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Features

As Microsoft Rolls Out Windows for Clusters, Early Adopters Begin Porting Bfx Apps to New Platform

Next week, Microsoft will begin offering evaluation versions of Windows Compute Cluster Server 2003 — the first version of the Windows operating system designed specifically for high-performance computing.

The product, which has just been released to OEM manufacturers and is expected to be generally available in August, signals the software giant's official entry into the high-performance computing market — and another step in an ongoing strategy to court the bioinformatics sector.

Kyril Faenov, director of high-performance computing at Microsoft, told *BioInform* that the company has identified life sciences as one of its primary markets for CCS 2003. "We're certainly viewing life sciences as the key pillar, together with engineering, as one of the largest markets," he said.

Microsoft said that CCS 2003 will be priced at \$469 per node when it is broadly available in August, but added that prices will vary depending on license and volume.

The release follows the launch of Microsoft's BioIT Alliance, a network of industry partners that will work with the company to ensure that its productivity software tools meet the demands of biomedical research [[BioInform 04-07-06](#)]. Faenov said that the HPC group works "very closely with the team that's driving the BioIT Alliance."

Microsoft is "certainly viewing life sciences as the key pillar, together with engineering, as one of the largest markets."

Microsoft first signaled its interest in the HPC sector with a preview of CCS 2003 at the Supercomputing 2004 conference [[BioInform 11-15-04](#)] and followed it up with a "beta 2" release at Supercomputing 2005 [[BioInform 11-21-05](#)].

The company has maintained for several years that its HPC offering would play a large role in its strategy for targeting the discovery informatics market. Last March, a company official told *BioInform* that Microsoft had been "slow" in approaching life science computing, and said that the firm's "initial play" in that area would be

"in the high-performance computing area to drive value through those areas through clustering" [[BioInform 03-21-05](#)].

The company's goal has been to design an operating system for cluster computing that combines performance with ease of use and integrates easily with other Microsoft tools.

According to several early adopters that *BioInform* spoke to, CCS 2003 lives up to these expectations, although none of these users had yet run performance benchmarks on the operating system against Linux or Unix clusters.

"We have not done any benchmarks — neither numeric nor empirical — but subjectively, [CCS 2003] stays out of the way when you're doing heavy computations, and that's the only thing that's important," said Michael Athanas, a principal at bioinformatics consulting firm the BioTeam.

Ron Elber, a professor in the department of computer science at Cornell University's Computational Biology Service Unit, noted that the system should be useful for end-user biologists.

"Even the wet lab these days, because of genomics, has become data-intensive in many respects," he said. "They need their own high-performance local computing facility, which is relatively small — not necessarily

the fastest on Earth, but something that will include 20 or even 40 nodes and will be able to accept genomics data — and they need it in a way that is very transparent, and that is the advantage of what we see here."

Matt Wortman, director of computational biology and IT at the Genome Research Institute at the University of Cincinnati, agreed that the system should interest scientists that aren't necessarily HPC experts.

"I don't see this replacing Linux in the supercomputer centers — those guys know what they're doing," he said. "It's the folks that are just getting into HPC for the first time, and they're not computer people — it's those people who I think will benefit. So I don't see it replacing Linux in a lot of ways, but I see it opening up a new market."

Microsoft's Faenov said that the company is indeed targeting "departmental and group" deployments for the system — market segments with IT budgets in the range of \$50 million to \$250 million and under \$50 million, respectively.

"It stays out of the way when you're doing heavy computations, and that's the only thing that's important."

Nevertheless, he said, it is important for Microsoft to demonstrate its supercomputing prowess in the highly competitive HPC market, and the firm is shooting for a spot on the next Top500 supercomputing ranking. Faenov did not disclose details of the Top500 run, but noted that all of its potential HPC customers "want to make sure that they have the headroom and scalability and that the vendor knows what it takes to build large-scale systems, and that's certainly where we'll have proof points to demonstrate that."

The operating system actually debuted on the Top500 list last November when a 660-processor Dell PowerEdge cluster at the Cornell Theory Center reached the No. 310 spot.

Where are the Apps?

