Progress Report:
**The Computational and Scientific Graphics
Laboratory at MSRI**
DE-FG03-95ER25250

David Hoffman

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

at **MASTER**

62

Progress Report: The Computation and Scientific Graphics Laboratory at MSRI

David Hoffman

1 Staff and Software Development

Hoffman continued his research in differential geometry with applications to the study of the microstructure and singularities in compound polymers. This work takes place at MSRI, where he has set up a computation and graphics laboratory.

James T. Hoffman was hired as senior graphics programmer for the laboratory project. Hoffman held a similar post at the Center for Geometry Analysis Numerics and Graphics at the University of Massachusetts when David Hoffman was the Director of that center. J. Hoffman is the principal author of the software MESH for studying minimal surfaces and TEMsim, laboratory software used for the identification of mathematically defined surfaces in periodic microstructures found in compound polymers. (This is discussed in more detail below.) Here is an outline of J. Hoffman's software-related work from August 15, 1995 to Jan 10, 1996.

- For all of the software developed at GANG:
 - upgraded most code with an improved error reporting mechanism
 - continued upgrading code to conform to a consistent coding standard using ANSI C prototypes, module-based naming, structure localization, to achieve an OOP-like encapsulation
 - created tcl/tk macro library to simplify crafting of graphical user interfaces
- Objects & algorithms:
 - implemented network objects (with full vertex/edge/face connectivity) to supersede less flexible polygon and triangle set objects
 - implemented slicing operations on network objects – the basis for clipping, and for extracting planar sections of surfaces
 - implemented a JPEG image input/output module

- Mesh:
 - created a new version of mgen (client setup utility) with a tcl/tk user interface.
 - added support for network objects, and made default output format
 - generalized output module to support storing of additional attributes, such as domain coordinates, in output object
- TEMsim
 - upgraded to support network data sets in addition to triangle sets
 - added a sample translation control
 - implemented operations on the File menu (save and restore state of system parameters)
 - added default preference loading capability
 - added ability to re-load dividing surface(s) in same session
 - added support for up to four volume classes; including a new model for the assignment of surface sides to volume classes
 - generalized the method for assignment of opacity/color values to volume classes
 - replaced method of computing light transmission with a more realistic one, and added a contrast control
 - made default window port equal to one period, making volume fraction calculations accurate using default parameters
- SolSurf
 - added support for network objects as output format
- VPS renderer
 - added support for network objects, including operators to parallel most supported operations on polygon and triangle set objects
 - began upgrade of visual editor to use tcl/tk user interface
- miscellaneous
 - created an application to interactively apply planar mappings to images using a complex algebraic function entered via a tcl/tk interface

In addition, a student programmer, Edwin Ng, worked for three months doing programming and systems administration work.

1.1 MESH and TEMsim

We are in the process of producing a final stable version of MESH. The principal users of the MESH software are now located in many different places in the United States, Japan and Europe. Users naturally have developed libraries tailored to their own research and some have not updated their clients (example-specific code) to newer versions of MESH. We are in the process of creating a WWW-site that will contain all relevant MESH clients written in C or C++ (some older ones exist only in Fortran!) with sufficient documentation (and links) to scientific papers. The site will contain images and animations, as well as code that will work with MESH, which will also be available for down-loading from the same site. These surfaces are of use not only to differential geometers but also to researchers in material science.(See the discussion of TEMsim below.) It will be important to have a repository of examples in both pre-computed and manipulatable form that are easy to down-load linked together with the necessary scientific explanations.

