INTEGRATING SIMULATION RESEARCH INTO CURRICULUM MODULES ON MECHANICAL BEHAVIOR OF MATERIALS: FROM THE ATOMISTIC TO THE CONTINUUM

MRS Workshop Proceedings

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Abstract

We describe the development of modules for teaching a senior level course, Mechanical Behavior of Materials, that incorporate the results of state of the art simulation techniques. The modules are Web-Java based and make extensive use of materials available through the Internet. The most important characteristic of these modules is that they teach the basics of materials mechanical behavior using research simulation codes that are state of the art in the materials simulation community. The simulation results span various length scales and start at the atomistic level, using embedded atom method techniques reaching finite element simulations at the continuum level. The modules attempt to stress the way in which macroscopic properties are controlled by phenomena at the atomistic and microstructural levels. Advanced computation and visualization techniques, including CAVE™ [=] virtual reality technology, are used to convey some of the more basic concepts. The course was taught by an interdisciplinary team of material scientists and engineering mechanicians. We will discuss our experience in teaching the course and the lessons learned.

Keywords: Atomistic-Models; Continuum-Models; WWW modules; Java

Introduction: Module Development Background

Modules were developed and distributed on our SUN-VNI Wave-Java Web server, Ref [1]. Early efforts to create a distributed, Web-based, visual computing environment were funded by SUN Microsystems, Visual Numerics, and Virginia Tech's Advanced Communications and Information Technology Center (ACTIC). This project was largely motivated by a student project, "Educational Atomic Models Using PV-WAVE & Java" by Arturo Falck, in ESM4714: Scientific Visual Data Analysis and Multmedia, Spring semester 1996, Ref [2]. The purpose of this project was to create a user-friendly Web-based interface to interact with large computer simulation models of cracks and dislocations in crystal lattices by using CGI (Common Gateway Interface). With CGI, an interactive Web-based form was created that students used to: 1) enter information required by the simulation, 2) compile that information into a data file, and 3) submit this file as a batch job to a remote supercomputer. Upon completion, the results from the supercomputer simulation were transferred back to the server for viewing at remote-site workstations. Unique to this project was the level of industrial participation by SUN Microsystems and Visual Numerics in the creation of a general Java Web-based interface, see Ref [3]. Early Java prototypes developed at Virginia Tech have been replaced with JWave interfaces developed by Visual Numerics except for the

[=] CAVE™ is a trademark of the Electronic Visualization Laboratory of the University of Illinois

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Network Programming Interface Builder (NPIB) which creates a user-friendly interface that non-Java programmers can use to build forms that were originally created by CGI. An example of a NPIB form used to calculate vacancies in iron is shown in Figure 1 (a).

Development of the Java-Web server continued with additional funding from the NSF Combined Research and Curriculum Development (CRCD) Program. With NSF funding the server was upgraded to a SUN Sparc10 with 640Mbytes of memory and the authors developed an undergraduate class where students learned about material behavior using the atomistic and continuum simulation modules, Ref [4]. Although still under development, the Web-Java interface that links students at their personal computers to remote-site supercomputers was created entirely in Java so that the same Java-Web server could be implemented at other universities using standard Java based technology on affordable UNIX workstations. A UNIX web server was selected as a more compatible interface with remote-site UNIX supercomputers.

The class was organized on the Web server with hyperlinks to Web modules that were divided into lectures, assignments, and examples, Ref [4]. Professor Farkas focused on Atomistic Models, Ref [5, 6], and Professor Batra focused on Continuum Modules, Ref [7]. Spanning the length scale from the atomistic to the continuum is a research topic of current interest, Ref [8]. Professor Kriz also developed wave-surface representations of fourth order stiffness tensors, Ref [9, 10], that will be used in subsequent classes. Professor Kriz was also responsible for creation of the Java-Web server and NPIB interfaces developed by Graduate Research Assistants Randy Levensalor [†] (Department of Computer Science) and Sanjiv Parikh[†] (Engineering Science and Mechanics).

Atomistic Modules

Atomistic modules consisted of lectures, assignments and examples. The examples consisted of NPIB forms that the student used to create information that was used to run simulations of various topics presented in the class lectures. Using the NPIB forms students can change values of physical properties interactively where simulations of crystal systems were created which produced results within 10 seconds or less. This quick feedback of information allowed students to experiment with a much broader range of parameters. Because this parametric study was based on numerical solutions, calculations could be completed quickly on the SUN Sparc10 Ultra with crystalline structures where the limiting factor was the size of the crystalline structure. A computational speed of less than 10 seconds was realized if the crystalline structure did not exceed 100 atoms.