One challenge for Microsoft in the bioinformatics HPC market is a dearth of life science applications that run on the new operating system.

Broad adoption of the platform in the life science market "is really going to require third-party applications to become available, or a nice open source bioinformatics package," Wortman said. "It's really going to depend on the availability of those applications."

However, he added that it's probably "just a matter of time" before these applications start emerging. "Part of the reason there are no applications is because [CCS 2003] hasn't been released yet, but I think that once it's been released — and because a lot of the bioinformatics programs are open source — I don't have any doubts that these things will appear quickly."

In fact, Elber's lab at Cornell's CBSU has begun porting a number of bioinformatics applications to the new platform that it intends to make publicly available. Several such applications, including P-Blast, P-HMMer, P-IPRSCAN, MrBayes, and MDIV, are already available for CCS 2003 via a web-based interface (<http://cbsuapps.tc.cornell.edu/index.aspx>).

Jaroslav Pillardy, senior research associate at the CBSU, said that his team plans to upgrade InterProScan to the newest version in around two to three weeks, and to port LOOPP and MKPRF to CCS 2003 shortly.

In addition, the BioTeam has ported its iNquiry suite of open source bioinformatics analysis tools to CCS 2003. Athanas said that the package will be ready to ship when the operating system is broadly available.

Athanas said that porting iNquiry to the Windows platform was straightforward. "It's a very different

platform than what I was used to, in terms of a Unix platform, but once I learned how to approach the platform, I found it to be very powerful in terms of development and ease of integration," he said.

The University of Cincinnati's Wortman agreed that it was "pretty easy" to port a Linux application to CCS 2003.

Wortman cited a number of other advantages of the Windows system. "We only use Linux and Unix for things that we have to," he said. "Our entire security and identity management is based on Windows, so it's kind of a pain to have these few very expensive complex machines that are not Windows in our environment."

In addition, he said, "the more heterogeneous my environment, the more support people I need. Linux HPC support people are expensive, and so far the computer cluster is just like any other part of our Windows domain. The guy who's managing it now doesn't have HPC experience, and that was key."

While Microsoft is going head-to-head with Unix and Linux in the HPC market — and will certainly find many entrenched Linux users in the academic bioinformatics sector — Faenov said that he has been pleasantly surprised to find that many academic researchers are actually "very agnostic in terms of their platform — they just want to get their research done."

Faenov acknowledged that there are many labs that "have access to graduate students that have computer science expertise and they can really spend the time building up a Linux cluster from scratch and make the necessary modifications and figure out which MPI stack to run and how to configure the job scheduler and what's the proper security model," but noted that "a lot of folks just want to get their science done, and it becomes a very attractive proposition for them to use a familiar environment and drop in a cluster they can get up and running pretty quickly with their existing skill set."

— *Bernadette Toner* (btoner@genomeweb.com)

Proteomics Software Vendors Applaud PSI and ISB's Plan to Merge mzData, mzXML Formats by Year End

It's a familiar adage in the informatics world that the great thing about standards is that there are so many of them. But that way of thinking is about to change in the proteomics community, which has released a roadmap for merging two leading mass spec data formats into one.

Last week, the Human Proteome Organization's Proteomics Standards Initiative issued a list of deliverables that should enable the new format to be completed by the end of 2006. The format, called dataXML, will include features from two mass spectrometry data formats currently in use: mzXML, from the Institute for Systems Biology; and mzData, from HUPO-PSI.

The merger of the two formats is expected to alleviate some confusion in the proteomics community that some view as a barrier to adoption of either mzXML or mzData.

"It was very important to have HUPO-PSI and ISB agree to this because they're both seen as the leading groups in proteomics data standards, and one issue with the data standards today was just a bit of unclarity," James DeGreef, vice president of product management at GenoLogics, told *BioInform*. "Is mzXML going to be the de facto standard, [or] is mzData the community-supported standard? And it sort of made it difficult for large software vendors to get behind and support one or the other or both."

"It was very important to have HUPO-PSI and ISB agree to this because they're both seen as the leading groups in proteomics data standards, and one issue with the data standards today was just a bit of unclarity."

