Visualization Value: Understanding and Developing Smart Materials from First Principles

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The development of "smart" materials is of wide-ranging, significant interest to the Department of Defense (DoD). These materials are aptly named as they inherently sense and respond to changes in their environment.

This ability is the primary reason that smart materials show promise in handling the extreme conditions and stringent requirements of military applications. In addition, there are a great many potential applications for this technology, many of which have remained unexplored.

However, smart materials tend to have complex properties that are difficult and expensive to study and experiment with in the real world. Some sort of computational model is preferable to experimental material design because of the reduced cost and time.

To that end, a method of chemical modeling known as first principles is being used to simulate specific behavior and predict suitable compositions of smart materials for future use. Given the various applications of smart materials, the research described in this article has been narrowed to the following two objectives:

1. Study the salient features of chemical processes on metallic surfaces to reveal the behavior of corrosion and how smart materials can affect corrosion.
2. Analyze the complexities of piezoelectric ceramics, a type of smart material that can be utilized as sensors in SONAR devices.

These two objectives have significant relevance to several branches of the DoD.

The first research objective–in which a smart material could be chemically combined with or used as a coating for a metallic surface and its properties might allow it to prevent or reduce corrosion–is of particular interest to the United States Navy and Air Force.

Both services are engaged in a continual search for new means to reduce maintenance and extend the lifetime of ships, planes, and other vehicles and equipment by limiting the effects of corrosion. The second research objective is of particular interest to the Navy–it could lead to improvements in the understanding of piezoelectric ceramics, which would contribute to the development of next-generation SONAR. Both lines of research are being conducted at the University of Pennsylvania (UPenn) as part of a Naval Oceanographic Office Major Shared Resource Center (NAVO MSRC) Challenge Project.

The researchers have developed a first principles model using a combination of several well-known methods and novel techniques that is both flexible and powerful. Truly understanding the output of such a complex model requires visualization to interpret the large volume of data and discern the potential intricacies within that data. The NAVO MSRC Visual Analysis and Data Interpretation Center (VADIC) provides assistance with the development of visualization applications for this research effort. This article describes how the model output is transformed so it can be visualized, how it was integrated into the software, and the techniques that were used for rendering the visualizations.

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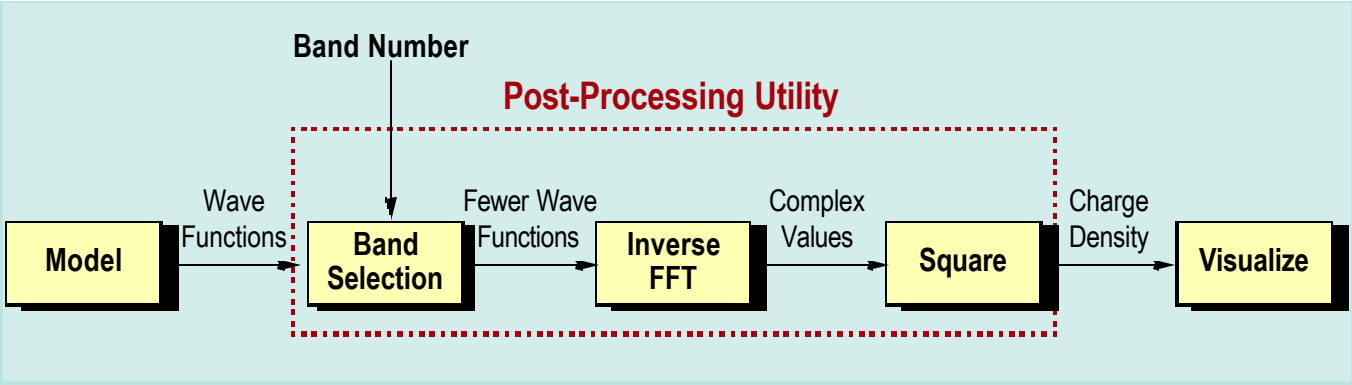

Figure 1. Step-by-step diagram of the Post-Processing Utility.

First Principles and Quantum Simulations

A first principles simulation refers to predicting the behavior of a system from a governing equation without any experimental inputs or fitting.

