Debugging Cement Hydration Numerical Simulations using D3.js and a CAVE

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Abstract

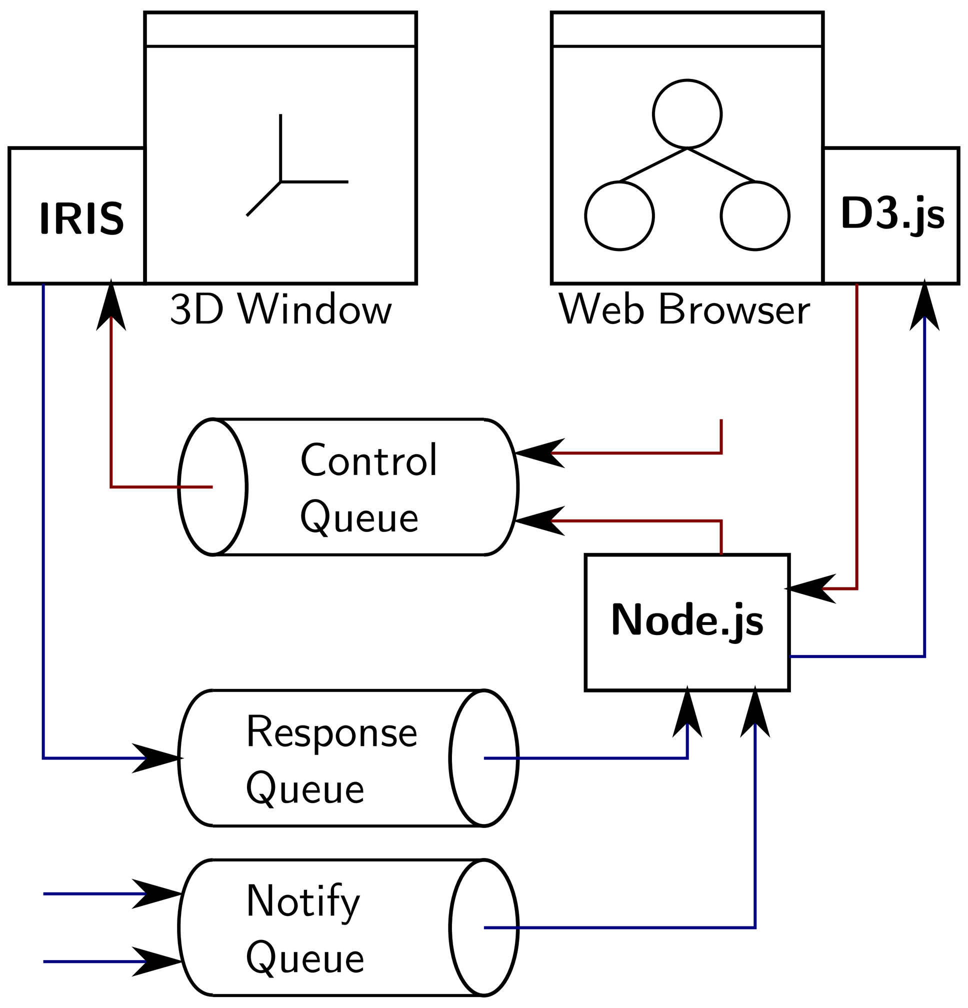
We have created an integrated interactive visualization and analysis environment that can be used immersively or on the desktop to study a simulation of microstructure development during hydration or degradation of cement pastes and concrete. Our environment combines traditional 3D scientific data visualization with 2D information visualization using D3.js running in a web browser. Both the data visualization and information visualization components are interactive and support bi-directional updates.

Introduction

Concrete provides strength and structure to a large part of our world. The cement binder in concrete undergoes multiple interacting chemical and structural changes as it transforms from a liquid suspension to a solid mass. Understanding the nature of these transformations is important for building a sustainable civil infrastructure. The Inorganic Materials Group within the Engineering Laboratory at NIST is developing computational models capable of predicting the flow, hardening, and strength of cement.

To help understand and validate the models, we have developed an integrated interactive visualization and analysis environment for the model outputs. Our environment provides a variety of visual modes to enable precise quantitative measurements and visual information. We also combine 3D scientific data visualization with information visualization using D3.js running in a web browser.