For atomistic models, lectures on the following topics were presented.

- Bonding in Crystals
- Crystalline Structures
- Mechanical Properties of Crystalline Materials
- Dislocations in Crystals
- Fracture Behavior of Bulk Crystalline Materials
- Fracture Behavior of Interfaces

Two NPIB interfaces were created in the examples section of the module: 1) Crack in NiAL and 2) Vacancy in Fe. The NPIB Web interface form is shown in Figure 1 (a) and a VRML

[†] Graduate Research Assistants

(Virtual Reality Modeling Language) of the resulting structure is shown in Figure 1(b). With the NPIB interface students were first asked to look at the numerical summary of results to determine if the simulation ran correctly. With a VRML Web browser plugin students could immediately view simulation results at their personal computer interactively. The NPIB interface also returned the simulation raw data in a format that could be viewed with WebLabViewer which was downloaded from the MSI (Molecular Simulations Inc) Web page. With WebLabViewer students could again view the simulation results interactively on their personal computer, but unlike VRML, the students could make measurements such as bond angles, bond lengths, volumes, etc, see Figure 1(c). If the simulation resulted in large complex crystalline structures, the results could also be viewed in the Virginia Tech CAVE, see Figure 1(d). In the CAVE the same VRML 1.0 file, shown in Figure 1 (b), could be loaded "as is" into the CAVE using a commercially available navigation tool called Performer Navigator ("pfnav"). The Web server was configured such that students can simply load the VRML files directly into the CAVE from the Web page projected on the front wall of the CAVE.

With the lectures and subsequent assignments using the NPIB interface, students were introduced to a fundamental understanding of how dislocations and crystal structures relate to ductile behavior at an atomistic level. Energies associated with the generation of a crack at the atomistic level were compared to continuum models that predict energy released in new crack formation in brittle behavior. Research topics in atomistic models, Ref [5, 6], were introduced where the embedded atom method could then be explained.

Continuum Modules

Continuum modules consisted of lectures, assignments and examples. The examples consisted of JWave interfaces that the student used to create information that was used to run simulations interactively of various topics presented in the class lectures. With the JWave interface students could change values for parameters interactively and view the results within 10 seconds or less. This quick feedback of information allowed students to experiment with a much broader range of parameters. Because this parametric study was based on exact closed form solutions, calculations could be completed quickly on the SUN Sparc10 Ultra where the limiting factor of these modules was not the computational speed but the network connection speed.

For continuum models lectures on the following topics were presented.

- Concepts of Stress
- Equations of Equilibrium
- Concept of Strain
- Strain-Displacement Relations
- Material Characterization
- Boundary Conditions
- Work done by External Forces
- Principle of Minimum Potential Energy
- Uniqueness Theorem
- Deformation Field in a Axially Loaded Bar
- Bending of Beams by Terminal Couples

For the continuum modules JWave was used as the interactive parametric tool. For example, following the lecture on Strain-Displacement Relations, students could experiment and explore which physical parameters influenced the pressure distribution in a thick walled cylinder. Figure 2 shows a typical JWave interface where students can input numerical values for the parameters that influence stress distribution. The lower Web frame in Figure 2 shows the governing equations together with a schematic diagram, which aids in the physical interpretation of the input parameters.

Students were introduced to continuum research topics in material behavior with an assignment where the objective was to run a range of impact velocities and to study how these impact velocities influenced different materials to undergo different ductile to brittle transitions. To run these simulations students were introduced to a commercially available simulation code that was designed to run only on standalone workstations. Each of the professors also provided Web link summaries of current research and the students submitted all of their homework assignments on the anonymous ftp server, ftp.sv.vt.edu/crcd/, which is open to public access.

Summary, Lessons Learned, Future Developments

The NSF -CRCD class is being taught this fall semester, 1998. Therefore the Java-Web server and modules described above, although mostly complete, are still under development. The class was taught as a three-credit hour class, which met for one hour three times a week: Monday, Wednesday, and Friday. Mondays and Wednesdays were reserved for lectures and on Fridays students met with instructors in the Scientific Modeling and Visualization Classroom (SMVC) which like the Virginia Tech CAVE is an ACITC facility.