In this project, the researchers begin with the Schrodinger equation and model the behavior of atoms and electrons starting at the quantum mechanical level. This is a difficult problem computationally and requires the solution of thousands of simultaneous equations.

The model discussed in this article uses Density Functional Theory (DFT). DFT is an accurate and efficient method of simulating electron interactions that uses electron charge density as the basic variable for systems of equations. This is faster than traditional quantum simulations.

The model also uses the Fast Fourier Transform (FFT) to operate in both real and reciprocal spaces, which allows the use of the most efficient computations for a given space.

The direct output of the model is a set of wave functions, given as complex numbers in the reciprocal space. A post-processing utility must be used on this output to produce the desired data for visualization.

A smaller group of the wave functions is culled from the output, based on the electron's energy, enabling the user to focus on electrons participating in important chemical or physical processes. An inverse FFT is performed on this smaller group of wave functions, effectively transforming the data from reciprocal space to real space.

The data points produced by the inverse FFT are still complex numbers, but when squared, produce real numbers that correspond with electron charge density. Figure 1 illustrates this process.

Visualization Software

The VADIC staff is developing a visualization application to examine charge density three-dimensionally. A standard, open-source software toolkit, OpenDX, is used to implement the visualization application.

OpenDX is a flexible software package allowing a wide range of graphics techniques, image processing tools, and visualization methods which are provided as modules in a visual programming environment. Each module performs some operation, such as importing data, processing data, producing visual output, rendering isosurfaces, etc.

These modules are connected together into what is known as a visual program. The connections are made graphically in OpenDX's visual programming editor. Figure 2 is an example of a simple visual program that: (1) imports data; (2) creates an isosurface; (3) colors the isosurface; and (4) displays the results on the screen. Figure 3 is a more complete example that shows parts of the visual program used specifically for this project.

One attractive feature of OpenDX is that it also provides modules that implement user interface components. These modules are placed within the visual program, but also have an interface object that allows the user to type in or select values. The selected values are passed from the output tab of the interface module to the input tabs of connected modules. Groups of interface objects can be arranged together into control panels.

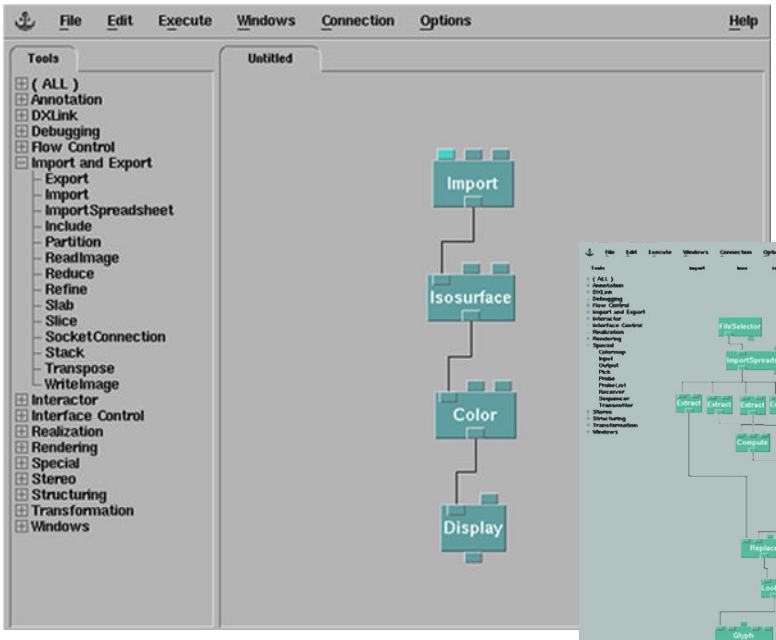

Figure 2. (Above) A simple example of an OpenDX visual program.

