especially for complex curve surfaces. The idea is to use computational molecular modeling to understand and predict possible interactions between nanomaterials and nano-biosystems (Yanamala, Kagan, & Shvedova, 2013).

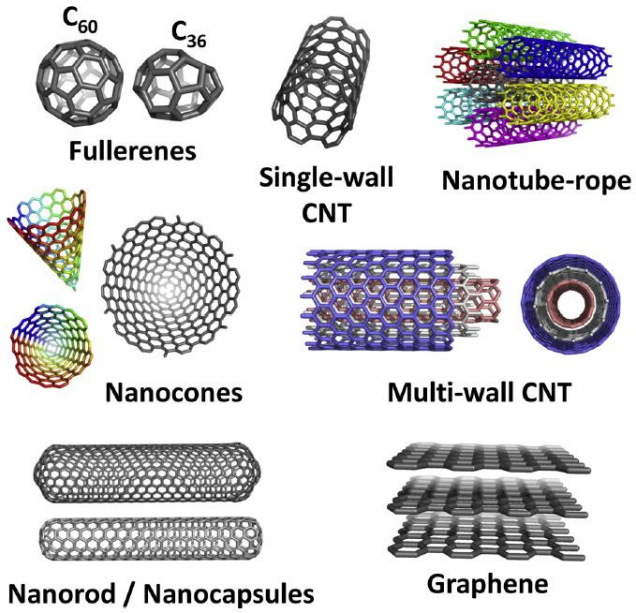

Figure 4: Carbon based nanoparticles (Yanamala, Kagan, & Shvedova, 2013).

Example of a few nanoparticles this research will try to explore using computational geometry to perform the analysis is in Figure 4. There are now more paper with computational

geometry focus on experimental and theoretical aspects of computational modeling of nanoparticles and nano-biointerfaces.

The technique to understand these nanoparticles comes from using computational approaches to study the nanoparticles shape, size, structure, and chemical properties. This includes the nanoparticles interactions with biomolecules and nanomachinery in living cells (Yanamala, Kagan, & Shvedova, 2013).

The method of computational geometry here comes from the algorithms that are written into to build sound integrity models that could represents nanoparticles. Using these models size shape, and structure could be studied. Computational geometry are great methods for modeling structures as it can perform complex curves using NURBS to simple lines and triangulation. Three dimension models using a CAD could create the nanoparticle model. Then if desire the model could even be enlarged for 3D printing by converting to STL file.

These models all require computational geometry algorithms to produce. It may be possible to simulate simple situation of these nanoparticles. In one article, it say that computational approaches to molecular interactions of nanoparticles with proteins and various other biomolecules are possible (Yanamala, Kagan, & Shvedova, 2013). This research has been discussed in a few articles.

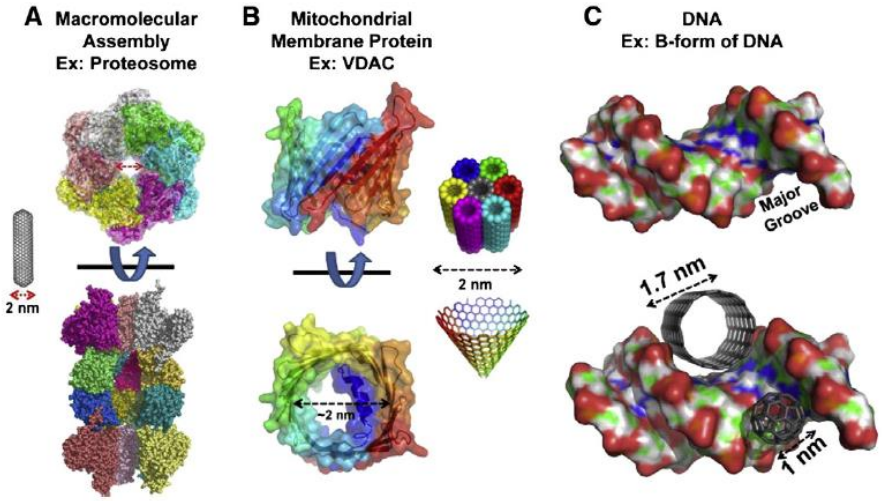

Figure 5: Carbon based nanoparticles and proteins comparison (Yanamala, Kagan, & Shvedova, 2013).