Things that worked well:

Except for the occasional server downtimes the NPIB and JWave interfaces worked well. Until the final evaluation is completed, conclusions are speculative. From first impressions however, it appeared that the most productive time spent using these modules were when students and instructors met in the SMVC on Fridays. Fridays were more like lab sessions where students could ask questions and try out their ideas out with comments from the professors who helped them interpret the simulation results. This also gave the instructors valuable feedback on how the JWave and NPIB forms were working and what needed to be improved. Friday sessions also built student confidence for successful completion of their homework assignments.

Things that need more work:

Although the NPIB form worked well, the “builder” part of the NPIB was improved with more features but was not stable enough for the instructors to build their own forms. Consequently the technical support team members built all the NPIB forms using a scripting syntax. When completed, NPIB will allow the instructor who is not Java literate more freedom in building their own interactive Java forms. The NPIB form only worked on the SMVC UNIX workstations with Netscape 4.5. Only near the end of the semester did we get the NPIB forms to work on Windows-NT.

Lessons Learned:

Java interface development is a difficult, if not an impossible task, for most professors who do not have backgrounds in computer science. These same professors are also not capable of routine systems administration needed for configuring and maintaining Java-Web servers.

In this class we found that programmers and system administrators need to work more closely than in years past where typically all that was needed was to install a standard language compiler and a user service hot line was created to answer any questions. With the advent of the network, professors and technical support staff can no longer afford to isolate themselves in the new world of computing where standards are like web pages which are always in a state of construction. Successful projects now require that professors devote more time learning computing skills and how to work more closely in teams. We experienced first hand how Java needs to be maintained as a standard: early interfaces developed in IFC had to be rewritten. Our experience in team teaching this class was a rewarding but difficult task. More time was spent solving technical problems than was spent developing course content.

To continue the learning experience, witnessed on Fridays in the SMVC, students need access to the Java-Web server from outside the SMVC. Some universities, because of security issues, prefer to isolate these resources from remote access. Such policies are counter productive when every student is required to own his/her own personal computer and professors are expected to create courseware materials for those students.

Future Developments:

Another course will be taught this spring semester, 2000, at a first year graduate level. As a graduate class the same material can be taught at a more comprehensive level and new simulations of cracks at or near bi-material interfaces will be modeled both at a continuum and atomistic level and comparisons made. The Java-Web server will be upgraded to Jwave 2.0, better security measures will be implemented without restricting access to the anonymous ftp site, and the NPIB builder feature will be completed so that professors can build their own Java forms.

