Scientific Problem Solving in a Distributed and Collaborative Multimedia Environment*

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Abstract

We describe a distributed and collaborative environment for cooperative scientific problem solving. SHASTRA is a highly extensible, distributed and collaborative design and scientific manipulation environment. At its core is a powerful collaboration substrate – to support synchronous multi-user applications, and a distribution substrate – which emphasizes distributed problem solving. The design of SHASTRA is the embodiment of the following idea – scientific manipulation toolkits can abstractly be thought of as objects that isolate and provide specific functionality. At the system level, SHASTRA dictates architectural guidelines and provides communication facilities that let toolkits cooperate to utilize the functionality they offer. At the application level, it provides collaboration and multimedia facilities that let users cooperate. A synergistic union of these two elements yields a sophisticated problem solving environment.

Sample applications that we have attempted in SHASTRA include custom design of human hip prosthesis, shape optimization of the connection between a jet engine and an airplane wing, and efficient computation of molecular "docking" algorithms for drug screening.

1 Introduction

Harnessing of current advances in computing technology has made it possible to tackle progressively larger problems. In project SHASTRA we consider the research and development of the next generation of scientific software environments where multiple users (say, a collaborative engineering design team) create, share, manipulate, simulate, and visualize complex three dimensional geometric designs over a heterogeneous network of workstations and supercomputers. SHASTRA consists of a growing set of interoperable tools for geometric design networked into a highly extensible environment [1]. It provides a unified framework for collaboration, session management and data communication along with a powerful numeric, symbolic and graphics substrate, enabling the rapid prototyping and development of efficient software tools for the creation, manipulation and visualization of multi-dimensional geometric data. These software tools are primarily tailored for use in both scientific experimentation and education, with an emphasis on distributed and collaborative geometric problem solving.

In this paper we briefly describe the SHASTRA toolkits: GANITH a curve and surface manipulator, SPLINEX a surface modeler in Bernstein-Bezier form, SHILP, a free-from solid modeler, VAIDAK, a medical image reconstructor, BHAUTIK, a front end to mesh generation and physical analyses, RASAYAN a

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Figure 1: Video Support for Design Confirmation in a Model Reconstruction Session in SHASTRA

molecular modeler and simulator and GATI an animation server. We also show how these interoperable tookits, can be used in the design of custom artificial implants[12], the optimization of the connection between a jet engine and an airplane wing[11], and the efficient computation of molecular "docking strategies" for drug screening[10].

2 SHASTRA : An Overview

The SHASTRA environment [1] consists of a growing group of interacting applications. Some applications are responsible for managing the collaborative environment (the Kernel applications), whereas others provide specific services (the Service Applications), while yet others provide scientific design and manipulation functionality (the SHASTRA Toolkits). Service applications are special purpose tools for multimedia support – providing textual, graphical, audio and video conferencing. Different tools register with the environment at startup, providing information about what kind of services they offer (Directory), and how and where they can be contacted for those services (Location). The environment provides mechanisms to create remote instances of applications and connect to them in client-server mode (Distribution). In addition, the environment provides support for a variety of multi-user interactions spanning the range from master-slave electronic blackboarding to simultaneous multiple-user interaction (Collaboration). It provides mechanisms for starting and terminating collaborative sessions, and joining or leaving them.

Scientific manipulation computations are often highly compute intensive. SHASTRA's information integration infrastructure intelligently distributes the input of low-computation tasks – to benefit from distribution, and the output of high-computation tasks – to emphasize sharing of resources among applications. It provides mechanisms to support a variety of multi-user interactions spanning the range from demonstrations and walk-throughs to synchronous multi-user collaboration. In addition the infrastructure facilitates the exchange of multimedia information which is often useful to successfully communicate at the time of design, to share the results of scientific tasks, and often necessary to actually solve problems. For example, a researcher uses a live video image in SHASTRA to verify femoral topology of a reconstructed femur model in Figure 1. Finally, SHASTRA provides a convenient abstraction to the application developer, shielding him from lower level details, while providing him with mechanisms to flexibly tailor cooperative interactions.