In Figure 5 C it the image show the binding site for the single wall carbon nanotube and the binding site for the fullerene.

Some examples of nanoparticles with proteins interaction simulations are possible with computational approaches. The 3D structures of ligand binding pockets and catalytic sites of various proteins are practically the same size and dimension as artificial nanoparticles. Examples of these nanoparticles include fullerene and single wall carbon nanotubes (SWCNT). These computational approaches reveal that fullerenes as well as SWCNTs of certain size can interact effectively with the hydrophobic ligand-binding site of enzymes (Yanamala, Kagan, & Shvedova, 2013).

With more molecular dynamics simulation studies using computational geometry it become possible to propose that the binding of SWCNT prevents enzyme flaps at the active site from opening and binding with polypeptides (Yanamala, Kagan, & Shvedova, 2013). This means that the computational simulation was able to depict some details of the interaction between the nanoparticles and the biomolecules. This type of simulation using computational approaches made it possible to speed up the process of testes and improve information gathering.

Other computational simulation includes investigation in fullerene-based inhibitors. Fullerenes are found during docking simulations that they bind to a cleft at the GST interface. This means that fullerenes blocks the binding at the site and suppresses the function increasing the oxidative stress in cells (Yanamala, Kagan, & Shvedova, 2013). This computational approach was able to provide research data and reduce the time necessary to perform other more extensive research.

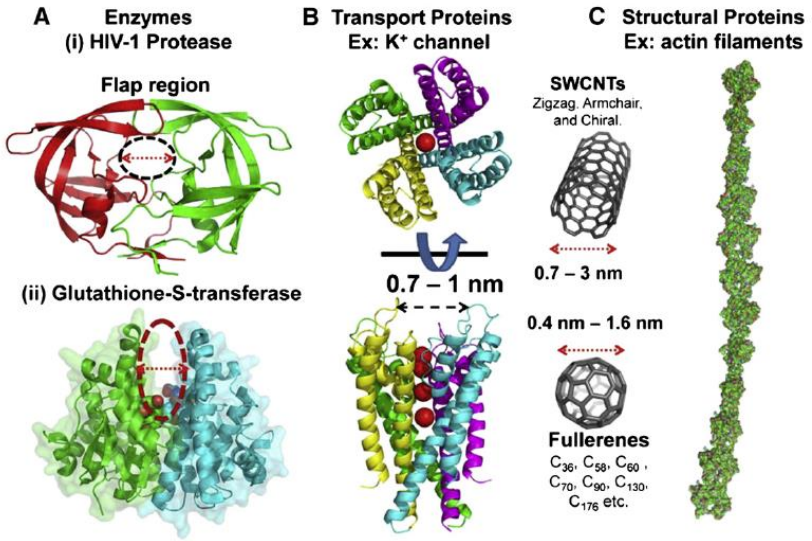

Figure 6: Carbon based nanoparticles and proteins comparison (Yanamala, Kagan, & Shvedova, 2013).

It is clear that computational geometry plays an important role in helping researchers devise algorithms that are more efficient and perform better simulations of nanoparticles interaction with biomolecules.

7.2 *Computational Geometry Techniques for Advanced Feature of Atom Probe Data (2nd article)*

Computational geometry plays an important role in atom-probe-tomography data that provide useful applications in materials characterization. The computational approach here uses Voronoi subvolumes and piecewise linear approximations along with delineation based on the distance to the center of mass (Felfer, Ceguerra, Ringer, & Cairney, 2013).

Using computational geometry technology for atom probe tomography this technology have proven to be useful in identifying atomic scale features like grain boundaries, dislocations, thin film layers, etc. of a material (Felfer, Ceguerra, Ringer, & Cairney, 2013). This is only possible because of the nanometer-scale resolution and extremely high chemical sensitivity (Felfer, Ceguerra, Ringer, & Cairney, 2013). An example of how atom probe tomography data results are analyzed is display in Figure 7.

