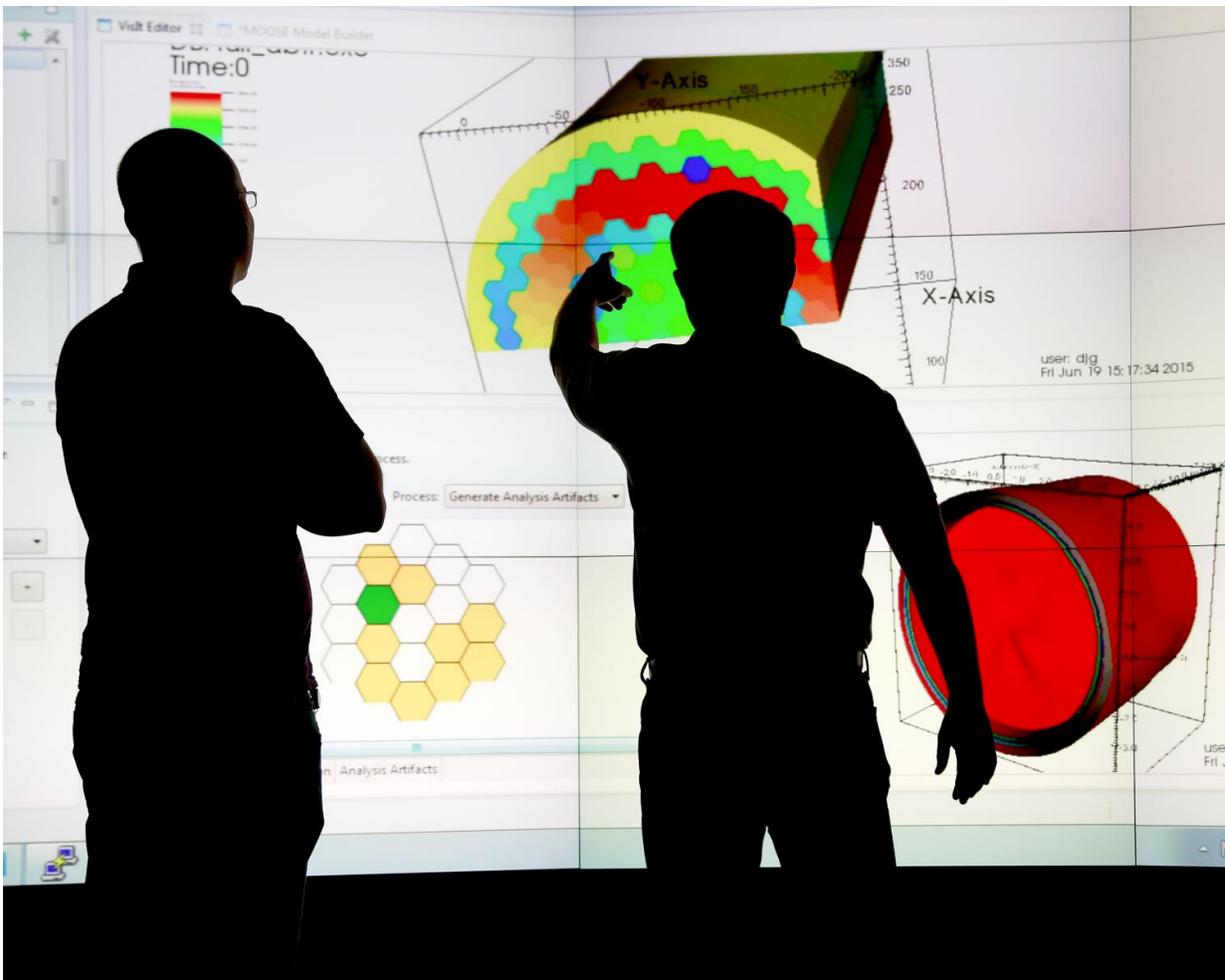


Collaboration yields open source technology for computational science

October 28 2016, by Scott Jones



The Eclipse Integrated Computational Environment (ICE) is a scientific workbench and workflow environment developed to improve the user experience for computational scientists. Credit: ORNL

The gap between the computational science and open source software communities just got smaller - thanks to an international collaboration among national laboratories, universities and industry.

The Eclipse Science Working Group (SWG), a global community for individuals and organizations who collaborate on commercially-friendly [open source software](#), recently released five projects aimed at expediting scientific breakthroughs by simplifying and streamlining computational science workflows.