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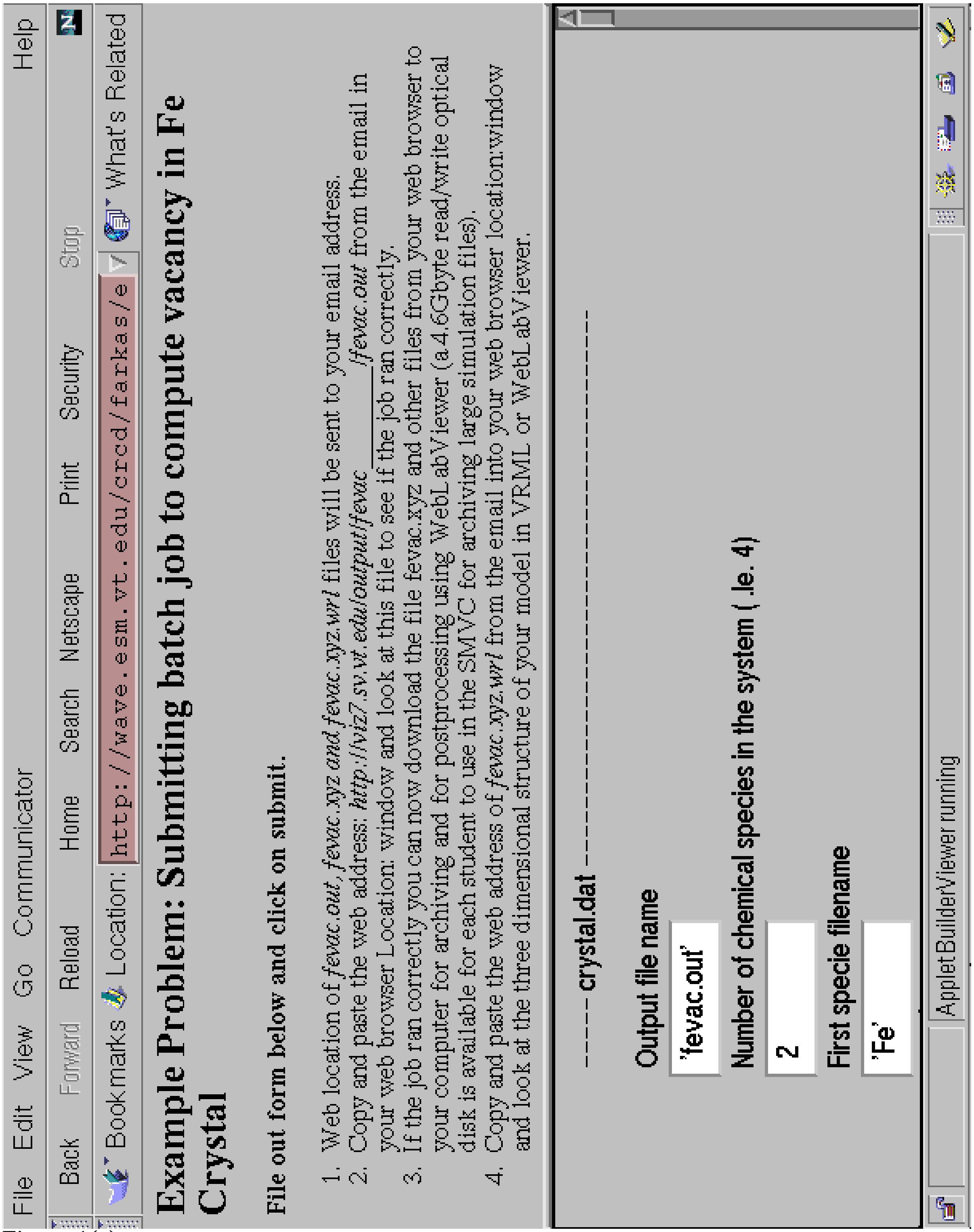
List of Figures

Figure 1. (a) NPIB (Network Programing Interface Builder) form used to create a simulation of a vacancy in an iron crystalline structure with appropriate boundary conditions, (b) navigable VRML file of crystal lattice simulation results showing a vacancy in iron, (c) WebLabViewer image from student homework assignment showing vacancy in iron, and (d) CAVE simulator image of the same vacancy in iron using the same VRML file in Fig. 1 (b).

Figure 2. Interactive JWave interface used by students to investigate how various physical parameters influence stress distribution in a thick-walled cylinder.


File Edit View Go Communicator Help
Back Forward Reload Home Search Netscape Print Security Stop
Bookmarks Location: http://wave.esm.vt.edu/crcd/farkas/e
What's Related
Example Problem: Submitting batch job to compute vacancy in Fe Crystal
File out form below and click on submit.
1. Web location of fevac.out, fevac.xyz and fevac.xyz.wrl files will be sent to your email address.
2. Copy and paste the web address: http://viz7.sv.vt.edu/output/fevac ______ /fevac.out from the email in your web browser Location: window and look at this file to see if the job ran correctly.
3. If the job ran correctly you can now download the file fevac.xyz and other files from your web browser to your computer for archiving and for postprocessing using WebLabViewer (a 4.6Gbyte read/write optical disk is available for each student to use in the SMVC for archiving large simulation files).
4. Copy and paste the web address of fevac.xyz.wrl from the email into your web browser location:window and look at the three dimensional structure of your model in VRML or WebLabViewer.
------ crystal.dat --
Output file name
'fevac.out'
Number of chemical species in the system (.le. 4)
2
First specie filename
'Fe'
Applet BuilderViewer running
Figure 1(a)