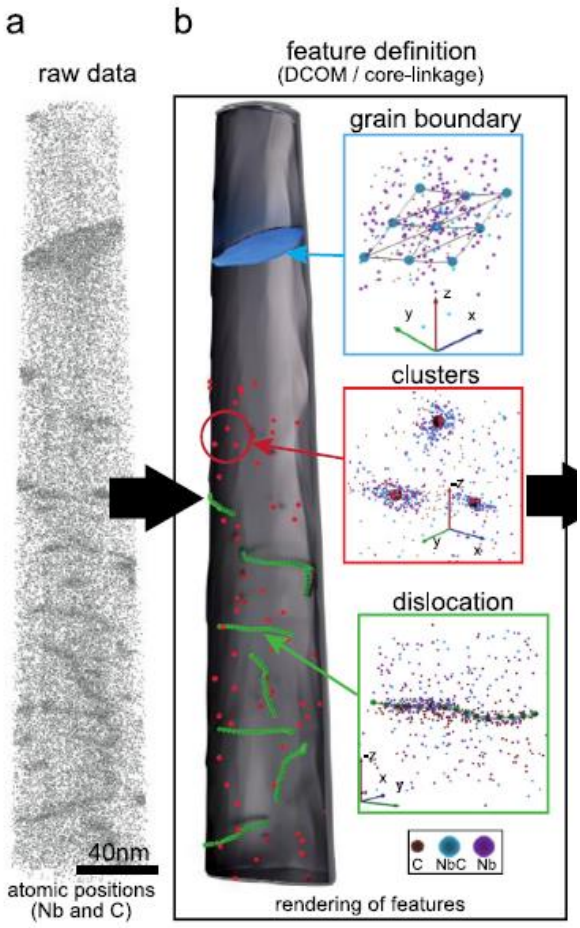

Figure 7: Atom probe result and analysis for grain boundary, clusters, and dislocation (Felfer, Ceguerra, Ringer, & Cairney, 2013).

In recent year with the development of computational geometry as well as sample preparation techniques, scientist now are capable of capturing and analyzing more features and large volume of samples at a shorter time frame (Felfer, Ceguerra, Ringer, & Cairney, 2013). The development of atom probe

tomography is now developed near atomic scale phenomena. This lets scientist analyze many features such as interfaces and defects in the material. This analysis sometime requires manual analysis using more primitive geometric cylinders and aligned boxes.

With the development of computer hardware and software, improvement in measurement in data is to be expected for atom probe tomography. The advancement in instrumentations and sample preparation will make analysis of various microstructure features possible and widespread in the future (Felfer, Ceguerra, Ringer, & Cairney, 2013).

These new features at the atomic scale still need structural standards for analyzing. This means that new designs in analysis framework are created to allow for both structural and chemical analysis of the atomic size microstructures (Felfer, Ceguerra, Ringer, & Cairney, 2013). To build these framework new algorithms must be introduced using computational geometry or computational approach to detect the new features in the data (Felfer, Ceguerra, Ringer, & Cairney, 2013).

Computational geometry lets scientists calculate the feature's spatial domain from the data and then define local coordinate systems based on those features. So from this atoms relative to specific coordinates systems are devised using new analysis methods (Felfer, Ceguerra, Ringer, & Cairney, 2013).

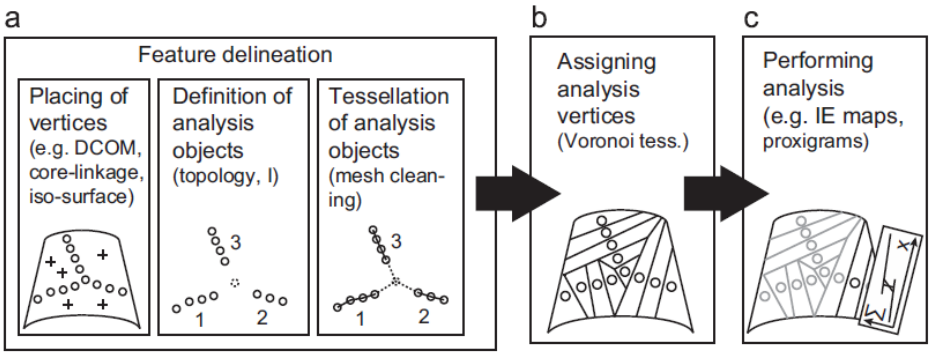

Figure 8: Schematic of the computational approach in analyzing the results of grain boundary, clusters, and dislocation (Felfer, Ceguerra, Ringer, & Cairney, 2013).

The idea of computational approach here is to build the necessary tools for scientist to develop analysis technique to optimize the analysis of information contained in data results as much as possible and produce results with few set parameters. Computational geometry and

computational analysis create the possibility for scientist to perform analysis with as little testing as possible but still obtain comprehensive results.