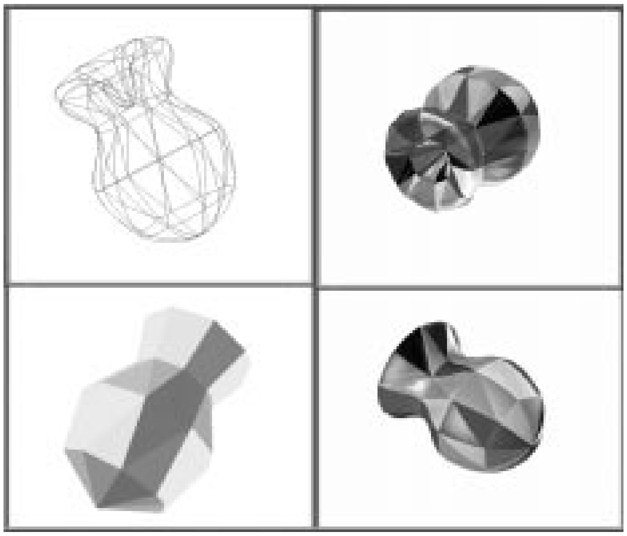


Figure 2: C^1 Implicit Splines over a Spatial Triangulation

3 SHASTRA Toolkits

Designed for extensibility, the SHASTRA environment is continuously growing. Currently GANITH, SHILP, VAIDAK, BHAUTIK, SPLINEX, RASAYAN and GATI are X-11 window based scientific toolkits under the SHASTRA umbrella. These toolkits have been integrated into the SHASTRA environment, and permit distributed problem solving by providing TCP/IP network access to their functionality to other toolkits.

1. The GANITH algebraic geometry toolkit manipulates arbitrary degree multivariate polynomials and power series [6]. It can be used to solve systems of algebraic equations, visualize its multiple solutions, compute and resolve singularities of curves, compute multivariate C^k interpolation and least-squares approximation, etc. We have also developed MathLink programs for a peer - peer connection between GANITH and MATHEMATICA (Computer Algebra Package of Wolfram Research Inc.).

2. SHILP is a boundary representation based solid modeling system As an example of distributed problem solving, SHILP calls upon remote distributed instances of GANITH for its interpolation capability (potentially one GANITH instance per face of the polyhedron), to smooth a polyhedral object and produce a curved surface solid model, as shown in Figure 2.

3. The VAIDAK Medical Image Reconstruction Toolkit can be used to construct accurate surface and solid models of skeletal and soft tissue structures from CT (Computed Tomography), MRI (Magnetic Resonance Imaging) or LSI (Laser Surface Imaging) data [5]. In a distributed problem solving scenario, medical images of the parts of the human body can be reconstructed in VAIDAK, solid models created and manipulated in SHILP. See Figures 1 and 3.

4. The BHAUTIK physical analysis toolkit provides mesh generation facilities as well as a graphics interface to set up, perform and visualize physical simulations on geometric models [7]. Problems can be 2 or 3 dimensional, using objects created in VAIDAK, SHILP, or other model creation toolkits. BHAUTIK has several finite element mesh generation options, including good bounded aspect ratio triangulations. Meshes can be subdivided repeatedly to gain more accuracy in analysis and visualization. A material database is maintained which contains both structural and heat properties of various materials. Boundary conditions including external forces, fixed nodes, and external heat sources can be specified interactively. Results of analysis, obtained through remote calls to any of a number of finite element solvers, can then be visualized in BHAUTIK. See Figures 3 (b), 4 and 5.

