

Chapter 13

Extending Measurement Science to Interactive Visualization Environments

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Abstract We describe three classes of tools to turn visualizations into a visual laboratory to interactively measure and analyze scientific data. We move the normal activities that scientists perform to understand their data into the visualization environment, which becomes our virtual laboratory, combining the qualitative with the quantitative. We use representation, interactive selection, quantification, and display to add quantitative measurement methods, input tools, and output tools. These allow us to obtain numerical information from each visualization. The exact form that the tools take within each of our three categories depends on features present in the data, hence each is manifested differently in different situations. We illustrate the three approaches with a variety of case studies from immersive to desktop environments that demonstrate the methods used to obtain quantitative knowledge interactively from visual objects.

Keywords Measurement, Metrology, Visualization, Immersive visualization.

13.1 Introduction

The National Institute of Standards and Technology (NIST) was established in 1901 as the National Bureau of Standards. Although NIST’s mission has expanded over the years, metrology, or measurement science, has remained a central theme. Measurement science has traditionally meant measurements on laboratory data that are made during the course of an experiment. However it is not always possible to perform desired measurements on laboratory data while the physical experiment is taking place. For example, a reconstruction phase may be needed to get the data into a form where it can be measured. An example is tomographic reconstruction, for which a great deal of information in the form of image data has to be carefully filtered, transformed, etc. to yield useful quantitative information. In addition laboratory experiments today are increasingly being replaced by computational experiments. Here, it may be too time consuming, expensive or impossible to do the laboratory experiment, and while quantitative data is typically gathered during

numerical simulations, there are also many reasons why additional measurements may need to be taken during a post-processing stage. Measurements and analyses from within interactive visualization environments provide unique capabilities in this regard.

There are a variety of other motivations beyond pure measurement for adding interactive analysis to visualizations. Computational and laboratory experiments are generating increasing amounts of scientific data, and often, the complexity of the data makes it difficult to devise a priori methods for its analysis. Also, data currently is derived from new landscapes, such as the nanoworld, where we have little experience. There may be ancillary data, from databases for example, that may be required for understanding. Finally, just having the capability at hand to quantify the visualization speeds understanding.

Most visualization techniques excel at providing a **qualitative** view of the visualized data. We are developing interactive measurement and analysis capabilities in desktop, three dimensional (3D) desktop, and immersive visualization environments, that bring **quantitative** data measurement into traditional qualitative visualization. We classify quantitative tools for visualization into three categories as follows:

Quantitative Measurement: These are of two types: (1) interactive measurement tools analogous to physical measurement tools such as tape measures, and generalizations thereof; and (2) interactive tools to measure more abstract properties of data

Quantitative Output: These are tools to perform interactive analyses and represent their output as quantitative data alongside raw data as it is visualized, and

Quantitative Input: These are tools using values or graphs as part of an interactive interface to help drive the direction of a visualization (visualization steering)

With real time qualitative and quantitative visual exploration and interaction, scientists can easily perceive complex relationships in their data, quickly ascertaining whether the results match expectations, and often obtain unexpected answers from visual observation. To support our classification for quantitative visualization tools, this chapter presents three case studies of visualizations at NIST incorporating quantitative tools for use by the domain scientist. In each of these three, the domain scientists played central roles, collaborating with computer scientists to develop visualizations and methods of interaction that produced valuable scientific measurements and insight.

13.2 Related Work

This work is not the first attempt to perform measurements in visualization environments [4, 3, 13, 15, 22, 23]. The most relevant work within immersive visualization environments is described by Reitinger et al. who present a set of virtual reality

tools for making measurements (distance, angle, and volume) for surgical planning [25]. They point out that the virtual environment affords more natural interactions, so the user is able to make measurements more effectively than could be done on a non-interactive system, and this has certainly been our experience. Our work involves the implementation of some similar measurement tools, as well as some novel measurement tools, and incorporates interactive tools for statistical analyses and investigation of the measurement data derived from the 3D scene. Moreover, our toolbox is not specific to any one application; the tools are general and can be moved from application to application.