The atoms imaging captured using atom probe tomography are assigned positions in space through reconstruction algorithms using computational approaches. The analysis of the field evaporation using computational approaches is needed to provide the necessary precision for the origin of the trajectories of the field evaporating ions and therefore provide the necessary information for the location of the atoms.

Once computational approaches are used to analyze the structure, the information is all stored in a point cloud with all the structural and chemical information (Felfer, Ceguerra, Ringer, & Cairney, 2013). This point cloud example is shown in Figure 7a.

With the point-cloud data stored in the computer, now come the crystallographic analysis using computational algorithms to identify certain common reoccurring structures. To identify these crystallographic structures delineation of features base on distribution of solutes is required (Felfer, Ceguerra, Ringer, & Cairney, 2013). Using the solute position (also known as analysis vertices) a model of the structure could be identify and feature using piecewise linear approximation can be build using common methods in computer graphics and computational geometry.

The point cloud data are stored as a lists of vertices, pair or triple of vertices, all depending on the dimensionality of the object analyzed (points, lines, and triangles)(Felfer, Ceguerra, Ringer, & Cairney, 2013). With this grouping, subvolumes can also be defined from the interface object.

Overall, computational geometry and computational approach is crucial in analysis for dislocation, grain boundaries, and clusters. This type of efficient analysis is only possible with the new advancement of computational geometry and data gathering techniques. By using computational geometry and approach to quickly sort through the various crystallographic structure results can be obtain much quicker and better prediction of grain boundaries, dislocation, and clusters could be predicted.

7.3 *Geodesic Polyarenes and Geodesic Domes (3rd and 4th articles)*

Geodesic polyarenes itself represents computational geometry base on its structure. Some of these Geodesic-arenes requires NURBS to predict energy density plot and more complex surface curve plots. Computational geometry sometime require finding geodesic pathways of a surface. Computational geometry is also used in developing nano-size geodesic domes. Researchers that have analyzed the assembly of grapheme on a surface of iridium have found out that the grapheme first grow out in carbon geodesic domes (American Physical Society, 2009).

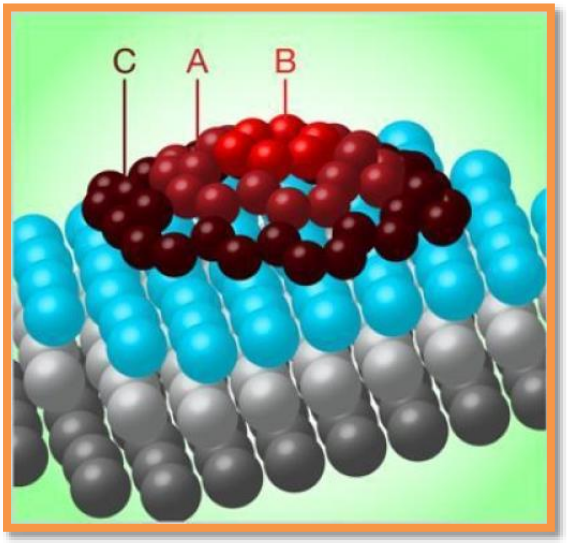

Figure 9: Carbon base geodesic dome (American Physical Society, 2009).

As for geodesic polyarenes they include the well-known fullerene C_{60}. Scientist are currently trying to control the shape of new geodesic polyarenes. These new shapes will be able to have high intrinsic curvature of geodesic arenes and will help with fusion to fullerenes.

The approach here is to generate large non-planar carbon-based nanostructures. These geodesic-arenes will have controllable curvature and holds key concepts to more nanostructure development in the near future. Computational geometry here plays a huge role here in providing the necessary tools for the scientist to analyze the results of these newly created nanostructures and their surface properties. NURBS, points, lines, and triangulation are all part of computational geometry that makes these analyses possible.

Some theory applied to computational geometry used to calculate for these geodesic-arenes nanostructures includes self-consistent charge-density functional tight binding (SCC-DFBT). The SCC-DFBT is used to calculate for the geometries of the investigated structures (Trzaskowski, Adamowicz, Beck, Muralidharan, & Deymier, 2014). Simple to complex computational models could be used to model the geodesic-arenes structures. Computational geometry modeling of these structures and using relative energy to control these structures are

all crucial development in nanotechnology for the future. Some curvature changes for these geodesic-arenes being developed are shown in Figure 10.