DeGreef added that for many software companies, particularly large ones, "reducing the risk of choosing the wrong format is very important, especially as people have big ISO processes around quality assurance that they have to meet. So it's not an easy decision going one way or the other."

Like with most bioinformatics firms that specialize in proteomics, it made sense for GenoLogics to support both formats, so the company's flagship Proteus software is compatible with both mzData and mzXML. Nevertheless, DeGreef added, "it will help to just support one." In addition, he noted, for larger software firms with a broader focus, or instrumentation vendors, "they wouldn't want to support two. They only want to support one, and because there were

two, they support none."

Echoing DeGreef's comments was Adam Rauch, a software developer at proteomics software consultancy LabKey and an affiliate of the Computational Proteomics Laboratory at the Fred Hutchinson Cancer Research Center.

"Right now, there's some confusion in the marketplace over, 'Should I do mzXML? Should I do mzData?' And traditionally when that happens, people do neither. They just kind of wait," Rauch said. "There are some tools that use mzXML, there are some tools that use mzData, but a lot of vendors of instruments and software are just sort of in a wait-and-see position. So having a single standard out there basically gives no one any excuses anymore."

Rauch said that while maintaining software for two formats isn't technically difficult, it can be a "distraction" for many labs. As an example, he said that the Fred Hutchinson Center has a new mass spec instrument, "but it doesn't export in mzXML, which is what our whole system uses right now." While the CPL team is working on a way to convert the data from the system into mzXML, "it's really provided a bit of a roadblock," Rauch said. "They could be using the machine and doing high-throughput data analysis today, but they're not because of this file format problem."

Why Two?

Brian Pratt, vice president of informatics at Insilicos, described the existence of two very similar — yet incompatible — formats within the relatively small proteomics community as a "historical accident."

Randy Julian, chairman of HUPO-PSI's mass spec working group, explained that the two standards were developed with slightly different goals in mind, at around the same time. HUPO-PSI very much wanted to ensure that its mass spec format was compatible with broader XML-based standards being developed by the American Society for Testing of Materials, and also wanted to create an interchange format that would work across different labs. "So the task of the group was to bring in instrument vendors and to do what was necessary to make it easy for the formats to be supported by the instrument manufacturers," he said.

"There are some tools that use mzXML, there are some tools that use mzData, but a lot of vendors of instruments and software are just sort of in a wait-and-see position. So having a single standard out there basically gives no one any excuses anymore."

The result was mzData, which a number of vendors — including Thermo Electron, Applied Biosystems, Agilent Technologies, Bruker Daltonics, Waters, Matrix Science, and Kratos — have since pledged to support.

ISB, meanwhile, was using several mass specs from a number of different vendors and needed a neutral exchange format to move data through its analytical pipeline, and it needed it quickly. Thus mzXML was born.

While the two groups kept abreast of each others' activities — and Julian stressed that "there was never a disconnect, there was never a rivalry between the two standards" — there were some important differences.

"Some of the techniques that were used in the early versions of mzXML were really designed to optimize its use in the lab, and they really inhibited the ability to interchange data using that format," Julian said. "They used some very specific non-XML types of technologies that both the vendors and the academic groups that we had assembled viewed as a little bit dangerous if you're asking multiple groups as a community to create these files."

On the other hand, within a single lab like ISB, mzXML offered better performance, making it a better option for some users.

Since the two standards initially emerged in 2004, they have actually begun growing closer together, Julian noted, "so by the time that mzXML 3.0 came out this year ... if you took a hard look at what the differences were, technologically, between the two formats, those differences weren't big enough to warrant having tools being built off of two different, roughly identical formats."

Recognizing this trend, the two groups agreed last summer to merge the two formats, and finalized the roadmap at a PSI workshop in San Francisco in April. HUPO-PSI officially released the roadmap at the American Society for Mass Spectrometry conference in Seattle last week (*see below for further details on the roadmap and the dataXML format*).

Will Vendors Adopt it?

The new standard is welcome news for those instrumentation vendors who have already committed to supporting mzData, and is expected to drive adoption among those who are still on the fence.

