



OpenEye
SCIENTIFIC



Gaussian, Inc.

OpenEye Scientific and Gaussian Collaboration Expands Quantum Chemistry Calculations

*Gaussian Software now is available on Orion[®],
the only cloud-native molecular design platform*

SANTA FE, N.M., and WALLINGFORD, Conn. – March 8, 2022 – OpenEye Scientific and Gaussian – both of which are leading computational chemistry software companies – today announced that OpenEye’s Orion[®] molecular design platform now is supporting Gaussian and its electronic-structure modeling software with automated scientific workflows to facilitate more rapid and comprehensive quantum chemistry calculations.

The Orion[®] Gaussian Module will help researchers in all fields using electronic-structure modeling software expand their quantum chemistry work by using Gaussian’s programs in conjunction with OpenEye’s Orion platform, which is built on top of Amazon Web Services’ (AWS) high-performance computing (HPC) infrastructure. Using Orion, pharmaceutical and biotechnology companies, as well as any industrial researcher who wishes to perform electronic structure calculations, can gain access to elastic and flexible computational resources in the Cloud.

Users of the Orion Gaussian Module also will enjoy cost savings through the Orion proprietary scheduler, which allows them to monitor computation job expenses in real time and set notifications and cancellation thresholds to lower costs.

Used by scientists globally, Gaussian’s software programs provide a wide-ranging suite of the most advanced modeling capabilities. “Now companies using Gaussian in their R&D, for example in pharmaceutical chemistry or materials science, can solve complex quantum chemistry calculations in OpenEye’s Orion platform without worrying about the cost of adding hardware capacity,” said Dr. Michael Frisch, President of Gaussian, Inc.

Orion is the only cloud-native fully integrated SaaS molecular design platform. The technology accelerates drug discovery science by combining the unlimited storage and computational

scalability of AWS with powerful tools for data sharing, visualization, and analysis in a customizable development platform. Orion features an easy-to-use, web-based graphical interface and sophisticated analysis and reporting workflows.

“Scientists often are limited by the computing resources they have available,” said Anthony Nicholls, CEO of OpenEye Scientific. “This collaboration between OpenEye and Gaussian will ensure customers have the powerful combination of Orion’s turnkey HPC and Gaussian’s world-leading quantum codes. As more and more molecular modeling requires quantum-level accuracy, this is a huge win for the community.”

For more information about OpenEye and its advanced technology offerings, visit www.openeye.inc.

About Gaussian

Gaussian Inc. develops, licenses, and supports electronic-structure modeling programs used worldwide by chemists, chemical engineers, biochemists, physicists, and others working on molecular-level chemical research. Gaussian’s programs enable researchers to study and predict the properties of molecules and reactions under a wide range of conditions, especially those that are difficult or impossible to observe experimentally. Gaussian is headquartered in Wallingford, Conn. For more information, go to www.gaussian.com.

About OpenEye Scientific

OpenEye Scientific is an industry leader in computational molecular design through rapid, robust, and scalable software, toolkits, technology and design services, and Orion[®], the only cloud-native fully integrated software-as-a-service molecular modeling platform. Combining unlimited computation and storage with powerful tools for data sharing, visualization and analysis in a customizable development platform, Orion offers unprecedented capabilities for the advancement of pharmaceuticals, biologics, agrochemicals, and flavors and fragrances. Founded in 1997, OpenEye is a privately held company headquartered in Santa Fe, N.M., with offices in Boston, Mass.; Cologne, Germany; and Tokyo, Japan. For more information, go to www.openeye.inc.

MEDIA CONTACTS:

OpenEye Scientific: Josh Segal | jsegal@punch-pr.com | 617-947-3795

Gaussian: James Hess | jhess@gaussian.com | 203-284-2501