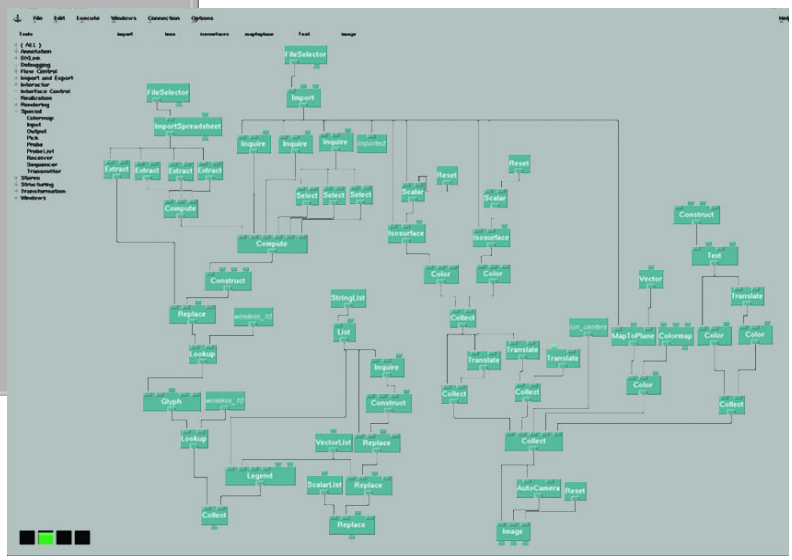

Figure 3. (Right) A more complex example of a visual program.

This allows developers, such as the VADIC staff, to build entire interface systems providing significantly more ease of use for the investigator. Figure 4 illustrates two user interface control panels with embedded interface objects.

Visualization Methods and Techniques

In the case of the UPenn research, one of the investigator's primary interests was to integrate the post-processing utility directly into the OpenDX visual program. This would result in a seamless visualization system that would work directly with the output of the model.

In addition, an interface object could be added to allow the investigator to select the desired band number for the post-processing utility. The post-processing utility was written by the investigator in Fortran90, but since it was compiled as an executable, OpenDX has the capability to execute it as an external program and "pipe" in the program's output. Furthermore, parameters such as file names and band number can be passed to the external program.

For this model, the investigator wanted to use some form of volume visualization to see specific values of charge density over the entire spatial volume of data. Given that requirement, the VADIC staff determined that semi-transparent isosurfaces are an excellent fit for this specific application.

An isosurface is a surface object that is rendered everywhere the data set is equal to a specific value. Figure 5 shows two isosurfaces of specific values, each transparent and with a different color.

The mere isosurfaces are not enough, however. It is helpful for the UPenn researcher to have contextual data in the form of ion center points and sizes. This provides the ability to correlate behavior and features in the data with the locations of certain types of ions. Types, sizes, and a color code for ions can be added via the user interface (the left control panel in Figure 4 shows the ion type lists).

The list of actual ion types and positions is provided by the user as a separate data file. This data file is imported by the OpenDX visual program and manipulated automatically to align with the data set.

The ions are rendered as spheres which are scaled in proportion to the atomic size of the specific type of ion. For further information, a legend can be displayed, indicating which color of sphere represents a type of ion. Figure 6 is an example of one data set with two isosurfaces and a set of corresponding ions.

Researcher Analysis

To understand how these visualizations benefit this smart materials research, it is necessary to consider some of the science that is present behind the scenes. The corrosion processes of Objective 1 occur through a sequence of steps:

1. A molecule, like oxygen, is adsorbed to a surface.
2. This adsorbed molecule disassociates into something more reactive.
3. It then interacts with the surface, resulting in corrosion.