Sean Seymour, a staff scientist in the mass spec R&D group at Applied Biosystems/MDS Sciex, noted in an e-mail message that the converged mzData and mzXML format will offer definite advantages for mass spec

vendors. "Although all vendors are now supporting the HUPO-PSI format, mzData, many of us have customers who are also using tools that require the ISB format, mzXML. Regardless of what portion of people use one or the other, this effectively doubles a vendor's development and support costs."

Seymour added, "All vendors are in agreement that a single standard is the right thing to do scientifically, and it's equally wasteful for all of us to spend on supporting multiple 'standards' instead of putting that money toward developing better technologies."

Erik Nilsson, president of Insilicos, noted that the field is in "an unprecedented age of productivity in mass spec instrument development, and people [won't] want to do new support for instruments twice if they don't really have to, so I think that having one standard that everyone is behind is going to drive faster adoption by the instrument companies."

LabKey's Rauch said that vendor buy-in is especially important for new instruments, because it's difficult for software developers to keep up with them. "There are converters from these vendor-specific formats into mzXML, but they don't cover every last machine that's out there. And new machines come out, they change their binary proprietary formats, so the converters have to change," he said.

Researchers want a single format that works out of the box and can be integrated with legacy analytical pipelines, Rauch said. "When we make recommendations to our clients, that's one of the things that we're going to recommend. Near the top of the list is exporting to this [format], being able to get the results quickly and easily in this common format. And instrument vendors that lag in that area are probably going to face some difficulty in the marketplace," he said.

— *Bernadette Toner* (btoner@genomeweb.com)

Best of Both Worlds? A Closer Look at the Planned dataXML Format

Randy Julian, chairman of HUPO-PSI's mass spectrometry working group, told *BioInform* that dataXML is expected to include the best features of mzData and mzXML, while eliminating some of the drawbacks of each one.

One difference between the two, he said, was that "in mzXML it was very easy to tell whether or not the file was valid, but it meant that you had very frequent revisions of the file format, which meant that there were lots of variants of the file out in the field, and people complained about that."

On the other hand, with mzData, "while we have not changed the file format in over a year, we had controlled vocabulary terms and so it's possible to create a 'correct' XML document, but somehow leave out an important controlled vocabulary term, like an instrument variable that's required to understand what's in the file."

In order to address this particular issue, the merged standard will include validation programs that take a file that describes an accepted nomenclature file for mass spectrometry, "and then combine that with an understanding of what the minimum expectations are about what gets reported, and determine whether or not a particular XML file has everything that it needs, and is in fact a valid file and can be read in without fear."

The merged format will also use IUPAC standard nomenclature for describing features of the spectra and features of the instrument, and will be developed with an eye toward digital signatures for clinical proteomics, biomarker discovery, and other research that may at some point be subject to regulatory approval.

The standard will also have "the performance characteristics of mzXML," Julian said. "It will have binary data integrity signature capability as well as binary pointers into individual spectra, which will make it perform almost as well as the vendor-proprietary file format, but instead of using a custom mechanism for doing that, we intend to use XML standards."

The format will also be compatible with new standards being developed for the Semantic web, Julian said, although he added that specific decisions along those lines have yet to be made.

Brian Pratt, vice president of informatics at Insilicos, said that while the "smithing" of the standard may be challenging, the implementation of it should be "pretty simple."

The primary difficulty in the process, he said, "is that every instrument manufacturer has something that makes their machine unique, that gives them a competitive advantage. So how do you describe in a single format all these different small variations? And that's a process that can take a while to put together because you do want to make sure that no one's been left out."

However, he noted, "once all that's been ironed out and all the big players agree that, 'Yes, we feel this format will describe what our instrument can do,' then for the software developer to implement readers and writers — that's not really a big deal."

As far as the timeline for the new format, HUPO-PSI plans to have a UML data model and ontology models ready by August; and documentation, a draft specification of the schema, and an API in place by September. By December, the group plans to have binary indexing and signature programs, a validation program, and reference implementations of converters available.

— *BT*

FDA and Pharsight to Collaborate on Drug-Disease Modeling Repository Under Critical Path Initiative

Drug-development informatics firm Pharsight said this week that it has signed a Cooperative Research and Development Agreement with the US Food and Drug Administration's Center for Drug Evaluation and Research to develop a data repository that will support drug-disease modeling within the agency.

