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Cycle Computing Ramps Global 50,000-Core Cluster For Schrodinger Molecular Research 04.19.2012

Utility supercomputing leader facilitates massive cluster for computational drug discovery

NEW YORK, NY – (Marketwire) April 19, 2012 – [Cycle Computing](#) provisioned a 50,000-core [utility supercomputer](#) in the Amazon Web Services (AWS) cloud for [Schrödinger](#) and [Nimbus Discovery](#) to accelerate lead identification via virtual screening. This milestone – the largest of its kind – is Cycle Computing’s fifth massive cluster in less than two years on the heels of a 30,000 cluster in October 2011, illustrating Cycle’s continued leadership in delivering full-featured and scalable cluster deployments. Cycle Computing revealed the cluster creation during today’s opening keynote at the [AWS Summit](#) in New York City.

Schrödinger’s widely used computational docking application, Glide, performs high-throughput virtual screening of compound libraries for identification of drug discovery leads. Computing resource and time constraints traditionally limit the extent with which ligand conformations can be explored, potentially leading to false negative while the same constraints may require a less accurate level of scoring, which can lead to false positives. Tapping into Cycle’s utility supercomputing, Schrödinger ran a virtual screen in collaboration with Nimbus Discovery of 21 million compounds against a protein target. The run required 12.5 processor years and completed in less than three hours.

“Typically, we have to weigh tradeoffs between time and accuracy in a project,” said Ramy Farid, President, Schrödinger. “With Cycle’s utility supercomputing, we didn’t have to compromise the accuracy in favor of faster throughput, and we were able to run the virtual screen using the appropriate levels of scoring and sampling.”

The global 50,000-core cluster was run with [CycleCloud](#), Cycle’s flagship HPC in the cloud service that runs on AWS. Replicating data across seven AWS regions while automating provisioned resources, CycleCloud run time per job averaged 11 minutes

and the total work completed topped 100,000 hours. Schrödinger's researchers completed over 4,480 days of work, nearing 12.5 years of computations in a few hours, with cost under \$4,900 per hour at peak requiring no upfront capital.

“By leveraging AWS, Cycle Computing is able to perform highly sophisticated computations in minutes at a fraction of what it would cost for businesses to purchase the high performance computing infrastructure themselves,” said Terry Wise, Director of Business Development, Amazon Web Services. “Cycle Computing brings an incredible amount of innovation to our partner ecosystem and we're excited to continue working with them to enable businesses to take advantage of AWS's highly scalable, elastic and low cost technology infrastructure.”

Cluster and performance analytics software CycleServer tracked utilization, diagnosed performance and managed scientific workflow. Replicating the success of employing next generation developments, Cycle engineers continued open source strategies, including Condor, Linux, and [Opscode's](#) Chef cloud infrastructure automation system. Cycle's Chef monitoring and analytics plug-in, called Grill, provided visualization into scaling the infrastructure environment and eliminated the need for additional Chef servers with alert technology supporting data around installations, driving down preparation and operational overhead.

Leveraging CycleCloud software and Cycle's HPC proficiency delivered these stats:

- Infrastructure: 6,742 Amazon EC2 instances /58.79 TB RAM
- Global-scale: Multi-datacenter clusters with simple user interfaces
- Cluster Size: 51,132 cores, 58.78TB RAM
- Security: Engineered with HTTPS, SSH & 256-bit AES encryption
- AWS Regions:7 (us-east, us-west1, us-west2, eu-west, sa-east, ap-northeast, ap-southeast)

The end-user experience for using CycleCloud is:

- User Effort: One-click global cluster at massive scale
- Start-up Time: Thousands of cores in minutes, full cluster in 2 hours
- Up-front Capital Investment: \$0
- Total Infrastructure Cost: \$4,828.85/hour

“Researchers can now meet their aspirations and bottom line through secure, mega-elastic and fully-supported utility supercomputers,” said Jason Stowe, founder and CEO, Cycle Computing. “By harvesting the raw infrastructure from AWS, we empower Schrödinger's scientific accuracy while allowing them to push the boundaries of

computation research. Creating robust, reliable and importantly repeatable supercomputers means any industry from life sciences, risk management, quantitative finance to product design can reap the benefits as we tip the scales towards the next generation of massive clusters.”