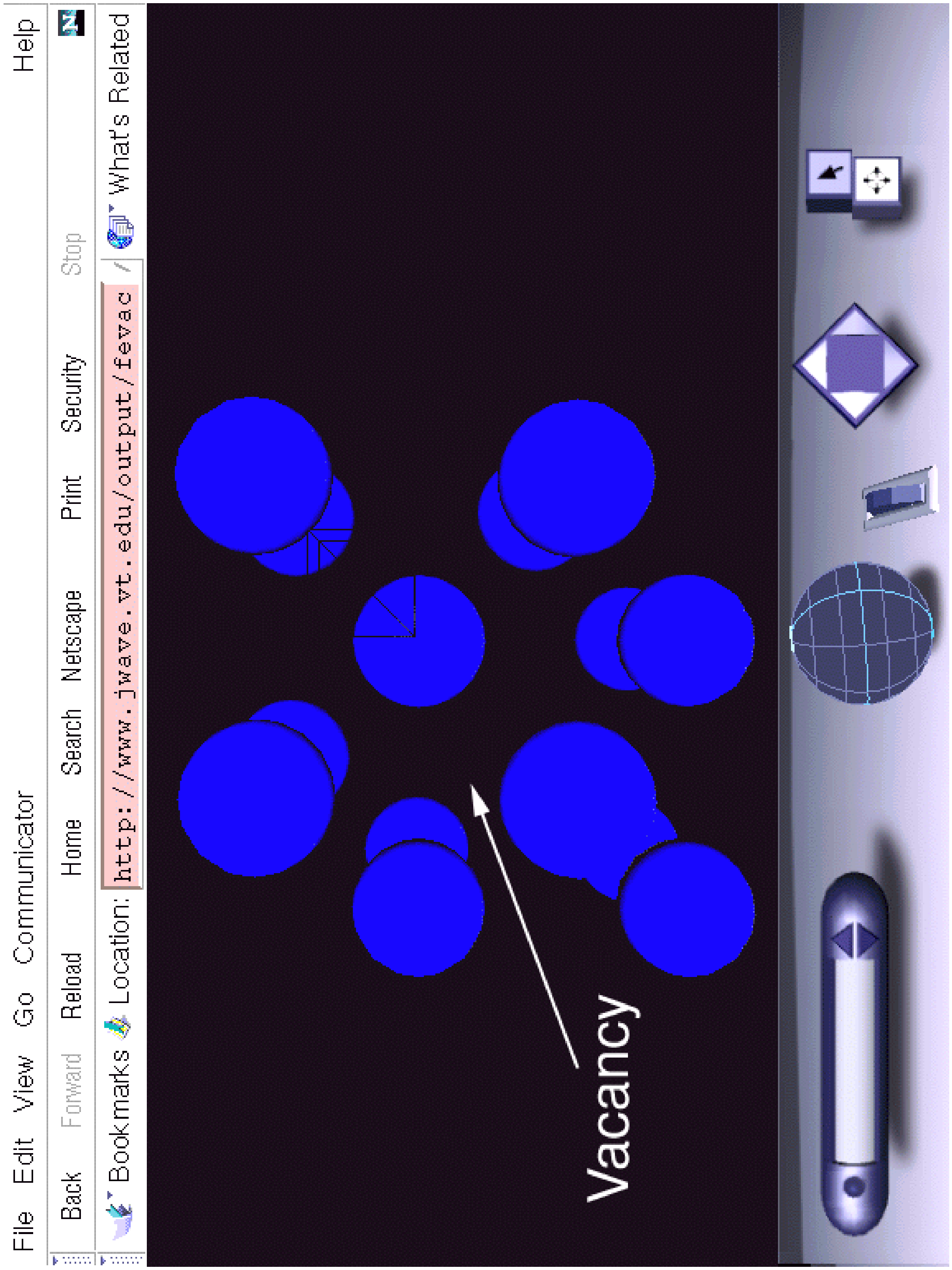

File Edit View Go Communicator Help
Back Forward Reload Home Search Netscape Print Security Stop
Bookmarks Location: http://www.jwave.vt.edu/output/fevac
What's Related
Vacancy

Figure 1(b)