On the commercial side, simple measurement capability has begun to appear in a variety of software e.g. Acrobat 3D [1], and Amira [19]. On the desktop, measurement of 3D objects requires the ability to directly access any point in 3D space. This 3D desktop capability has existed for years in CAD software, but CAD systems are design tools – the scales of interest are an integral part of the design. In scientific visualization, the investigative scales generally come out of the data, and are not usually designed. This chapter will not address how to build a 3D desktop but rather assumes it exists and describes analytical techniques to gather and understand data in the 3D world. Immersive environments by their nature allow access to any part of space. So measurement in these environments is straightforward. We design our applications to work both on the desktop and immersively.

13.3 Case Studies

A few widely varying examples of the use of a 3D visualization environment to gather new information from data are described below. Each uses one or more of our three types of quantitative techniques that add to the productivity of understanding and quantifying that particular application.

13.3.1 *Tissue Engineering*

Tissue engineering has been identified by NIST as a biotechnology area in which metrological analyses are required to lower the cost barrier for product commercialization. To this end, NIST is developing methods to measure tissue engineered scaffold structures and analyzing scaffolds interactively. Scaffold structure is known to have a large influence on cell response, and this in turn affects the success of the final tissue engineered product. These structures are manufactured and then scanned using X-ray microcomputed tomography. The 3D structure is then reconstructed mathematically. Thresholding enables extraction of the scaffold which is visualized using a polygon approximation. We study the visualization with quantitative methods.

For tissue engineering, we use all three classes of quantitative visualization tools within an immersive visualization environment to determine the fidelity of a manufactured tissue engineered scaffold to a design specification [12]. Each of the quantitative measurement tools places measurement objects into the virtual world that are, in some sense, surrogates for the features being measured. The user interacts with these objects in the immersive environment with a 3D cursor that is controlled by the position of the hand-held motion-tracked wand. The researcher can position and stretch those surrogate objects to fit the features of the data representations under study. The measurement of those features can then be taken from the known dimensions of the surrogates, and the user is able to analyze and interact with those measurements. So far, we have developed three such measurement tools: linear, cylindrical, and ellipsoidal. We envision these tools as the first of a set that will form a general purpose tool-box for the measurement of dimensional quantities in a virtual laboratory.

The linear measurement tool lets the user stretch line segments to measure the linear distance between any two points. This is a virtual tape measure that provides a continuous numeric display of the length while the user is stretching each line segment. The cylinder measurement tool places wire-frame cylinders into the scene which the researcher can move, orient, and stretch in any dimension in order to match tubular features in the scene. The resulting dimensions of the wireframe cylinders can then be recorded to measure these features of the scene. Similarly, the ellipsoidal measurement tool enables the researcher to place wire-frame spheres into the scene. These spheres can then be interactively stretched into any ellipsoidal form and moved and oriented to match features of the scene. The various quantitative features of each ellipsoid can be recorded to measure these features.

All these positioning and stretching interactions are direct manipulations of the objects. For example, the user manipulates a linear measurement by grabbing one end of the line segment (point and click) and moving it to a new location (drag and drop). During the interaction, the system shows a continuous display of the rubber band line segment, with a continually updated numeric display of its length.

As these linear, cylindrical, or ellipsoidal measurements are taking place, a second set of quantitative output tools allows the scientist to analyze the compiled measurements graphically, while they are being gathered. At any time, the user can display a histogram of the current set of measurements together with their mean and standard deviation. Finally, the histogram can be used as a quantitative input tool, allowing the user to sweep out a portion of the histogram and have the system highlight the corresponding line segment measurements whose lengths lie in that portion of the histogram.

This closes the loop between measurement, analysis, and visualization. Here it lets the researcher see the relationship between the spatial location of measurements and their positions in the distribution of measurements. For example, we are able to highlight and examine all fibers whose diameters are less than 30% of the design size to see whether they are spatially clustered within the scaffold. Note also that the highlighting based on interaction with the histogram could be regarded as a form of *brushing* [2]. In the immersive system, this interaction takes place

through a panel that is an element in the 3D virtual scene. Figure 13.1 shows the cylindrical measurement tool with its accompanying analysis panel as it might appear in the immersive visualization environment.