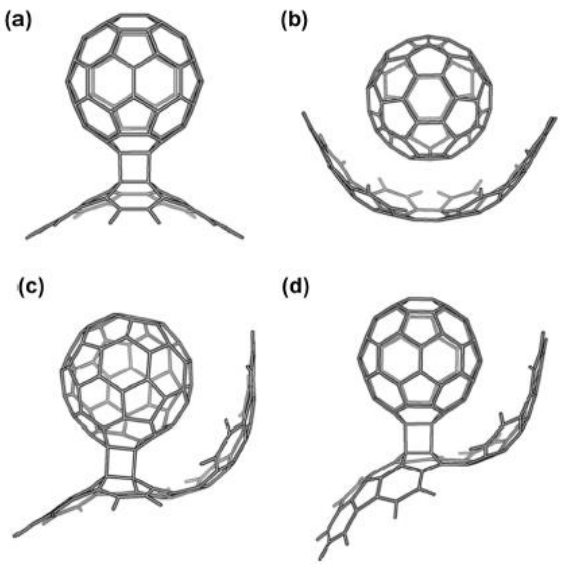

Figure 10: Geodesic-arenes structures with changing curvature (Trzaskowski, Adamowicz, Beck, Muralidharan, & Deymier, 2014).

8 Vision of Future Development in the Field

With new fields continuously being developed in the field of science, computational geometry will continue to play an important role in many field of science either in modeling or computational analysis. Since the start of development in computational geometry along with computer this field continue to prosper as techniques and algorithms are develop to face engineering, biological, and world issues. The same will go for the field of MEMS and nanotechnology. Computational geometry will probably develop better and more efficient algorithms to solve geometrical problems in MEMS and nanotechnology. Better simulation results could be achieve with time depend solutions. Modeling in with time dependent results could definitely be improved and made more efficient. Current points, lines, triangulation, NURBS, and other computational analysis techniques can still be improved on and more efficient sorting and optimization technique may be possible.

The field of computational geometry could build more efficient and complex geometry for modeling and analysis. With the many interdisciplinary field being integrated computational geometry and computational analysis should strive for better integration of various field and data analysis. Currently computational geometry and computational analysis have solve many technical problems that were not possible by hand quickly. The idea is to improve this field in a way to make it better in analysis.

This also applies to the computational geometry and analysis used in the MEMS and Nano field. Current development for nanotechnology can help identify dislocations, grain

boundaries, and clustering. I believe that with improvement computational analysis could bring forward better prediction of possible failure at grain boundaries or dislocations.

9 CONCLUSIONS

Our research here has shown that computational geometry and computational analysis have many future applications in either the design and prototype field or biomedical field. Computational geometry provides designer and visionary scientists with a feasible way to produce models and run simulations. Computational geometry plays a huge role in both MEMS and nanotechnology from algorithms identifying dislocations, grain boundary, clusters to new innovative geodesic-arenes designs. With continuous requirement enforce on computational geometry for further advancement, computational geometry will definitely continue to advance further.

10 ACKNOWLEDGEMENTS

I would like to acknowledge Professor Daniel Yang for their help and guidance.

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12 APPENDICES

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Exploring structures and properties of new geodesic polyarenes

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ABSTRACT

We have employed the self-consistent charge density-functional tight-binding, the density functional theory and the classical molecular dynamics methods to study new geodesic polyarenes, which can be synthesized via the regiospecific cove-region closure and HF elimination. We show that the shape of new polyarenes may be altered and controlled by the presence of C_{60} fullerenes. The high intrinsic curvature of the geodesic arenes facilitates fusion with C_{60} fullerenes. This propensity to fuse is consistent with the hypothesis of an optimal value of the bond-puckering angle at which graphene-like structures show maximum reactivity.

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1. Introduction

Geodesic arenes are a family of polycyclic aromatic hydrocarbons that has recently received a lot of attention, due to their potential use in the synthesis of fullerene isomers [1,2] and isomerically pure single-wall carbon nanotubes [3]. In a very recent paper Amsharov et al. presented an elegant method for obtaining geodesic arenes, which involves a regiospecific cove-region closure via HF elimination [4]. The method also uses activated γAl_2O_3 as catalyst, which mediates the reaction at slightly elevated temperatures (100–150 °C). The advantage of this approach is the high chemoselectivity and regioselectivity, since the chlorinated or brominated analogues remain completely intact under these conditions. The reaction only takes place if the fluorine atom is positioned directly in the cove region. The method allows for a total control of the geodesic-arenes synthesis process and can be used to generate large non-planar carbon-based nanostructures.