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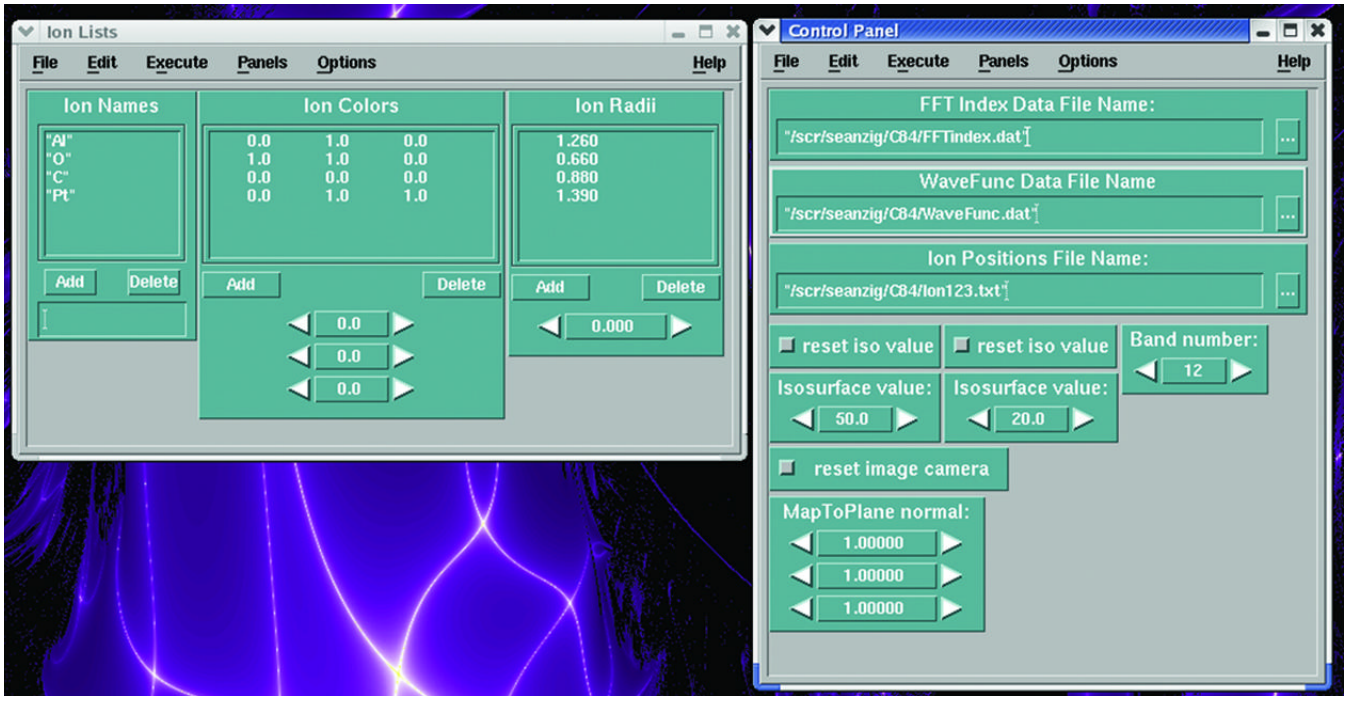

Figure 4. Control panels with interface objects from the visual program in Figure 3.

For Objective 2 the science behind piezoelectric ceramics is in how they respond to changes in their environment. An external mechanical force (such as a sound wave) can deform the crystals, thereby inducing an electric field within the piezoelectric ceramic.

The field can be monitored, resulting in information about the mechanical force that was observed. Conversely, an electric field can be applied to some other type of piezoelectric ceramic, causing it to deform and produce sound waves.

The above-mentioned processes involve the movement of electrons, i.e., a change in the charge density within these materials. An understanding of these fluctuations of the charge density would result in an understanding of either how the adsorption of a molecule occurs (helping with Objective 1) or how a change in piezoelectric response occurs (helping with Objective 2).

Observing charge distribution in such a way can give us a window into how smart materials respond to their environment and what modifications to the material will result in the desired behavior for the chosen application.

With charge density fluctuations in mind, it is often necessary to look at the induced charge density of a material. The induced charge density is simply the change in charge density of a material as a result of altering some external variable.

For example, the induced charge density of a metal surface after the adsorption of a molecule such as oxygen will provide information as to which metal electron orbitals are most involved with the bonding of this molecule.

Once a clear understanding of how oxygen molecules bind to the surface is obtained, it is possible to think of ways to modify the particular orbitals involved in the binding of oxygen to the surface. By weakening these interactions it will be possible to slow down the corrosion processes within these metals.