We performed linear measurements both on the “as-designed” scaffold model (generated synthetically from the design) and on the image of the actual manufactured scaffold material in the visualization environment. The former are intended to validate the measurement method, while the latter are used to understand the scaffold structural characteristics and fabrication method. We derived descriptors such as gap width, spacing of fibers, angles between intersecting struts, etc., and compared the results to those from the as-designed scaffold. We found that the inter-junction strut diameter was about 19% smaller than the as-designed model and the at-junction strut diameter (or layer thickness) was about 33% smaller than the as-designed model. However the angular measurements correspond very closely to the design [10].

The manual nature of these measurement tools presents some ease-of-use issues for the user. For example, when making large numbers of measurements in the immersive environment, user fatigue becomes a substantial issue. We also found that it was often difficult to align the surrogate objects with the surfaces that represent the objects being measured. The steadiness of the hand became a factor and many small adjustments were often required to get the desired result. This alignment problem was ameliorated in the immersive environment by interactively

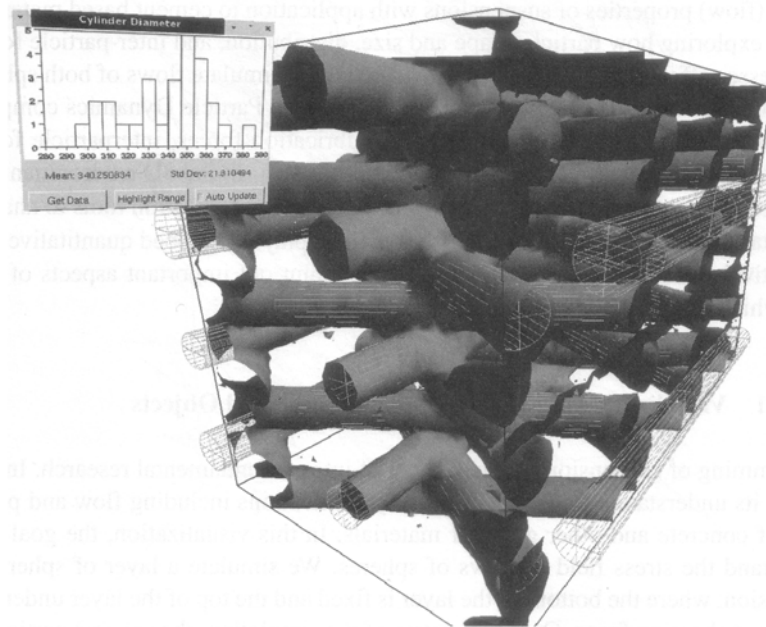


Fig. 13.1 Cylinder measurement and analysis tool used on rendered objects derived from measured data taken from a tissue engineering scaffold (See Color Plates)

enlarging the virtual scene so that small mis-positionings would have less impact. However, it is also important to keep in mind that the (typically polygonal) representations that are displayed in the virtual environment are themselves only approximations of the real objects being measured. The researcher may choose not to place a surrogate object exactly aligned with the data representation based on his or her scientific judgment about how the virtual object approximates the real object.

Researchers reported that interactive measurement of the data provides valuable quantitative information for the scaffold manufacturers and scientists. They were able to look at multiple attributes at the same time, enabling the identification of manufacturing defects. The ability to interactively make physical measurements of objects in the virtual world and to display and interact with statistics derived from these measurements has let researchers efficiently collect and understand the data that they need. These domain scientists identified several areas in which this work could be extended: the integration of a fluid flow simulation to quantitatively understand nutrient transport issues in the scaffold; the imaging of cells growing on the scaffold structure; and inclusion of automated measurement techniques used side-by-side with the manual measurement methods described above.

13.3.2 Flow of Suspensions

This research is focused on advancing our fundamental understanding of the rheological (flow) properties of suspensions with application to cement based materials. We are exploring how particle shape and size, distribution, and inter-particle forces and stresses affect the properties of suspensions. We simulate flows of both spheres and more realistic particle shapes using a Dissipative Particle Dynamics computational model that includes hydrodynamics, lubrication forces, interparticle forces and takes into account the local surface curvature [18]. In the 3D environment, we create both *quantitative input* and *quantitative output* visualization tools to analyze computational output. We use analysis tools to display and embed quantitative data interactively as it is investigated. Visual clues point out important aspects of data from which quantitative information can be derived.