Inspired by the geodesic-arenes study we perform a computational investigation of novel geodesic arenes, which can be obtained via the cove-region closure method. In the study we aim to answer the following three main questions: what are the common features of the 3-dimensional structures of various geodesic arenes; how the curvature and the shapes of the geodesic arenes be controlled when they are synthesized; does the intrinsic curvature of the geodesic arenes facilitate their fusion with C_{60} fullerene and production of hybrid nanostructures. To answer these questions we use a combination of theoretical methods including DFT, SCC-DFTB, and MD. All these methods have been previously used to describe various properties of carbon-based systems and, in most cases, the results and predictions derived from the calculations have been quite accurate.

2. Computational methods

The SCC-DFTB method (as implemented in the DFTB+ software [5]) is used in all calculations in this study to obtain the geometries of the investigated structures. These geometries are staring points for the DFT and MD calculations. Some information on the energetics of these systems are also obtained from the SCC-DFTB calculations. DFTB is based on the second-order expansion of the Kohn–Sham total energy in the Density-Functional Theory (DFT) with respect to the charge density fluctuations [6,7]. The zeroth-order approach is equivalent to the standard non-self-consistent tight-binding scheme, while at the second order a transparent, parameter-free, and readily calculable expressions for the generalized Hamiltonian matrix elements can be derived. These are modified by a self-consistent redistribution of the Mulliken charges (SCC) [8]. The DFTB method has been extensively used for modeling of carbon nanostructures and was shown to be in good agreement with more sophisticated methods in the determination of equilibrium geometries, energies and vibrational modes [6,9–12].

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Molecular modeling in structural nano-toxicology: Interactions of nano-particles with nano-machinery of cells ☆

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ABSTRACT

Over the past two decades, nanotechnology has emerged as a key player in various disciplines of science and technology. Some of the most exciting applications are in the field of biomedicine – for theranostics (for combined diagnostic and therapeutic purposes) as well as for exploration of biological systems. A detailed understanding of the molecular interactions between nanoparticles and biological nano-machinery – macromolecules, membranes, and intracellular organelles – is crucial for obtaining adequate information on mechanisms of action of nanomaterials as well as a perspective on the long term effects of these materials and their possible toxicological outcomes. This review focuses on the use of structure-based computational molecular modeling as a tool to understand and to predict the interactions between nanomaterials and nano-biosystems. We review major approaches and provide examples of computational analysis of the structural principles behind such interactions. A rationale on how nanoparticles of different sizes, shape, structure and chemical properties can affect the organization and functions of nano-machinery of cells is also presented.

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"As crude a weapon as the cave man's club, the chemical barrage has been hurled against the fabric of life—a fabric on the one hand delicate and destructible, on the other miraculously tough and resilient, and capable of striking back in unexpected ways." — Rachel Carson, In Silent Spring, (1962), 297.

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1. Introduction

In his epochal speech of 1959 [1] Richard Feynman, not only formulated new concepts in nanotechnology and, highlighted its significance for science and research, but also forecasted several new directions in nanobiology, nanomedicine and nanotoxicology. He introduced the idea of nanomaterials and alerted us: "At the atomic level, we have new kinds of forces and new kinds of possibilities, new kinds of effects. The problems of manufacture and reproduction of materials will be quite different. I am inspired by the biological

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Applying computational geometry techniques for advanced feature analysis in atom probe data

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ABSTRACT

In this paper we present new methods for feature analysis in atom probe tomography data that have useful applications in materials characterisation. The analysis works on the principle of Voronoi subvolumes and piecewise linear approximations, and feature delineation based on the distance to the centre of mass of a subvolume (DCOM). Based on the coordinate systems defined by these approximations, two examples are shown of the new types of analyses that can be performed. The first is the analysis of line-like-objects (i.e. dislocations) using both proxigrams and line-excess plots. The second is interfacial excess mapping of an InGaAs quantum dot.