The isosurfaces of induced charge density displayed in Figures 5 and 6 show specific values of interest to the UPenn investigator. Given renderings such as those, it is possible for a researcher to investigate the bonding of oxygen molecules to metallic surfaces. Additionally, the invaluable contextual information, i.e., the ion center points and sizes, allows the

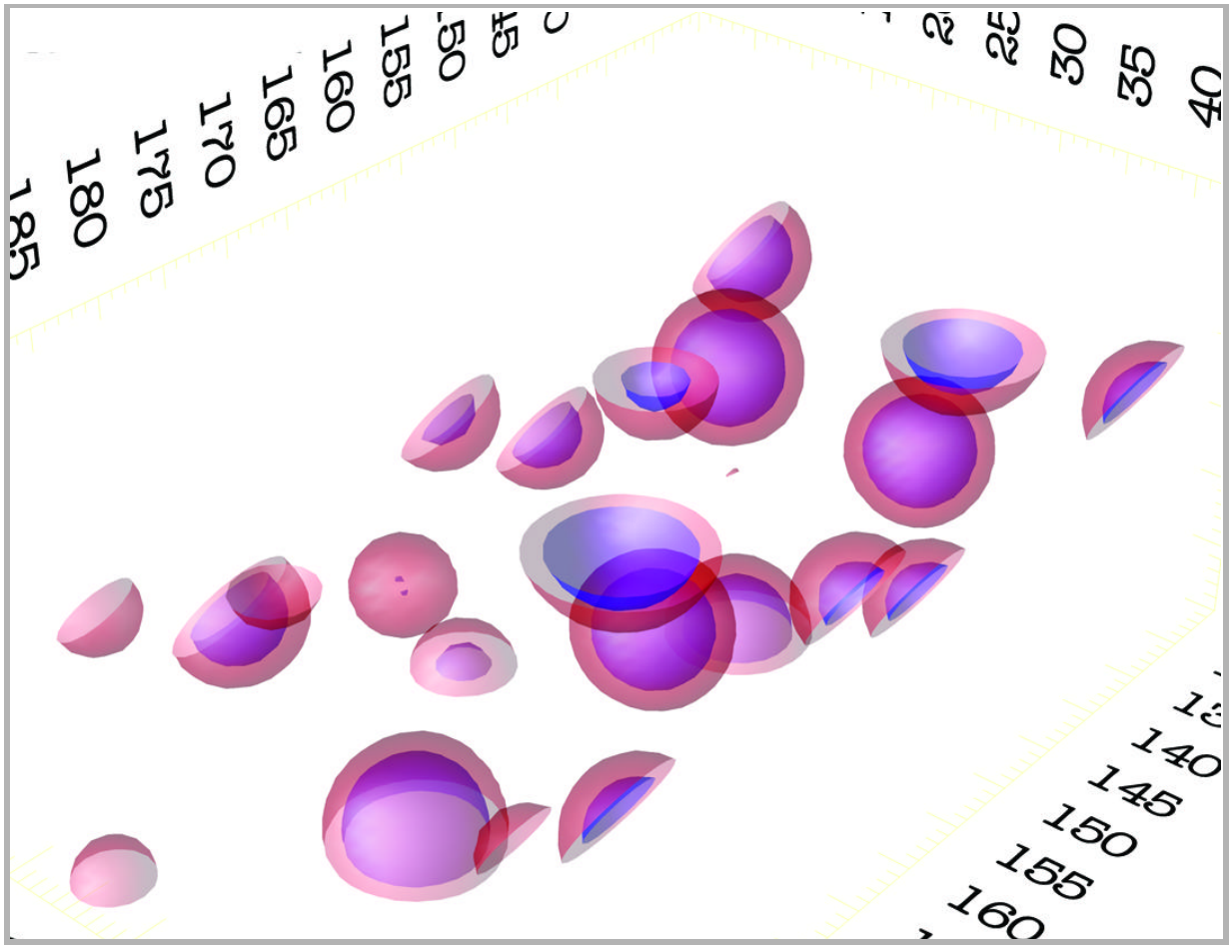

Figure 5. Isosurfaces of value 20 (red) and 50 (blue) respectively.

UPenn investigator to notice where certain interesting features in the induced charge density occur with respect to the oxygen molecules and metal ions.

Unfortunately, an isosurface rendering of induced charge density may not be enough. An example is in the case of oxide supported metal thin film surfaces.

Traditional isosurfaces of induced charge density would compare changes in the charge density of metal atoms in the thin film metal layer (supported on the oxide surface) with that of a block of metal (with no oxide support).