Implementation

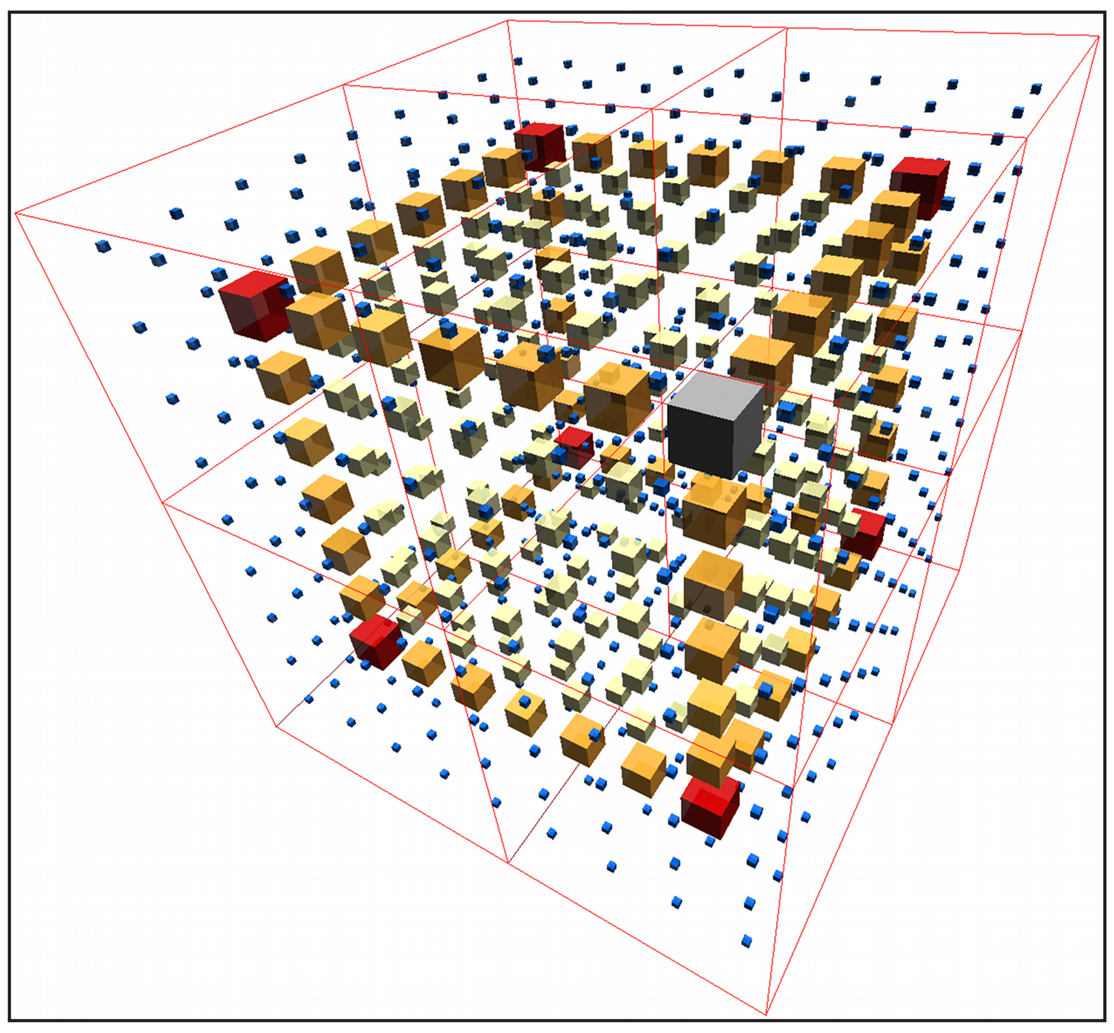


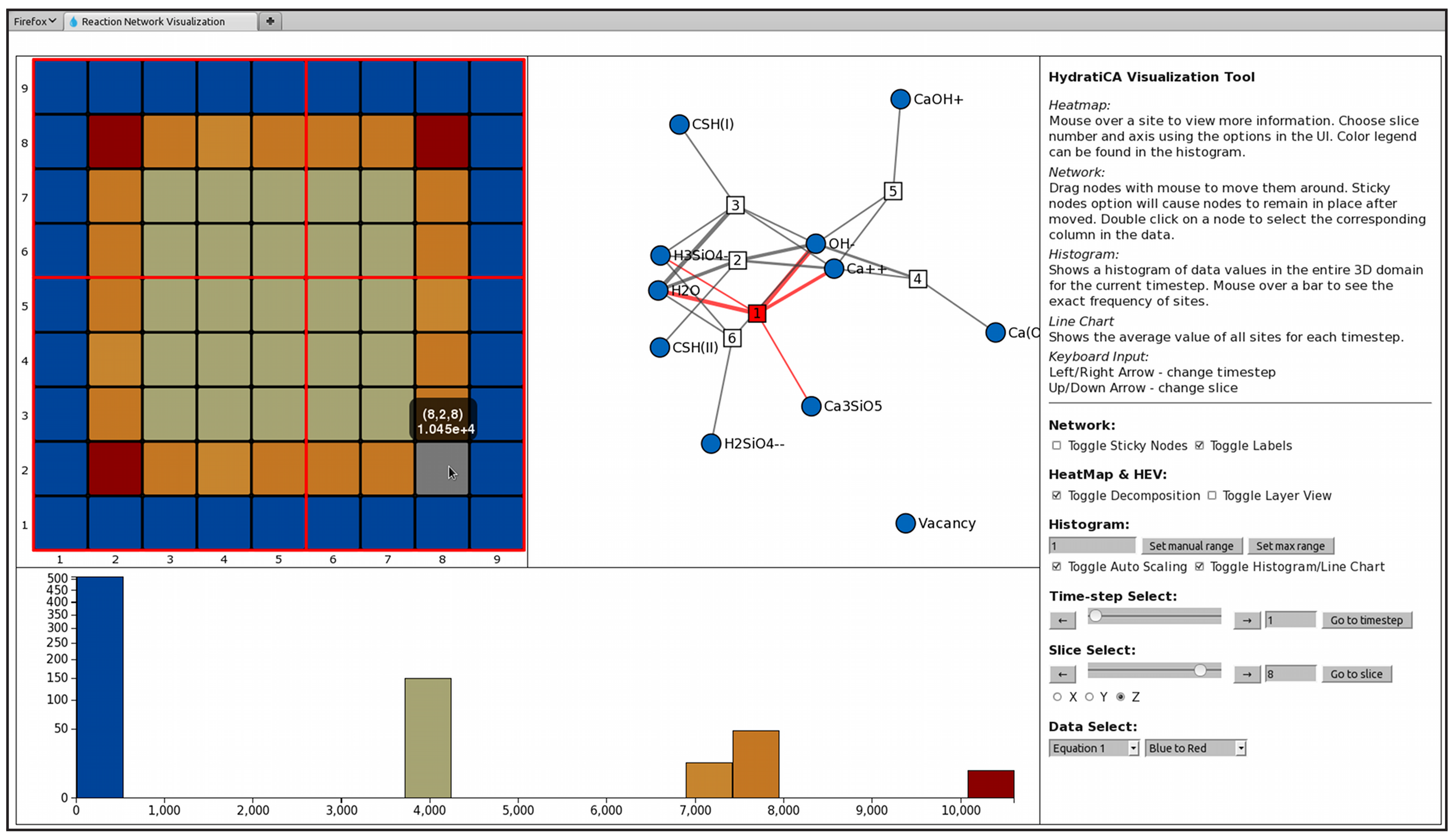
Our implementation, illustrated on the left, consists of three main pieces: 1) **IRIS**: the 3D data visualization component; 2) **D3.js**: the 2D information visualization component; and 3) **Node.js**: the bidirectional communication server. In the figure, processes are illustrated by squares, interprocess communication queues by cylinders, graphical user interface windows by squares with titlebars, and data flow by arrows which are colored based on the specific flow: red for data into **IRIS** and blue for data into **D3.js**.

IRIS is the immersive 3D scientific data visualization. This component runs either in a 2D window on the desktop or in stereo in an immersive virtual environment with tracking. **IRIS** supports a variety of visual modes and interactive tools to make precise quantitative measurements. One specific tool is the probe tool which is used to measure the specific concentrations of each reaction. As the probe tool is moved, **IRIS** updates **D3.js**.

D3.js is the web-browser 2D information visualization. This component is built on top of the D3 visualization library and thus supports any visualization that can be implemented in D3. This specific visualization is a heat-map of the reaction concentrations. As different layers and reactions are viewed, **D3.js** updates **IRIS**.

Results





The figures on the right show the 3D data visualization (**IRIS**) and the 2D information visualization (**D3.js**) windows respectively. The 3D visualization shows the full simulation grid while the 2D visualization shows a single z-layer of the grid. The z-layer of the grid currently being viewed in the 2D visualization is rendered with the same set of colors in both windows. The specific cell that the mouse is hovering over in the 2D visualization is highlighted in gray in the 3D window.