The project falls under the FDA's Critical Path initiative, which has highlighted computational modeling and simulation as areas that it expects to help speed drug development.

Under the terms of the CRADA, for which financial details were not disclosed, FDA will use a number of Pharsight's software products for analyzing, storing, and managing pharmacokinetic/pharmacodynamic data, including Pharsight Knowledgebase Server, PKS Validation Suite, WinNonlin Validation Suite, Drug Model Explorer, and Pharsight Trial Simulator.

Mark Hovde, senior vice president of marketing at Pharsight, said that in return for access to the company's tools, FDA will provide "feedback on the utility of the tools in their environment."

Hovde said that Pharsight is "keen" to hear what FDA has to say about its technology, because while the company claims that all of the top 50 pharmaceutical firms license at least one of its products, the agreement marks the company's first deal with the regulatory agency.

"As FDA looks at its need to do more modeling, to better understand sponsored drugs, it needs the infrastructure to support that modeling."

FDA serves as "a new group of people to analyze data, and potentially a different type of data; for example, looking at data maybe more broadly than the sponsors have an opportunity to," Hovde said.

He added that Pharsight may upgrade its products based on FDA feedback, and is also considering modifying the system "to foster better collaboration between sponsors and FDA."

The primary purpose of the agreement is to develop PKS into a repository for clinical trial data, particularly related to clinical pharmacology and clinical safety reviews, that FDA can use for modeling and simulation.

Hovde said that under the Critical Path, FDA is asking pharmaceutical companies to do more in the area of modeling and simulation, which requires computational modeling tools, but also poses "a significant data-management problem."

In order to do effective modeling, "you're looking at issues across studies, and even across drugs ... So you get these data sets, and you would like to be able to federate those datasets and incorporate them into a modeling analysis," he said. "So as FDA looks at its need to do more modeling, to better understand sponsored drugs, it needs the infrastructure to support that modeling."

Robert Powell, head of pharmacometrics in FDA's Office of Clinical Pharmacology, said in a statement that the CRADA with Pharsight is "concrete evidence of the FDA's commitment to the Critical Path Initiative," and that FDA expects Pharsight's software to "help us in applying model-based drug development skills to regulatory decisions, recommendations, and knowledge sharing."

In an interview with *BioInform*, Powell said that FDA's interest in drug-development modeling extends well beyond PK/PD.

"That's a part of it, but it's more going at disease modeling," he said. In the case of chronically degenerative

diseases like Parkinson's or Alzheimer's, for example, "there can be a number of different subtypes of patients that can be partially explained by genotype, or it could be racial, or males versus females, but it's understanding the covariates, the factors that really characterize the disease."

Currently, Powell said, FDA is gathering data from prior NDAs, NIH databases, and the scientific literature to help develop disease models. "What we'd like to do is make this information more freely available and have people share it," he said, "although there are no concrete plans to do so at this time."

Nevertheless, Powell said, the field of model-based drug development "is a lot broader than what PK/PD was 15 or 20 years ago."

— *Bernadette Toner* (btoner@genomeweb.com)

BioInform's Licensing Roundup: May's Software and IT Deals

BioInform's Licensing Roundup: May's Software and IT Deals			
	Company	Product	Licensees
Software	Ariadne Genomics	PathwayStudio	Institut Curie
	BioWisdom	SRS, SRS Prism	Boehringer-Ingelheim (renewal)
	Genedata	Genedata Screener	Novartis Institutes for Biomedical Research (expansion of existing agreement)
	GeneGo	MetaCore	Peakadilly
	GenoLogics	Proteus	University of Dundee
	Geospiza	Finch Suite	SeqWright
	Nonlinear Dynamics	TT900 S2S, Progenesis PG240	University of York
	Partek	Partek Genomics Suite, Discovery Suite, QSAR Solution, Screener Solution	Chaim Sheba Medical Center, Weizmann Institute of Science
	Rosetta Inpharmatics	siRNA design algorithms	Sigma-Aldrich
	Teranode	Teranode XDA	Tehys Bioscience, Calibrant Biosystems, undisclosed "top-five pharmaceutical company"
Databases	Egenera	Blade server system	Shanghai Center for Bioinformation Technology

Locus to Use Computational Drug-Design Platform in Collaboration with Amgen

Locus Pharmaceuticals said this week that it has signed a research agreement with Amgen, under which it will use computational methods to design small-molecule compounds with activity against a target identified by Amgen.