Changes in charge densities in this case would relate to a metal suspended in a vacuum, and not to the block of metal, therefore leaving researchers with misleading information.

For this reason, using band population charge densities is a more useful tool. Each band corresponds to a particular electron orbital within the material. By mapping out these bands, the UPenn investigators expect that it will be possible to look at the charge density changes within a particular orbital and thereby be able to quantify the changes in the orbital as a result of changes in the external environment.

In this is seen the necessity of the post-processing utility discussed previously and shown in Figure 1. Selecting the band number within the post-processing utility should effectively select, from within the data, the induced charge density of a given electron orbital that is of interest to the investigator.

Conclusion

VADIC has provided a unified visualization system constructed within a standard framework.

This system shows a specific variable of interest, induced charge density, with multiple, specific values of interest using semitransparent isosurfaces. Furthermore, integrating the post-processing utility directly into the visualization application creates a system capable of even more flexible and powerful exploration of the data.

This ability has new implications for being able to accurately map out the flow of electrons within a material. The visualization system allows the researchers to investigate these changes, providing new insights into how to design more efficient smart materials.

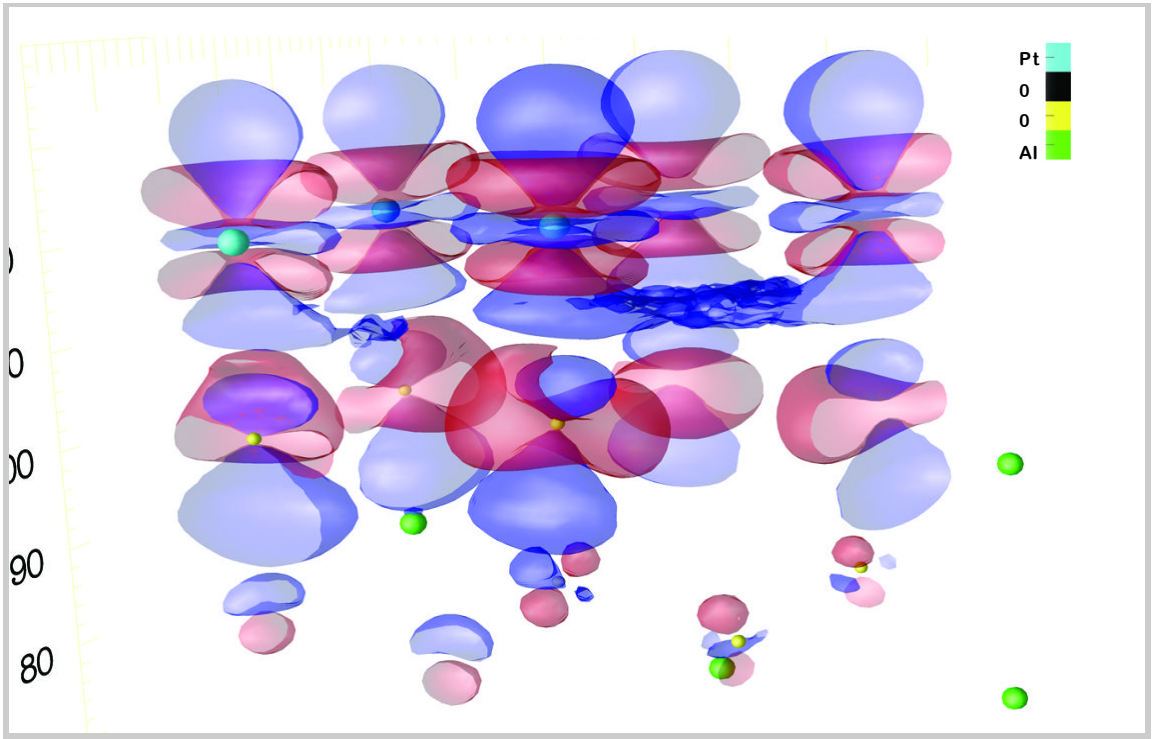

Figure 6. Isosurfaces of value -13.7 (blue) and 17.0 (red) with ions displayed as scaled spheres.

Acknowledgements

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