13.3.2.1 Visualization of Stress in Flows of Spherical Objects

The jamming of suspensions is the subject of intense fundamental research. In particular, its understanding is useful for many applications including flow and placement of concrete and other granular materials. In this visualization, the goal is to understand the stress field in flows of spheres. We simulate a layer of spheres in suspension, where the bottom of the layer is fixed and the top of the layer undergoes a constant shearing force. Over the course of the simulation, the spheres participate in multiple small low-stress interactions with neighboring spheres. Our scientist collaborator hypothesized that when the system jams, one or more high-stress

chains would form from sphere to sphere to sphere through the system, possibly dissipating quickly as the system breaks free.

In order to see the stress field, we create a visual representation of the stress value between each pair of spheres (an output of the simulation). As shown in Fig. 13.2, the stress between each pair of interacting spheres is represented as a line. The sphere positions are implied from the line end points. We do not visualize the actual spheres because with their simple, known shape, they would just obscure the important data in the visualization. 3D time sequence animation allows a qualitative understanding of the system stress. As can be seen from the representation of stress in the figure, patterns of the stress can be ascertained visually, illuminating the directions along which the stress is being transferred through the system. The stress chains of the system are of significant importance to the researchers. This quantitative information embedded in our data makes these chains explicit to the scientist during the visualization.

A slider selecting the upper and lower stress values to display gives real time quantitative interaction with the data. This provides the researchers with an interactive

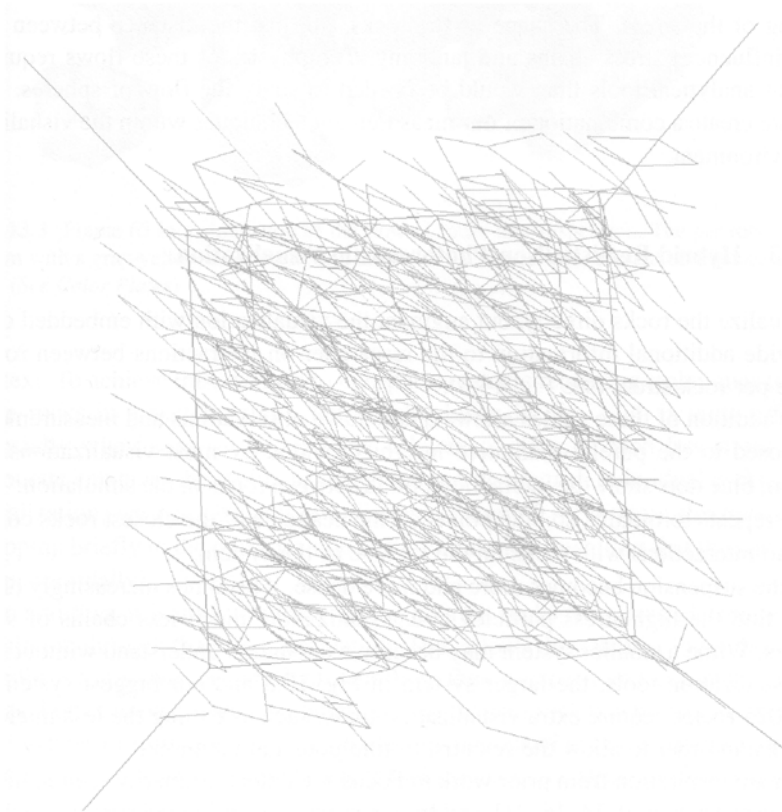


Fig. 13.2 Stress in flows of spherical objects. The spheres are not shown, but are centered at the endpoints of each line segment. Stress chains show the structure of the stress field

tool to visually explore the data by dynamically viewing the stress data through a data window defined by the slider controlled stress range, and allows the user to visually remove the data of low interest and focus on the areas where stress chains and potential jamming/locking occurs.

An example of an identified stress line propagating from top to middle to bottom of the system is shown in Fig. 13.2. Another slider provides control of the animation speed. When a stress chain in the system occurs, it typically exists for a short period of time. A higher animation speed allows for a quick overview of the system. Reducing the animation to very slow or to a full stop allows an identified area and time step to be studied in more careful detail. The capability to focus on particular lines of stress and study them in frame-by-frame detail provides information to the scientist not otherwise available without these visible clues.