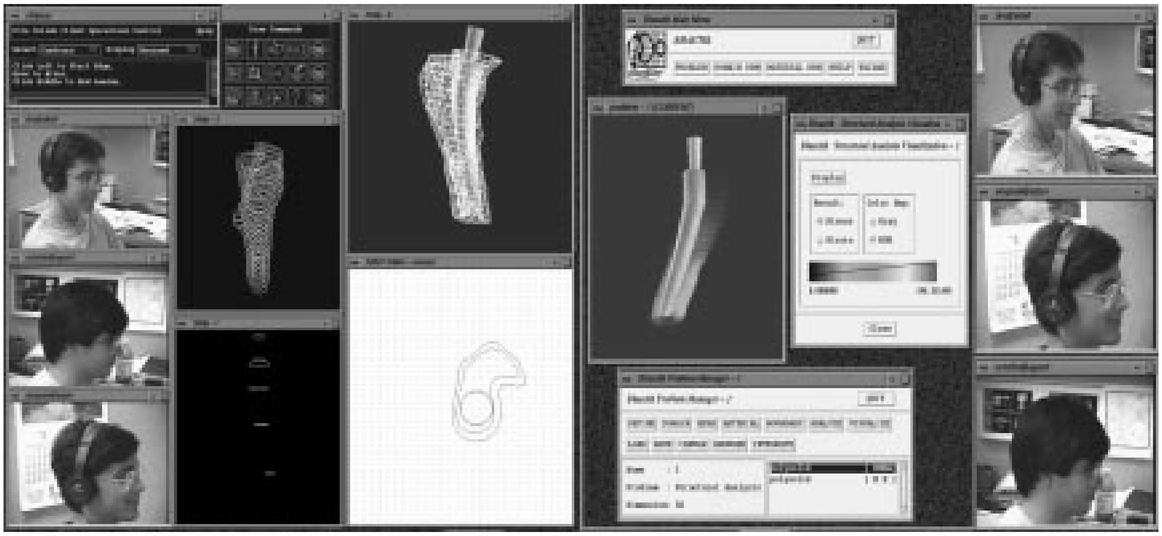
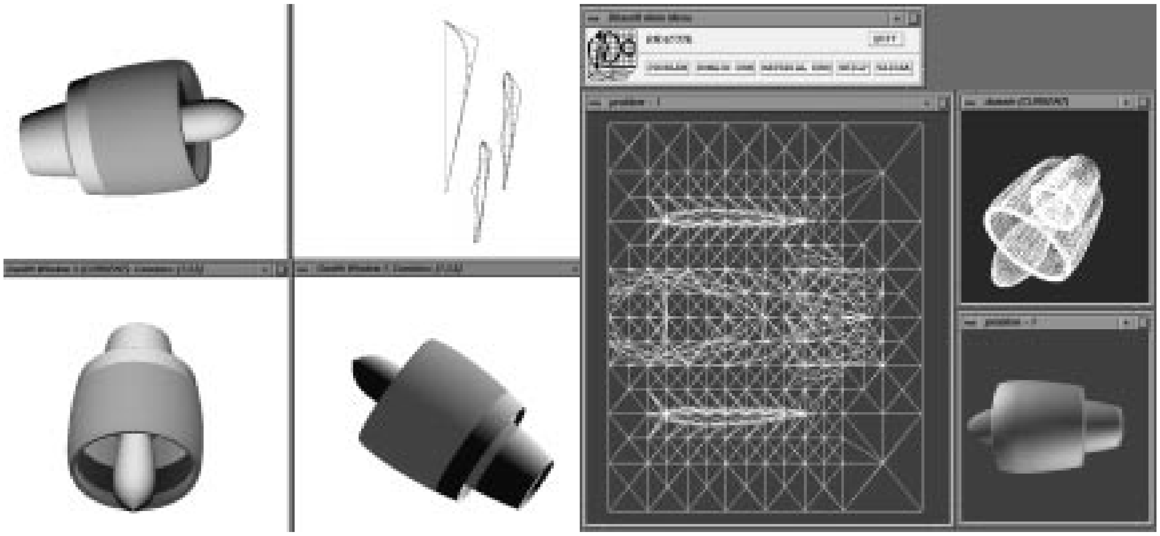


Figure 3: Custom Prosthesis Design and Stress Transfer Modeling from Prosthesis to Femur in SHASTRA

5. SPLINEX is a curve and surface modeling toolkit that provides interactive creation and manipulation of multivariate algebraic splines (A-splines, A-patches) in Bernstein-Bezier (BB) bases[8, 3]. Here the computation and rendering tasks of the multiple curves and surfaces making up the spline are automatically distributed over a network of workstations. See Figure 4 (a) where an A-spline cross-section is created in SPLINEX to fit given data and obey certain continuity requirements and then revolved in SHILP to produce the jet engine model.
6. RASAYAN is a molecular modeling and visualization toolkit that provides automatic creation and manipulation of the combinatorial and topological structure of molecules. This includes covalent bond structure determination and the computation of the union of balls model. Furthermore RASAYAN provides quantitative information such as length, surface area and volume of specified parts of molecular chains. In conjunction with GANITH and SPLINEX the RASAYAN toolkit also provides the computation and visualization of the potential energy surfaces of the molecules as well as the stationary points on these surfaces. See Figures 6 and 7.
7. GATI is an animation server that provides for distributed and collaborative real-time interactive animation in two and three dimensions [4]. The system supports a high level animation language based on a commands/event paradigm.