We have developed several algorithms for computer simulation of two-dimensional projections from structures determined by periodic, smoothly-varying dividing surfaces. Projection rays are sent through the model structure and subdivided into very small subintervals. The midpoint of each subinterval is checked to see on which side of the dividing surface it lies. These rays can be thought of as paths taken by electrons; the projection plane onto which the rays are projected represents the photographic film or image detector. We take the optical density at a given pixel to be a linear function of the fraction of subintervals lying on one particular side (e.g. phase A) of an inter-material dividing surface (IMDS). Recent work by the group headed by E. Thomas at MIT (and others) has established an additional equilibrium block copolymer microdomain structure with space group symmetry Ia3d (No. 230)[1]. This cubic structure appears in the same compositional range as the ordered bicontinuous double diamond (OBDD) structure space group symmetry Pn3m (No. 224). Small angle X-ray scattering (SAXS) and TEM evidence suggest a possible bicontinuous structure for the IMDS of the new microdomain morphology based on Schoen's G-minimal surface (the gyroid). This is quite intriguing, since the OBDD is well modeled by a constant mean curvature IMDS based on Schwarz's D minimal surface. (See Figure 2.2.) The D- and G-surfaces are associate surfaces and related by the Bonnet transformation- in the same family as the Schwarz P-surface. Until very recently there were no known theoretical or computable constant mean curvature surfaces known to exist close to the gyroid. This has now changed a great deal due to work of Große-Brauckmann, who showed that numerically that there exists a large deformation family of such surfaces. Prior to this, gross approximations were used by materials scientists to produce models to interpret TEM experiments.

There has been a great deal of progress made in the past year. The current state of things is communicated in the article "Triply periodic level surfaces as models for cubic

tricontinuous block copolymer morphologies” by Lambert, Radzilowski and Thomas which will appear in the Proceedings of the Royal Society of London.[7] (See Appendix 2.) The preparation of this paper was completely dependent on the existence of the software TEM-sim, written by J. Hoffman. Many of the level surface models used were computed using the software SolSurf also written by J.Hoffman. This application was modified a great deal to handle the needs of the authors. As practicing laboratory polymer scientists, they will prepare the guide for users that will accompany the next distribution of the software. D. Hoffman and E. Thomas are working on a Scientific American article about mathematical models for IMDSs in compound polymers.

2 Interaction at MSRI and LBNL

During the Fall of 1995, MSRI was host to special programs in Several Complex Variables and Holomorphic Spaces. We were able to use graphics to help in the understanding of several important examples in the subject. One is the Kohn-Nirenberg domain. (See included illustration.) The center of the flat-saddle surface is a point with the following property: every holomorphic curve tangent to the domain at the point must contain nearby points both inside and outside the domain. Yet the domain is pseudo-convex everywhere else. Another example, the worm domain, can be approximated from the inside by strongly-pseudoconvex domains, but it *cannot* be approximated from the outside by such sets. These illustrations are the first of their kind and were used in several of the conference presentations in the Fall of 1995. Several members reported that they were illuminating and very useful for understanding the underlying mathematics. In other related activity, a program for computing the Kobayashi metric of a domain in C^2 , written by S. Krantz and a former post-doc, was given a graphical interface by J. Hoffman. The algorithm for determining the extremal curves necessary to compute the metric is being rethought and improved. It will be rewritten.

Hoffman aided in the conception and coordination of the MSRI Multicast Backbone project. The Multicast Backbone software is being developed at LBNL in the networking group, which is in the the Computer Science Division, under the direction of Stu Loken. MSRI has put together a consortium of twelve centers and University mathematics departments. These units will each be able to send and receive Multcasts of seminars, the first series of which will come from MSRI. Funding has been requested from the National Science Foundation and there is preliminary indication that it will be forthcoming. We note that no equipment for this project has been purchased with funds from this grant. With the exception of Hoffman’s time in coordinating this project, no funds have been expended for personnel.