13.3.2.2 Visualization of Stress in Flows of Realistic Shapes

Flows of realistic random particulate shapes require new methods to obtain the qualitative and quantitative information needed by the scientists for a full understanding of the stress. The shape of the rocks, not just the distance between the rocks, influences stress chains and jamming. The physics of these flows requires different analytical tools than would be needed to study the flow of spheres. We therefore create a combination of our measurement techniques within the visualization environment.

13.3.2.3 Hybrid Realistic/Non-Photorealistic Visualization

We visualize the rocks directly, but augment the visualization with embedded data to provide additional information to the researcher on interactions between rocks and the per-rock stress (see Fig. 13.3).

The addition of these values allows quantitative observations and measurement, as opposed to the purely qualitative insight provided by most visualizations. In addition, blue dots show the interaction points between rocks in the simulation. The system repeats toroidally, so blue points on the near side of the closest rocks correspond to interactions with rocks on the far side of the system.

As the suspension becomes more and more dense, it becomes increasingly difficult to find the high-stress particles in a visualization, much less chains of such particles. While a smaller system may be simple enough to understand without further visualization tools, the larger system in Fig. 13.3 and our biggest system to date, 2025 rocks, require extra visualization tools, such as culling the less interesting rocks, in order to allow the scientist to find potential jamming.

We gain inspiration from prior work in Focus + Context, primarily seen in information visualization [9, 14, 16, 21], and from non-photorealistic rendering in graphics [7, 8, 17]. In this case, the scientist would like to focus on the highest stress rocks, but still have the indication of the other surrounding rocks to put the total system in



Fig. 13.3 Frame 63 in a simulation of the flow of rocks in a suspension. The per-rock stress is shown with a gray-yellow color scale, and also with a numeric value printed on the face for each rock (See Color Plates)

context. To achieve this, we turn to non-photorealistic rendering techniques to show these rocks in a sketchy style. The result, shown in Fig. 13.4, is quite effective, especially when seen in motion. The coherent motion of each low-stress rock's silhouette enhances the ability to recognize and distinguish individual rocks. In this visualization, we can clearly see a diagonal chain of rocks from the upper right, wrapping briefly to the opposite side of the simulation (recalling that the simulation wraps toroidally).

In addition, it is useful to track the high-stress rocks from a single frame of the simulation through the entire simulation. That allows the scientist to see how those specific rocks move into gridlock, and how they escape it and continue on afterwards. For example, in some simulation runs, a small rock can be seen to move and twist to a new location while larger rocks remain locked in place, almost like working a 3D jigsaw puzzle. Then the larger rocks release, the stress goes down, and the aggregate motion continues.

To assist the scientist in choosing a frame to display, we create a quantitative input visualization tool using a graph of the total system stress per frame as a form

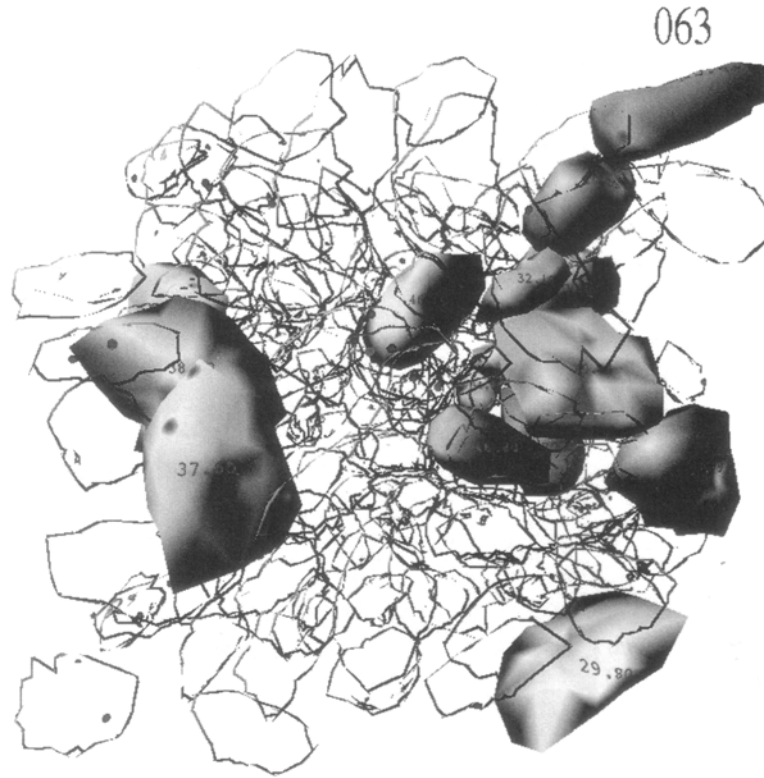


Fig. 13.4 Frame 63 in a simulation of the flow of rocks in a suspension. Lower stress rocks are shown in sketch mode