Financial and other terms of the agreement were not disclosed.

"Given our past molecular design experience across 10 classes of protein targets, we are confident that we will identify novel chemical classes of inhibitors for Amgen," said Jeffrey Wiseman, vice president of technology and informatics at Locus.

The company said that it has so far used its proprietary technology in six external collaborations.

Rosetta Biosoftware Uses Borland's ALM for Resolver Development

Borland Software said this week that Rosetta Biosoftware is using its Application Lifecycle Management product line as part of its ongoing development of the Rosetta Resolver analysis platform.

Borland said that Rosetta is using its CaliberRM, StarTeam, and Together lifecycle management products, as well as its consulting services, "to streamline and automate the processes of requirements management, software change and configuration management as well as visual modeling and architectural design."

Siena Biotech Licenses Aureus Pharma's ADME and hERG Databases

Aureus Pharma said last week that Siena Biotech has licensed its AurScope ADME/Drug-Drug Interaction and hERG databases.

Financial terms of the agreement were not disclosed.

The databases "complement our in-house knowledge-based drug design platform," Graeme Robertson, vice president of therapeutic research, said in a statement.

Pfizer to Use BioWisdom's Sofia KnowledgeScan

Pfizer has licensed BioWisdom's Sofia KnowledgeScan platform, BioWisdom said this week.

Sofia KnowledgeScan is a service based on the company's Sofia Intelligence Platform, and provides "contextually relevant information to support critical healthcare-related decision-making," BioWisdom said in a statement.

Financial terms of the agreement were not provided.

Downloads & Upgrades/People in the News

Downloads & Upgrades

Simulations Plus has released upgraded versions of its **ADMET Predictor** and **ADMET Modeler** software for predicting properties of new molecular structures and for building structure-property prediction models, respectively. ADMET Predictor now enables researchers to add their own data to embedded predictive models without retraining. ADMET Modeler now enables visualization of the sensitivity of predicted properties to different molecular features, and includes features that make it faster and easier for scientists to build predictive models.

The **Gene Ontology Consortium** has released **OBO-Edit 1.000**, an ontology editor, at http://sourceforge.net/project/showfiles.php?group_id=36855. OBO-Edit includes support for OBO 1.0 and OBO 1.2 specifications, basic reasoning capabilities, cross-product editing, and a user's guide.

Anami Communications, the IT division of **Cornet Technology**, has released the **Scientific Image Manager**, a software product that enables life science researchers to display and manage multiple microscope image files. Users can view thumbnails and preview images of multiple file types in a single window, "eliminating the need for multiple third-party image viewer programs," according to the firm. The software also enables users to search and store images either by keyword or description.

GeneGo said this week that its **MetaCore** pathway-analysis software is now fully integrated with **Agilent Technologies'** **GeneSpring** software.

Taverna 1.4 is available at <http://taverna.sf.net>. The new version includes a public preview of the provenance capture and exploration subsystem, expanded web service and biomart invocation plug-ins, and other minor enhancements.

People in the News

Definiens has appointed **Wolfgang Rencken** as vice president of research and development. Rencken will be responsible for all worldwide R&D activities, including Definiens' Enterprise Image Intelligence platform, Cognition Network, Language Competence Center, Life Sciences Solutions, and Geospatial Intelligence Solutions.

Rencken previously was vice president of engineering for **Siemens Medical Solutions'** software components and workstations business unit. He holds a PhD in engineering science from the **University of Oxford**.

Definiens also said that **Gregory Calaman** has joined the company as vice president of customer services in North America.

Calaman was most recently employed by **Pfizer**, where he was responsible for large-scale IT program delivery, internal customer relationship management, and large-scale IT investment portfolio management.

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