Hoffman wrote MSRI’s part of LBNL’s NERSC proposal to move the National Energy Research Supercomputer Center to Lawrence Berkeley Laboratory. In it we outlined

projects that would be undertaken jointly between the proposed Center and MSRI. These include a summer student workshop, joint post-doctoral students, common high-speed networking and conferences on mathematical topics relevant to scientific research using modern computational and networking tools. Due to the delay in the definitive decision to move NERSC from Livermore to Berkeley, the plans to implement these joint projects have been stalled. We have scheduled a meeting during the mid February will meet W. McCurdy, the Director of NERSC, and with Piermaria Oddone, who is an Associate Director of LBNL and S. Loken. Last year, Oddone strongly requested MSRI's participation in the proposal. At this upcoming meeting, we expect to clarify MSRI's role in the newly-moved Center. The delays in beginning our involvement have been frustrating.

2.1 Miscellaneous

At D. Hoffman's invitation, J. Colvin spoke to the MSRI Empennage Seminar in the Fall. Colvin is from Sandia National Laboratory and is a computational quantum chemist. Simulations in this area often require the repetitive use of geometric algorithms, whose complexity is the main contributor to their enormous computational expense. In a conversation last Spring, Hoffman suggested an algorithm of order n^2 for determining whether, given n points in R^3 , a new point can be separated from the others by a plane. Colvin's group was using an order n^3 algorithm at the time. The faster approach was developed in conversations with mathematicians at Stanford, T. Ilmanen in particular. W. Thurston pointed out that there was code, called QuickHull, developed at Princeton and distributed by the Geometry Center, that could be used to solve this problem faster than order n^2 , the speed depending on how many of the n points were extremal. Colvin spent several hours discussing this and other computational problems with members and staff of MSRI. He returned a week later with a colleague to continue the research discussions, this time focusing on the so-called solvent-surface problem. We expect that this sort of contact will continue.

We mention several other minor activities to indicate the scope of work in which we are engaged. Don Glaser, a Berkeley physicist and member of the Friends of MSRI, visited to discuss several graphics tools of use to him in studying the biology of human vision. J. Hoffman is preparing an animation for R. Osserman to illustrate upcoming talks in Washington.

3 Geometry

D. Hoffman continued his research in the theory of complete embedded minimal surfaces. With Wei and Karcher, he completed the manuscript "The periodic genus-one helicoid," [3] which has been submitted for publication in *Inventiones Mathematicae*. (See Appendix I) Wei and Hoffman have used the results of this paper to show that the genus one helicoid (see [4]) is embedded. This proof is not completely synthetic. In addition to a fair

amount new theoretical work concerning the asymptotic behavior of the constructed family of screw-motion-invariant periodic minimal surfaces—statements about monotonicity and asymptotic behavior—the work relies heavily on detailed computations to support statements about the behavior of the family. We know for example from these computations that the conformal structures of the screw-motion-invariant family converge to the conformal structure of the genus one helicoid. While our visualization software clearly shows that these surfaces—away from the two ends—are embedded this is convincing but not a proof. The theory shows that the ends are embedded separately and we have been able to prove that

Theorem 3.1. *If the initial periodic genus-one helicoid is embedded then the entire family of screw-motion-invariant surfaces is embedded. Furthermore, if properly normalized, they have as a limit the genus one helicoid (an aperiodic surface).*

Both the existence and embeddedness of the periodic genus-one helicoid are proved in [3].

As part of this newerwork we were able to characterize helicoidal-type ends that are “aligned,” in the following sense. Let E be a minimal annular end, conformally equivalent to a punctured disk. Suppose that the Weierstrass data dg/g and dh both have double poles at the puncture. We will say that E is *aligned* if it contains a vertical ray and a horizontal ray. Then

Proposition 3.2 *An annular end E is aligned if and only if it can be represented on a neighborhood of ∞ in C by Weierstrass data of the form*

$$dg/g = f(z)dz, \quad dh = idz,$$

with $f(z) = \sum_{k=0}^{\infty} r_{2k}z^{-2k}$, where all r_{2k} are real and $r_0 \neq 0$. Furthermore, any such end contains an embedded sub-end, which is asymptotic to a helicoidal end in the weak sense.

These results will appear in [6].