of slider (Fig. 13.5). The graph is generated in a preprocess using the statistical package [24], and a selection bar is overlaid on top of it. The scientist can drag this selection bar to choose a frame. For example, frames just before a steep drop-off in stress are of particular interest, since they may indicate a time step when the rocks in the aggregate were binding, then one moved to release the pressure. Other interactions with the GUI in Fig. 13.5 enable toggling features of the visualization: closest point spots, stress colors, stress values, and solid/sketchy style transition value.

The sparse visualization of Fig. 13.4 makes it much easier to see and understand the per rock digital stress measurements. The measurement value of total rock stress is centered on the face of the rock closest to the viewer, so as the system is rotated and manipulated, whether on the desktop or in the immersive visualization environment, the text always remains at the correct orientation. Some interactive rotation is generally necessary to see the values on hidden rocks, but with many fewer rocks displayed as solid photo-realistic entities, it is straightforward to find a suitable view to read the data from each rock.

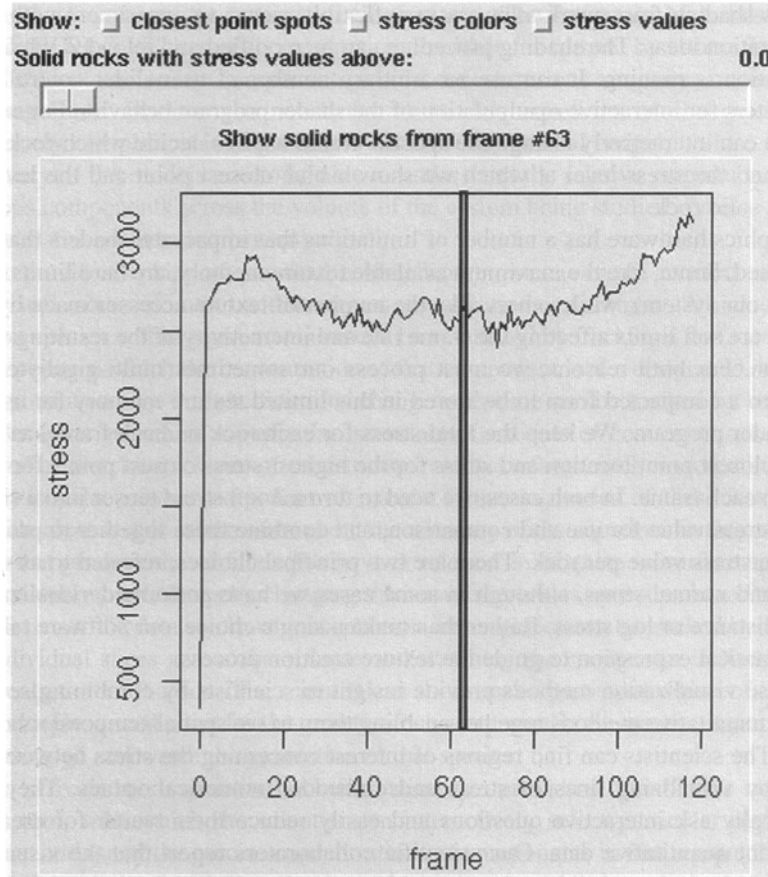


Fig. 13.5 GUI for interactive exploration of the visualization

13.3.2.4 Shading-Based Visualization Environment

This set of visualizations is created with a procedural-shading based add-on to our visualization environment [5, 12, 20]. A shader is a short procedure which determines the color (i.e. shading) and opacity of each point on a surface. Our shaders are written in the OpenGL Shading Language [26] and run in the graphics hardware at each pixel on each rock. This procedure determines the color and opacity of that pixel, referring to the current rock and frame number, position of the pixel on the rock, and data packed into a couple of floating point texture values. This procedure is responsible for creating the sketchy appearance for less important rocks, the stress color scale for solid rocks, placing the spots on the rock surface, and writing the numeric values on each rock.