While computational science has made a great impact across the scientific spectrum, from climate change to astrophysics to genomics, today's data-centric simulation environments require enhanced analysis, visualization, and workflow management to further reduce time to solution and increase the frequency of research breakthroughs. Hence Eclipse's software release.

"Oak Ridge National Laboratory is renowned for its hardware—like Titan, the world's third fastest supercomputer—but we are also leaders in scientific software development," said Jay Billings, the SWG Chair and a research scientist at Oak Ridge National Laboratory. "The Science Working Group has not only helped us create software to simplify complex [computational science](#) but it has also allowed us to become a part of a thriving community that focuses on collaboration, interoperability, and cutting edge research."

That community extends far beyond Oak Ridge into the wider national laboratory complex.

"The Eclipse Science Working Group provides an open, international forum for design and development of critical components of scientific software, bringing together a diverse set of application requirements drivers and software architects to address the challenges of next-

generation scientific computing," said Robert Clay of Sandia National Laboratory.

Likewise, small businesses are also engaged as either members of the group or consumers of its software. Dr. Gerald Sabin from RNET Technologies, Inc., a Dayton Ohio-area firm focused on high-performance computing research noted: "The ICE workflow environment is an ideal platform for us to develop a cutting-edge, cloud-based collaboration environment to support scientific computing. The licensing model and openness of the Science Working Group is to our advantage."

The open source projects, which represent years of development and thousands of users, are the product of intense collaboration among SWG members including ORNL, Diamond Light Source, Itema AS, iSencia, Kichwa Coders, Lablicate GmbH and others. The five projects are:

- The Eclipse Integrated Computational Environment (ICE). Led by Billings, this scientific workbench and workflow environment was developed to improve the user experience for computational scientists and make it possible for developers to deploy rich, graphical, interactive capabilities for their science codes and integrate many different [scientific computing](#) technologies in one common, cross-platform user environment. It is easily extended to new problems and has been successfully deployed for additive manufacturing, advanced batteries, advanced materials, nuclear energy, neutron science, quantum computing, and other areas.
- The Eclipse Advanced Visualization Project (EAVP). Likewise led by Billings, EAVP provides advanced visualization technologies for plotting, geometry and meshing and 3D visualization to address the needs of projects in the working groups. It provides a simple framework for exposing and developing visualization services.

- **January.** Led by Jonah Graham of Kichwa Coders and Peter Chang of Diamond Light Source, this set of libraries was created for handling scientific data in Java. It includes support for n-dimensional arrays, hierarchical data, and 3D geometry and mesh data. Originally created as a spin-off of other group projects to provide a common data structure library, January promises to provide a large portion of the common code base of the group in the future.
- **Triquetrum.** Led by Erwin De Ley of iSencia and Christopher Brooks of the University of California, Berkeley, Triquetrum delivers an open platform for managing and executing scientific workflows. Its goal is to support a wide range of use cases, from automated processes based on predefined models to replaying ad-hoc research workflows recorded from a user's actions in a scientific workbench UI.
- **Chemclipse.** Led by Philip Wenig of Lablicate GmbH, Chemclipse supports users who analyze data acquired from systems used in analytical chemistry. In particular, chromatography coupled with mass spectrometry (GC/MS) or flame-ionization detectors (GC/FID) are used to identify and/or monitor chemical substances, which is important for quality control issues.

The software downloads are available here:

Eclipse ICE -

<https://projects.eclipse.org/projects/technology.ice/downloads>

EAVP - <https://projects.eclipse.org/projects/technology.eavp/downloads>

January -

<https://projects.eclipse.org/projects/technology.january/downloads>

Triquetrum -

<https://projects.eclipse.org/projects/technology.triquetrum/downloads>

Chemclipse -

<https://projects.eclipse.org/projects/technology.chemclipse/downloads>

"Open source is having tremendous impact on both productivity and innovation in industry, government, and academia," explained Eclipse Foundation Executive Director Mike Milinkovich. "The Eclipse Science Working Group is a great example of how world-leading scientific research organizations like Oak Ridge National Laboratory, Diamond Light Source, and others can collaborate on delivering free software that will enable the next major scientific breakthrough. This is an important advancement for the scientific research community, and we are proud to be hosting the collaboration at the Eclipse Foundation."

More information on the Science Working Group is available [on their website](#).

Provided by Oak Ridge National Laboratory

Citation: Collaboration yields open source technology for computational science (2016, October 28) retrieved 10 April 2024 from <https://phys.org/news/2016-10-collaboration-yields-source-technology-science.html>

<p>This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.</p>
--