Anaconda + OpenEye Scientific

How Anaconda Helps Power OpenEye Scientific's Cloud-Native Molecular Design Platform

OpenEye Scientific is an industry leader in computational molecular design, based on decades of delivering rapid, robust, and scalable software, toolkits, and technology and design services. Its scientific, physics-based approach to molecular design historically focused on molecular shape and electrostatic potential to inform and guide molecular discovery and optimization. OpenEye now has integrated its applications and toolkits into Orion®, the only cloud-native, fully integrated molecular design platform. Combining unlimited computation and storage with powerful tools for data sharing, visualization, and analysis in an open development platform, Orion offers unprecedented capabilities for advancing pharmaceuticals, biologics, agrochemicals, and flavors and fragrances.

Powering the Scientific Community

OpenEye Scientific turned to Anaconda as a partner because they needed a reliable way to manage Python environments within Orion. At the time, the Python community didn't have an answer for managing dependencies, especially when they require compilation. Other open-source tools for managing Python environments were either too slow, too unreliable, or didn't provide the necessary features such as shared library support and multiple interpreter versions. When looking to embed a solution in its software, OpenEye knew they could turn to Anaconda. "Anaconda is an established leader in Python package management, with a track record of responsible behavior," said Jharrod LaFon, Vice President, Cloud Development, for OpenEye. "It's not just OpenEye; the entire Python ecosystem trusts Anaconda."

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>
> **Jharrod LaFon**
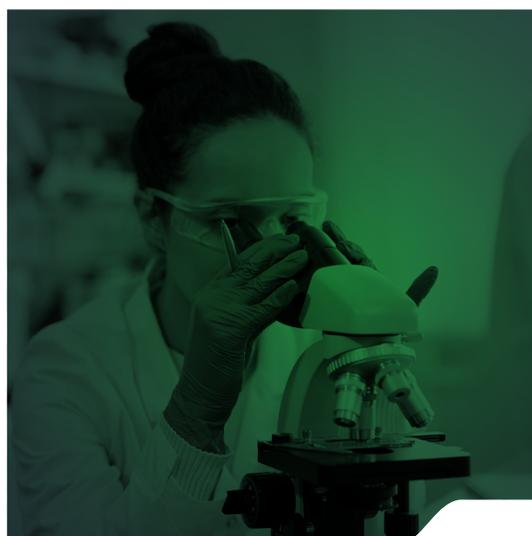> Vice President of Cloud Development

How Leveraging Anaconda Benefits Orion Users

Anaconda embedded in OpenEye's software helps provide reliable and straightforward access to many scientific libraries. "Using those libraries without Anaconda would be quite challenging, and would only be possible for experts who can compile all of their dependencies from source," LaFon said. "The main benefit of including Anaconda as a part of our software is that it allows scientific developers to leverage the entire scientific ecosystem in Orion."

Most importantly, Anaconda makes the experience seamless. "Anaconda has played a key role in enabling novel scientific calculations running on the cloud with Orion," said LaFon. Most Orion users don't notice Anaconda is powering the backend; all they see is their ability to access many scientific libraries, manage conda environments, and use a deterministic dependency resolution.

Creating a Seamless Experience for the Scientific Community

Anaconda provides OpenEye Scientific with a reliable solution for Python package management in its Orion platform. Anaconda allows Orion to utilize Python environments and provide essential features, including computation, storage, analysis, and more. Having easy access to scientific libraries is a powerful benefit for scientific developers working with Orion, and without Anaconda, this would not be feasible. Additionally, Anaconda's seamless user experience plays an invaluable role in contributing to Orion's cloud-native molecular design platform. At Anaconda, we're happy to offer solutions that support growth in the scientific community.

Power your product with proven open-source tools. To learn more about Anaconda Embedded and other partner programs, contact us today.

With more than 35 million users, Anaconda is the world's most popular platform to develop and deploy secure Python solutions, faster. We pioneered the use of Python for data science, champion its vibrant community, and steward the open-source projects behind tomorrow's artificial intelligence (AI) and machine learning (ML) breakthroughs. Our solutions enable practitioners and institutions around the world to securely harness the power of open source for competitive advantage and groundbreaking discoveries. Visit anaconda.com to learn more.