HydratiCA is a parallel simulation of the cement hydration process designed to run on distributed memory machines. The software is parallelized with a spatial decomposition and the boundary layers between the processors are transferred into *ghost* layers for the iterative updates. Recent modifications to the code, however, were yielding questionable results and bugs were also introduced into the checkpointing code. By visualizing the model output in both 3D and 2D (including the specific spatial decomposition shown as red lines in the figures), our combined visualization immediately revealed implementation issues in the computation model, specifically the ghost layers. This issue can be see as the dark blue nodes in the figures, which should be purple. This quickly pinpointed the location in the code that needed to be fixed.

Conclusion

We have presented an integrated interactive visualization environment that can be used immersively or on the desktop and combines 3D scientific data visualization and 2D information visualization. Both visualization components are interactive and support bi-directional updates. Our combined visualization revealed implementation issues in the computational model. These issues were quickly pinpointed by the scientist and the implementation was corrected.

Future Work & Acknowledgements

We are currently extending this visualization into a more general tool that can be used on datasets of varying size and spatial decomposition. This version displays the 2D information visualization directly in our immersive environment. We plan on incorporating a hand-held tablet to display the 2D visualization thus leaving more display space for the immersive 3D data visualization. We also plan on applying this technique to additional data sets. This work used the Extreme Science and Engineering Discovery Environment (XSEDE) supported by National Science Foundation grant OCI-1053575.