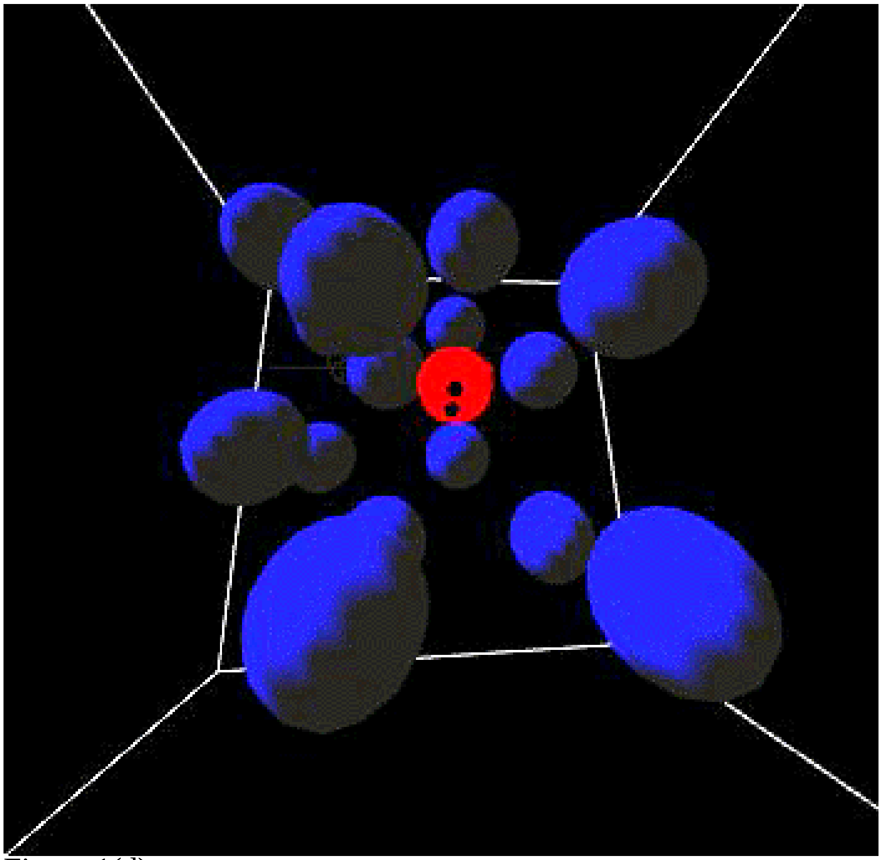


Figure 1(d)

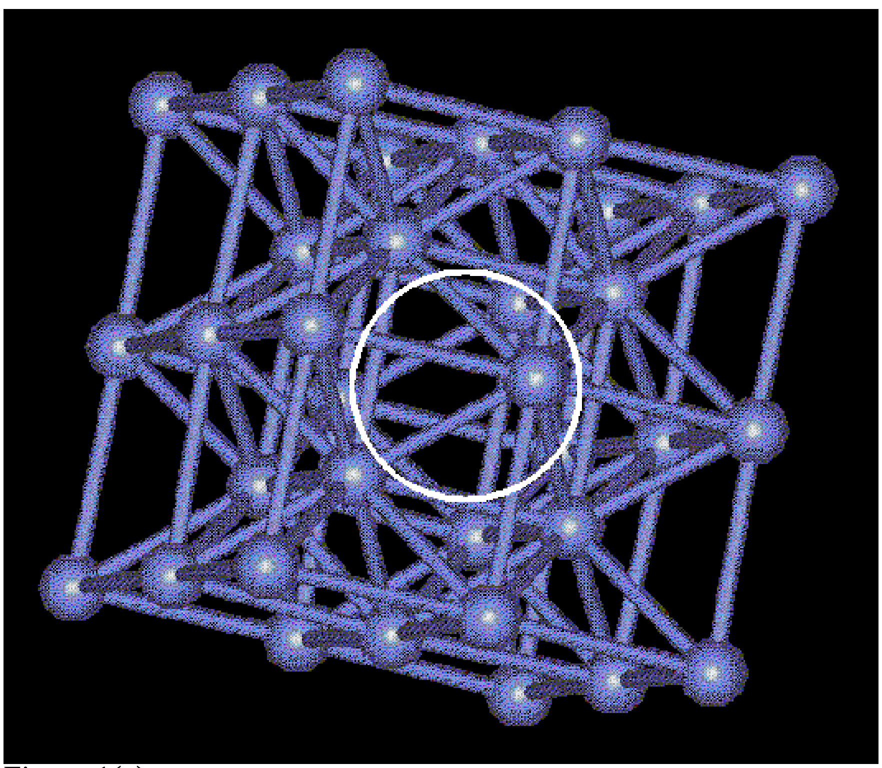


Figure 1(c)