4 Custom Hip Prosthesis Design

The SHASTRA toolkits provide a distributed environment for the interactive design and analysis of a hip prosthesis. VAIDAK accurately reconstructs a solid model of a patient's femoral bone, which SHILP can use as a guide for the design of an artificial hip replacement. Using these two models, BHAUTIK can analyze the interaction of the prosthesis with the original bone of the patient, and provide feedback for possible modifications for the bone and the prosthesis design. If a region on the bone is under too much stress, the bone may be reamed out more in that region. If the bone is not thick enough to modify at that point, the implant can be redesigned to redistribute the stress to other areas. Traditional implants vary in the length of the femoral portion of the implant. Changing the length may help to distribute the stress. The orientation of the implant with respect to the femur may also be altered. Figure 3 shows a collaborative problem solving



(a) (b)

Figure 4: C^3 Cubic A-splines, A Jet Engine Solid Model, and a Volume Finite Element Mesh for Flow Analysis

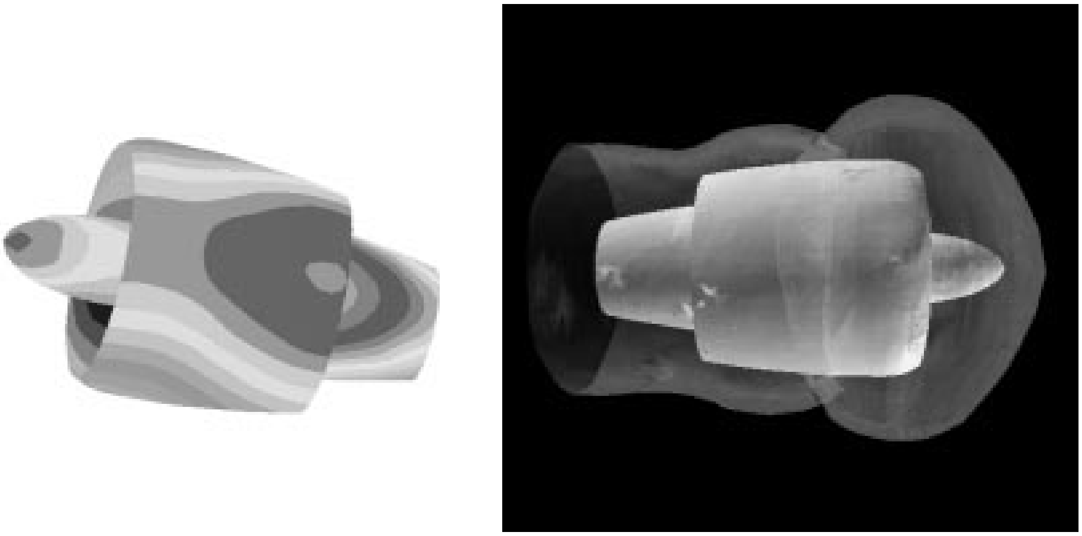


Figure 5: Visualization of Iso-Pressure Contours

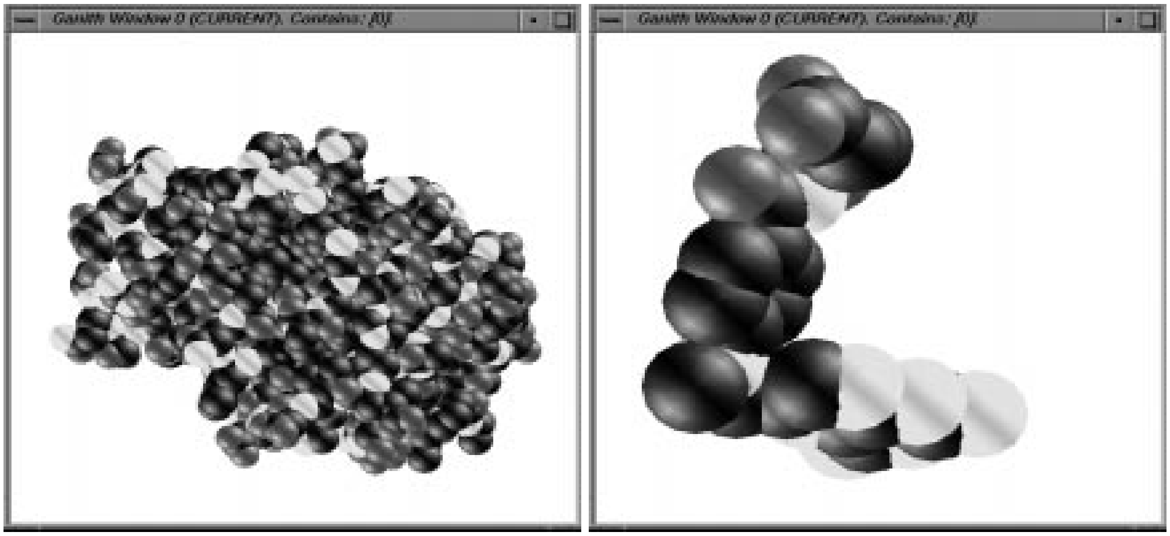


Figure 6: Modeling of Protein and Drug Molecules

session in which implant shape optimization is being performed based on load transfer structural analysis from the implant to specific regions of the femur.