This shading framework allows a very flexible means to experiment with new visualization ideas. The shading procedure can be modified and reloaded while the application is running. It can use an arbitrary number of user-slider controllable parameters for interactive manipulation of the shader program behavior. For example, we can interactively change the specific frame used to decide which rocks are solid, and the stress level at which we show a blue closest point and the level to show a solid rock.

Graphics hardware has a number of limitations that impact the shaders that can be created. Some, like the maximum available texture memory, are hard limits (512 MB on our system), while others, like the number of texture accesses made by the shader, are soft limits affecting the frame rate and interactivity of the resulting visualization. For both reasons, we must process our sometimes multi-gigabyte raw data into a compacted form to be stored in this limited texture memory for use by the shader program. We keep the total stress for each rock on each frame, as well as the closest point location and stress for the highest-stress closest points for each rock on each frame. In both cases, we need to turn a 3×3 stress tensor into a single scalar stress value for use and comparison, and combine these together to produce a single stress value per rock. There are two principal choices, referred to as shear stress and normal stress, although in some cases we have performed visualization using distance or log stress. Rather than make a single choice, our software takes a mathematical expression to guide the texture creation process.

These visualization methods provide insight to scientists by combining several of our quantitative methods together enabling them to see spatial-temporal relationships. The scientists can find regions of interest concerning the stress between the rocks by visualizing lines of stress and embedded numerical values. They can graphically ask interactive questions and easily reduce their search for areas of important quantitative data. Our scientific collaborators report that the visualizations enable them to validate the physical correctness of the simulation, to detect problems, and to tune parameters of the model. The quantitative displays and interactions also enable the researchers to find and to focus on locations and periods of rapid change in stress.

13.3.3 Cement Hydration

Scientists can also use the 3D visualization environment to test the accuracy of their experimental methods, whether they are using computational or laboratory bench methods. This is an example of an application in which visualization was useful for debugging a complex numerical model. Both physical and graphical measurement tools can be used to understand the model and collect valuable numerical results.

As a basic construction material, it is important to understand the complex properties of cement. Providing strength and structure to a large part of the man-made world, concrete has a complex mechanism for phase changes and development over time once it is poured. Models that can successfully predict the flow, hardening, and

strength of concrete are currently being created. The Inorganic Materials Group within BFRL/NIST has new computational models for cement hydration that track both solvent and solute components whose concentrations vary over many orders of magnitude. Because the new software models equations of change that are extremely complex, it is important to have detailed visual output, both to test the accuracy of the models and to be able to understand the relative magnitudes of the various components across the volume of the system being studied. Precise quantitative visual information is required.

To provide this kind of quantitative visualization, we can create a variety of different visual modes of output within a given visualization environment. A high concentration species within a given volume can be visualized by tracking a surface created from points at which the concentration of that component is at a designated isovalue. Components whose volume fractions change with time can be tracked by watching the decay or growth of a particular isosurface. Gradients of concentrations can be viewed by watching a series of semi-transparent isosurfaces, each representing a different isovalue of the component of interest. Time sequences of these isosurfaces provide clear visible information about the accuracy of the equations in the computations that produce the surfaces. We have developed an adaptive isosurface approach that reveals more features by changing the isosurface values over time based on characteristics of the data set. Low concentration ionic species can be tracked by looking at individual slices across the volume and watching the changes in isolines of the concentration of that ion. The scientist can zoom into a particular region of interest, for example, a seed point for the growth of a new species in the system, and carefully step through and watch the generation of that species.

To provide more quantitative information, we provide a quantitative measurement tool, with which the scientist can interactively select particular regions of interest and query the precise concentrations of components in that region. 2D plots can be brought up in the visualization environment to show the volume fractions of each species at a particular point in space and time during the time analysis. In Fig. 13.6, we see a 3D display of isosurfaces of the various components in the modeled system together with graphs depicting the volume fraction of each component and the values used for the adaptive isosurface display.

The system allows for flexibility in choosing exactly which components and in which sub-volume the scientist would like to generate quantitative information. Testing the accuracy of the models and outputting this type of quantitative information are essential to the understanding of cement hydration. Because of the complexity of the system, quantitative visualization provides a creative way to obtain more information from the output of this model than purely qualitative methods. The ability of scientist to visually query locations of interest within the data and graphically examine those regions helps to narrow the search for important information.