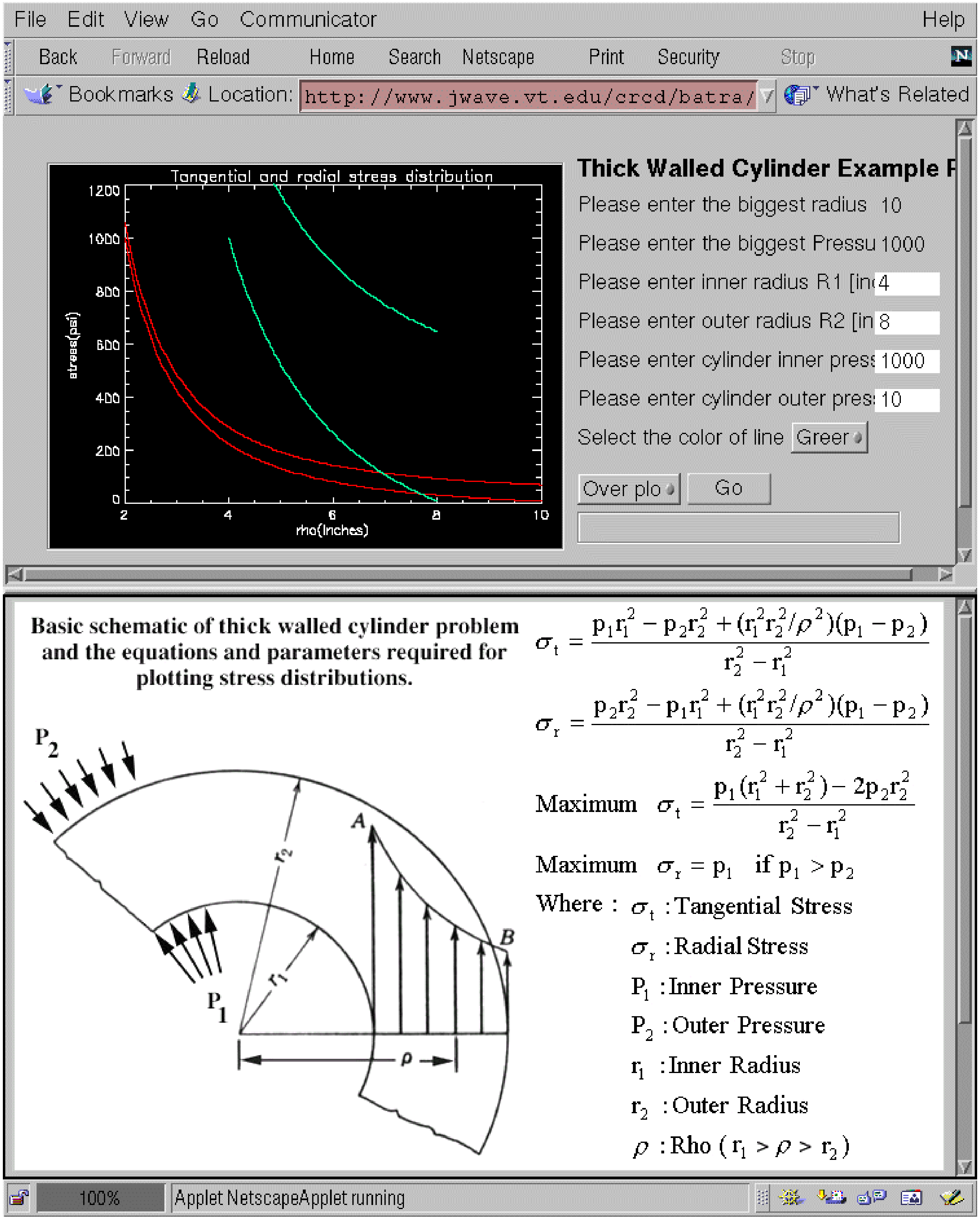

File Edit View Go Communicator Help
Back Forward Reload Home Search Netscape Print Security Stop
Bookmarks Location: http://www.jwave.vt.edu/crcd/batra/ What's Related
Tangential and radial stress distribution
stress(psi)
rho(Inches)
Thick Walled Cylinder Example F
Please enter the biggest radius 10
Please enter the biggest Pressu 1000
Please enter inner radius R1 [in 4
Please enter outer radius R2 [in 8
Please enter cylinder inner press 1000
Please enter cylinder outer pres 10
Select the color of line Greer
Over plo
Go
Basic schematic of thick walled cylinder problem and the equations and parameters required for plotting stress distributions.
P2
P1
A
B
r2
r1
ρ
Maximum
Maximum
Where :
Tangential Stress
Radial Stress
Inner Pressure
Outer Pressure
Inner Radius
Outer Radius
Rho
100%
Applet NetscapeApplet running

Figure 2