5 Shape Optimization of Engine and Wing Connections

We are also using the SHASTRA environment to study the effect of geometry for connections between jet engines and aircraft wings using 3D air flow simulations around reconfigurable geometries.

Figure 4 (b) shows a volume mesh, generated in BHAUTIK, of the fitted 3D model of the engine and a bounded surrounding region. The geometric design task of creation and modification of the engine model is accomplished in SHILP in conjunction with remote calls to SPLINEX for A-spline fitting operations. As shown in Figure 4 (a) an A-spline cross-section is created in SPLINEX, to fit given data and obey certain continuity requirements, after which SHILP performs a revolve operation on the cross-section to generate a solid model for the jet engine nose and cowling. We are linked to available CFD (computational fluid dynamics) solvers (like FIDAP 7.01), while handling all the geometry, mesh generation and graphics visualization tasks in SHASTRA. See Figure 5 where iso-Pressure contours on the surface of and surrounding the jet engine.

6 Molecular Docking for Drug Screening

New algorithms are being developed in SHASTRA to exploit the domain geometry represented by:

1. molecular structure – approximated by Weighted Alpha-Shapes[9]. See Figure 7.
2. the potential energy surfaces – approximated by piecewise algebraic surface interpolants [2].

. An interactive application is being developed in RASAYAN to compute and visualize the "docking" of drug and protein molecules [10] under molecular Brownian motion. The application reads in a description of the atom locations of a molecule from a file, computes the bonding information and then displays the molecule through SHASTRA's visualization toolkits. Both the computation and visualization of the potential energy surfaces of the molecules and the stationary points on these surfaces require sophisticated surface fitting (interpolation) techniques. Here RASAYAN interoperates with the GANITH and SPLINEX toolkits.

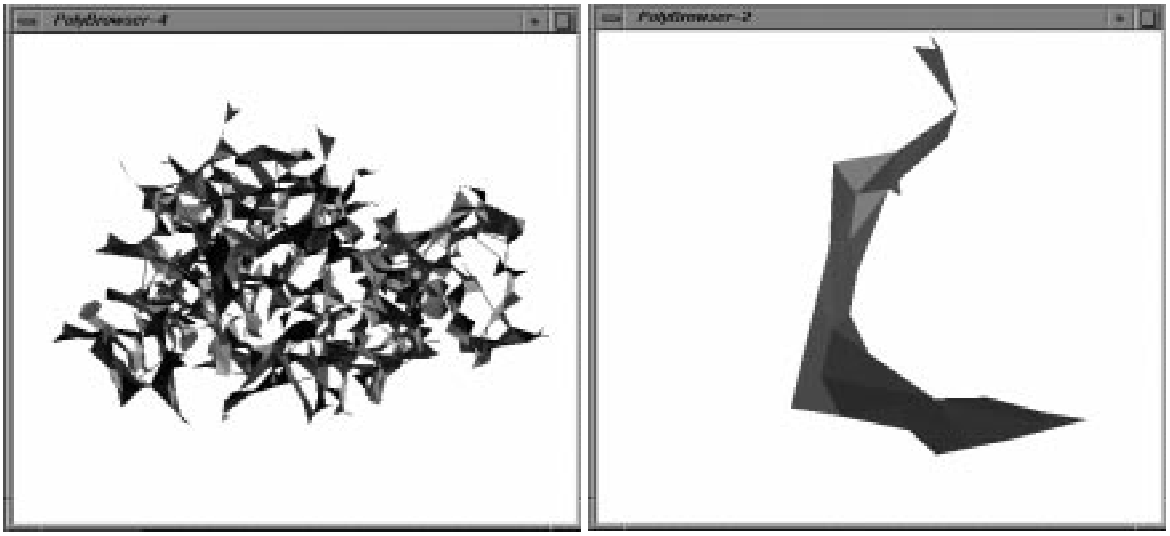


Figure 7: The Combinatorial Structure of the Protein and Drug Molecules

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