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1. Introduction

Atom probe tomography has proven to be an invaluable tool for the analysis of atomic scale features such as grain boundaries, dislocations, thin film layers, *etc.* due to its nanometre-scale resolution and high chemical sensitivity. In recent years, both the increased field of view of wide-angle atom probes and progress in sample preparation techniques now allow the capture of many more features and larger volumes in a shorter time [1]. So far, while advanced analysis methods for atom probe data have been developed for near atomic scale phenomena such as clustering and precipitation [2] and second phases [3], other features such as interfaces and defects have mostly been analysed manually using geometric primitives, *e.g.* cylinders and aligned boxes. Due to the advances in instrumentation and sample preparation, we expect the analysis of a wide variety of microstructural features to become more widespread in the foreseeable future. The problem, however, is the lack of a clear standard for describing and analysing these features. Therefore we have designed a new analysis framework that allows for both structural and chemical analysis. In this framework, the algorithms introduced below are used to detect features in the data. The feature representations allow us to automatically calculate the feature's spatial domains within the dataset, and to define local coordinate systems on the features. Based on this information, new analysis methods were then devised based on the positions of the atoms relative to these coordinate systems. The aim of developing this analysis technique is to use as much of the information contained in the data as possible and to produce results that depend on as few parameters as possible. The underlying computer programs will be available freely with open source code from the authors of this article under the working title 'Open VA' [4].

Atom probe tomography is currently able to analyse volumes of material of $\sim 100 \times 100 \times 200\ nm^3$ through field evaporation and to determine the chemical nature of the atoms within this volume through time-of-flight mass spectrometry. The atoms that have been captured by the position sensitive detector (~57% of all atoms or ~35% if an energy compensating mirror is used) are assigned positions in space through reconstruction algorithms [5]. Both the field evaporation process itself and the precision with which the origin of the trajectories of the field evaporating ions can be approximated limits the precision of the 3D data, which has to be taken into account when analysing the data.

After reconstruction, the 3D spatial position and chemical nature of the captured atoms are stored in the form of a point cloud, which bears all the structural and chemical information. This point cloud is the basis of our analysis. Crystallographic analysis can be used to identify features in atom probe data [6,7]. However, in this work the delineation of features is based on the distribution of solutes. Solutes that are segregated are used to define points that delineate the features of interest within the data. Using these specific solute positions (or analysis vertices), a model of the feature using a piecewise linear approximation can be built up by using methods commonly used in computational geometry and computer graphics. The reader is referred to the vast literature in this area, especially the ACM SIGGRAPH publications [8]. The analysis can then be based on the position of the atoms relative to this approximation. This means that the analysis objects are stored as lists of either vertices, pairs of vertices or triples, depending on the dimensionality of the object (point, line, and triangle). Each list defines an analysis object

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Application Challenges to Computational Geometry

CG Impact Task Force Report*

Abstract

With rapid advances in computer hardware and visualization systems, geometric computing is creeping into virtually every corner of science and engineering, from design and manufacturing to astrophysics to molecular biology to fluid dynamics. This report assesses the opportunities and challenges this presents for the field of computational geometry in the years ahead. Can CG meet the algorithmic needs of practitioners? Should it look to applied areas for new sources of problems? Can CG live up to its potential and become a key player in the vast and diverse world of geometric computing? These are some of the questions addressed in this document. It was prepared by a group of computer scientists, engineers, and mathematicians with extensive experience in geometric computing. This report is intended as a wake-up call rather than an agenda setter. It is hoped it will engage a community-wide discussion on the future of computational geometry.

1 Preamble

The fraction of computing falling under the loosely defined rubric of "geometric computation" has been on the rise and is likely to become dominant in the next decade. Computer graphics, manufacturing, scientific visualization, computer vision, astrophysics, molecular biology, and fluid mechanics are just a few in a crowd of avid users of geometric computing. Where does computational geometry fit into all this?

Twenty-odd years ago, the nascent field of computational geometry set sail on a mission to build general tools — analytical and computational — to satisfy the algorithmic needs of geometric computing [45, 64, 98, 108, 114, 120, 129]. The intention was to create a body of knowledge to which computer programmers could turn for help when wrestling with geometric problems. The vision was that of a two-way pipeline: applications areas feeding CG with important practical problems, and CG in turn providing answers in the way of algorithmic tools and mathematically sound analyses.

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