Researchers have reported that these methods provide insight into cement paste microstructure, particularly the 3D spatial relationships among the cementitious compounds. This enables the scientists to: validate the computational algorithms; to gain insight into the chemical relationships among phases (common reactants,

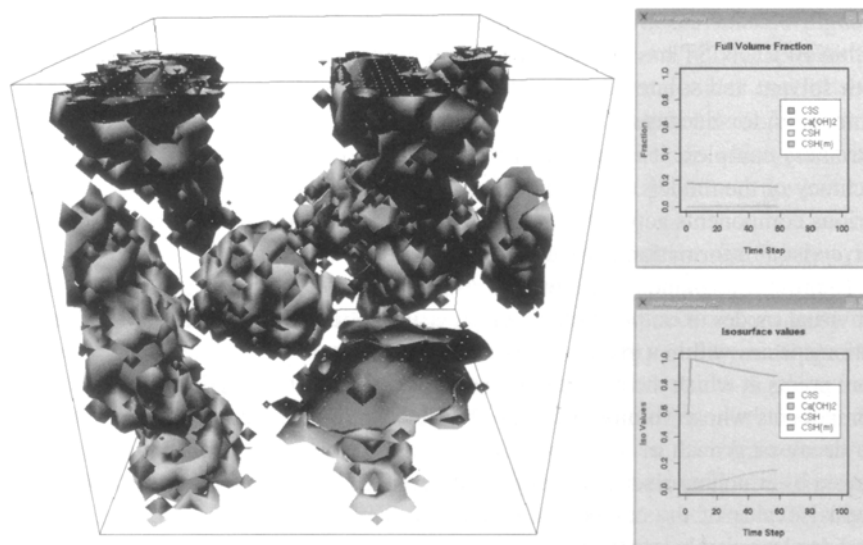


Fig. 13.6 Visualization of the cement hydration model with quantitative displays (See *Color Plates*)

nucleating agents, etc.) based on the spatial proximity that these phases have with each other; and to interpret macroscopic properties of cement in terms of changes in the three-dimensional microstructure. Future work could include the integration of interactive quantitative local chemical analysis, virtual microcalorimetry, the measurement of the thickness of cementitious compounds, and other numeric methods in the virtual environment.

13.4 Summary

Most visualizations excel at presenting a qualitative view of complex data, allowing scientists to quickly make overall judgments and locate interesting features in their data. The focus at NIST on measurement science has led us to introduce quantitative measurement tools into our visualizations. In this chapter, we present a classification of these tools into *Quantitative Measurement*, *Quantitative Output*, and *Quantitative Input*. Quantitative measurement tools allow direct in-visualization measurement of derived quantities such as lengths, volumes, etc. Quantitative output tools analyze the visualized data and present concrete values or graphs alongside the visualization or embedded in it. Quantitative input tools use direct, physically meaningful values or graphs as input to the visualization. These quantitative visualization tools can be used alone or together to enhance traditional qualitative visualizations. Through measurement, visualization can become a more effective instrument for quantitative science.

This chapter also presents three case studies demonstrating the use of quantitative visualizations in collaboration with domain scientists. We present quantitative input and several forms of quantitative measurement for analyzing X-ray micro-computed tomography data of a tissue engineering scaffold. We show quantitative output and several types of quantitative input for flow of particles in suspension. Finally, we present quantitative output and quantitative measurement within a cement hydration simulation. These case studies have shown how the integration of these quantitative methods can direct scientist(s) to otherwise unknown features of interest and then provide tools to single out and analyze those features. These tools allow scientists to view large amounts of numerical data from computational simulations and see subtle problems with the numerical calculations when resulting output has inconsistent features. They also provide data mining information on large data sets, assessing statistically important features in the data.

Future work includes the implementation of additional quantitative interactive measurement and display tools, the application of these methods to non-spatial data [6], and development of methods for analysis and display of uncertainties in the input data and in our interactive measurements. We note that laboratory measurements on physical objects always have an uncertainty associated with them. We will be applying this same standard to measurements and analyses of virtual objects.

Disclaimer Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

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