To learn more about the development of the 50,000 core-cluster and Cycle’s projects leading up to this accomplishment, please visit the Cycle Computing blog: Compute Cycles (<http://blog.cyclecomputing.com/>).

About Schrödinger

Schrödinger is a scientific leader in developing state-of-the-art simulation software for use in pharmaceutical and biotechnology research. The Company’s products range from a complete suite of drug design software employing both ligand- and structure-based methods to general molecular modeling programs. Additionally, the Seurat platform provides enterprise-wide data management, sharing, and visualization. Most recently, Schrödinger debuted BioLuminate for modeling biologics. The predictive power of Schrödinger’s software allows scientists to accelerate their research and development, reduce costs, and make novel discoveries. Schrödinger operates from locations in New York, Oregon, California, Massachusetts, Maryland, Germany, the UK, and Japan. For more information, visit www.schrodinger.com.

About Nimbus

Nimbus Discovery is applying advances in computer-based drug discovery to develop new medicines against important drug targets and thereby unlock fundamental biological pathways. Nimbus has established a first-of-its-kind partnership with Schrödinger, the leader in computational drug discovery, to gain privileged access to cutting-edge technology and exclusive rights to key targets. Nimbus has already delivered selective, potent, and differentiated compounds within the first year for two disease targets that are pivotal in the progression of an aggressive form of Non-Hodgkin’s lymphoma and obesity, respectively. Nimbus has built a virtually integrated, globally distributed R&D organization that leverages an experienced internal drug discovery team across an external network of R&D partners. The resulting organization is scalable, capital efficient and has attracted world-class talent. Nimbus seeks to partner its programs with larger pharmaceutical companies early in the development process allowing Nimbus to focus on its competitive advantage in novel drug discovery. Nimbus programs are held in target-specific subsidiaries under an LLC umbrella. Nimbus Discovery was founded in 2009 by Atlas Venture and Schrödinger, Inc. In 2010,

Nimbus received three Qualifying Therapeutic Discovery Project Tax Credit (QTDP) grants for its programs. For more information please visit www.nimbustx.com.

About Cycle Computing

[Cycle Computing](#) is the leader in [Utility Supercomputing](#) software. As a bootstrapped, profitable software company, Cycle delivers proven, secure and flexible high performance computing (HPC) and data solutions since 2005. Cycle helps clients maximize existing infrastructure and speed computations on servers, VMs, and on-demand in the cloud. Our products help clients maximize internal infrastructure and increase power as research demands, like the 10000-core cluster for Genentech and the 30000+ core cluster for a Top 5 Pharma that were covered in Wired, TheRegister, BusinessWeek, Bio-IT World, and Forbes. Starting with three initial Fortune 100 clients, Cycle has grown to deploy proven implementations at Fortune 500s, SMBs and government and academic institutions including JP Morgan Chase, Purdue University, Pfizer and Lockheed Martin.

About Amazon Web Services

Launched in 2006, Amazon Web Services (AWS) began exposing key infrastructure services to businesses in the form of web services – now widely known as cloud computing. The ultimate benefit of cloud computing, and AWS, is the ability to leverage a new business model and turn capital infrastructure expenses into variable costs. Businesses no longer need to plan and procure servers and other IT resources weeks or months in advance. Using AWS, businesses can take advantage of Amazon's expertise and economies of scale to access resources when their business needs them, delivering results faster and at a lower cost. Today, Amazon Web Services provides a highly reliable, scalable, low-cost infrastructure platform in the cloud that powers hundreds of thousands of enterprise, government and startup customers businesses in 190 countries around the world. AWS offers over 28 different services, including Amazon Elastic Compute Cloud (Amazon EC2), Amazon Simple Storage Service (Amazon S3) and Amazon Relational Database Service (Amazon RDS). AWS services are available to customers from data center locations in the U.S., Brazil, Europe, Japan and Singapore.