At the present time, we do not know a how to give a non-computational proof of the facts we need to make a limiting argument. Here, the detailed information we can get out of MESH is extremely important. The reliability of this program is absolutely critical for this work.

The paper “Limit surfaces of Riemann examples,” written with W. Rossman, was accepted for publication by the *Journal of Geometric Analysis*. The survey “Complete embedded minimal surfaces of finite total curvature,” written with H. Karcher will appear soon in the Springer *Encyclopedia of Mathematics*. In addition to surveying what is known about complete embedded minimal surfaces, there are results in this paper that appear in print for the first time; existence and growth estimates for the deformation family of three-ended minimal surfaces of genus $k \geq 2$. For the deformation of Costa’ surface ($k = 1$),

these estimates are more delicate and will appear in the paper "One-parameter Families of Embedded Complete Minimal Surfaces of Finite Topology" (with Karcher and W. Meeks III), which is in preparation.

Hoffman is working with J. McCuan, an MSRI Post Doctoral Associate on problems involving constant-mean-curvature surfaces bounded by convex plane curves. Consider a membrane bounded by a convex plane curve, Γ . The surface, bounded by Γ , that minimizes area among all such surfaces that also surround a region of volume V has constant mean curvature. For small values of V , the surface is a graph in a halfspace defined by the plane of Γ . The conjecture that for all $V > 0$ the solution lies in a halfplane is almost certainly false. Several years ago Hoffman was able to compute and view graphically numerical simulation of solutions this problem and it appears that for V suitably large, the conjecture is not true; this is the case for all Γ computed so far, with the exception of close polygonal approximations to a circle. For a circle—the only curve for which the solution is known for all V —solutions are always spherical caps. On the basis of these experiments, Rosenberg conjectured that the first spill-over into the other half-plane would occur at a point of Γ where the curvature was minimized. Recent work of Ros and Rosenberg on theoretical aspects of this problem inspired a construction that indicates that this Rosenberg's conjecture is false; if it is the case that there is spill-over for every non-circular curve, then one can construct a curve for which spill-over happens first at a point where the geodesic curvature of Γ is not extremal. We are in the process of constructing just such a candidate for numerical testing. McCuan has outlined a procedure for proving that for every non-circular convex plane curve Γ , there is a volume $V(\Gamma)$ such that for $V > V(\Gamma)$ the constant-mean-curvature surfaces bounded by Γ have points on both sides of Γ . We will work in the coming year on proving this result—first observed in computer experiments—to be true.

4

We will continue the research described in this report and the original proposal.

References

- [1] D. Hadjuk, P. Harper, S. Gruner, C. Honeker, G. Kim, and E. Thomas and L. Fetters. The gyroid: a new equilibrium morphology in weakly segregated diblock copolymers. *Macromolecules*, 27:4063–4075, 1994.
- [2] D. Hoffman and H. Karcher. Complete embedded minimal surfaces of finite total curvature. 92 pages. To appear in the Springer Encyclopedia of Mathematics.
- [3] D. Hoffman, H. Karcher, and F. Wei. The periodic genus-one helicoid. MSRI preprint. Submitted for publication.

removed
DLE

- [4] D. Hoffman, H. Karcher, and F. Wei. The genus one helicoid and the minimal surfaces that led to its discovery. In *Global Analysis and Modern Mathematics*. Publish or Perish Press, 1993. K. Uhlenbeck, editor, p. 119–170.
- [5] D. Hoffman and W. Rossman. Limit surfaces of Riemann examples. To appear in *J. Geom. Analysis*.
- [6] D. Hoffman and F. Wei. The genus one helicoid as the limit of embedded, singly periodic screw-motion-invariant minimal surfaces. In preparation.
- [7] C. Lambert, L. Radzilowski, and E. Thomas. Triply periodic level surfaces as models for cubic tricontinuous block copolymer morphologies. To appear in the Phil. Trans.R. Soc. London A (1995) Vol. 13.

removed
(AT)