

## Global computational grid takes on smallpox threat



Biological weapons have been around for decades. For most of us, it was the stuff of entertainment — novels and movies involving Cold War secret agents.

The end of the Cold War did not make the world a safer place. Fear of terrorists around the globe gave rise to an unprecedented sense of urgency in how we deal with the threat posed by biological weapons such as smallpox.

In response to the potential threat of smallpox being used as a weapon of bio terrorism, an international consortium of researchers recently completed a massive global collaborative computing project to find new treatment options for the deadly smallpox virus.

Dr. Grant McFadden has led the project at the

university and research level. McFadden, an expert on viruses that can cause pox diseases such as smallpox, is the Canada Research Chair in Molecular Virology at The University of Western Ontario and Co-director of the Bio-Therapeutics Research Group at the Robarts Research Institute.

Speaking at the ORION --CA\*net4 Advanced Networking Day workshop hosted by the University of Western Ontario earlier this month, McFadden drew on his experience with this project to illustrate the enormous power and impact that collaborative computational efforts can have in areas where the size and complexity of the challenge traditionally made researchers shy away.

"I think that most researchers are, like myself, computationally challenged," said McFadden

in an interview. "This project demonstrated to me the enormous potential of research combined with high speed computation capabilities, the kind that ORION provides for Ontario researchers."

"Viruses are difficult to 'weaponize'," says McFadden. "However, smallpox is a particular concern because it was suspected to have been developed as a bio-terrorism tool by the former Soviet Union and these stocks could have fallen into rogue hands."

The smallpox virus has an incubation period of one to two weeks and is extremely contagious. It is estimated that thirty per cent of those who get smallpox will die and those who don't may become disfigured or blind. Since smallpox was eradicated in the late 1970s by vaccinating

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## Network on track for connected users



The ORION network is on-track for its target of connected users at year-end, reports Andre Quenneville, ORION's Manager of Marketing and Communications.

Ryerson University and the University of Toronto are the most recent institutions to sign-up to connect to ORION, bringing the network's list of users to 34 earlier this week, heading into the New Year.

"We're on track with our target of at least 40 user organizations by the end of 2003," he said. Users now include 15 universities, eight colleges, two teaching hospitals, four school boards, three research centres, one Centre of Excellence and one major project (SHARCNET).

A few more users are planning to sign up by December 31. To date, at least a third of Ontario's 25 colleges of applied arts and technology are connected to the ORION network - for some enjoying connectivity to CA\*net 4 and global research and education networks for the very first time.

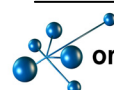
"There will be a transition period. Part of our work is introducing ORION users to the benefits of high-speed connectivity among institutions and to other networks in Canada and around the world. ORION opens up new possibilities and new opportunities for colleges in research, education and learning" he said. "For many of them, ORION levels the playing field. They can now enjoy the same level of connectivity as the institutions in the larger cities."

ORION will hold information sessions at some of the colleges in the near future. "We'll bring speakers and give demonstrations of how the ORION network can be put to use in several areas, from distributed computing, to resource sharing and administrative efficiencies, to advanced video conferencing, to access to large databases and online services," he said.

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The ORION Research and Discovery News is a monthly electronic publication providing news and information of interest to users of the Ontario Research and Innovation Optical Network and to the worldwide research and education community.



# Smallpox Research Grid – just the facts

## Smallpox Background

- There is no specific treatment post infection, and the only prevention is vaccination.
- Smallpox was eradicated by 1978
- Vaccination ended in 1972 and the population is highly susceptible.
- Availability of new anti-viral drugs to counter the virus would be a major defense.

## Grid computing

- Some computational problems are so big and complex that researchers refrain from tackling them.
- Grid (or distributed) computing works by taking large tasks and dividing them into many smaller tasks, all of which are disseminated to many computers running simultaneously via a network or the Internet.
- After the tasks are processed via individual computers, the data is transmitted back to a central server that then assembles an answer.
- Computers are typically idle 90% of the time. Grid technology takes advantage of this idle resource and mimics the power of a virtual supercomputer at a tiny fraction of the traditional cost.

## The Grid

- United Devices' (UD) Global MetaProcessor Grid computing software harnesses the computational power provided by 2 million PCs worldwide to create the largest Grid and fastest computer known.
- UD's software is powered by IBM infrastructure: servers, DB2 on AIX and Linux. IBM -- The Global MetaProcessor Platform (GMP) includes IBM eServer running DB2 database software on AIX and Linux operating systems. DB2 will handle 15 million SQL queries a day provided by the approximately two million personal computers analyzing billions of virtual drug screens.
- Accelrys' Ligandfit docking and scoring algorithm is used to predict and prioritize the suitability of potential lead drug candidates for subsequent drug development.
- Evotec OAI's drug modeling expertise identified and defined active sites.
- Oxford University, assisted by researchers at Essex University, prepared the protein structures for use with LigandFit, contributed the large molecular library and prepared the web site.
- Leading Universities and Research Institutes -- The project at the university and research level is led by Dr. Grant McFadden, (UWO and RRI); Dr. Stewart Shuman (Sloan Kettering, NYC); Dr. Graham Richards (Oxford), and Dr. Chris Reynolds (Essex University).
- Robarts Research Institute is Canada's only independent medical research centre. Physically close to and affiliated with The University of Western Ontario and London Health Sciences Centre, Robarts makes full use of the many opportunities that arise to bring research full circle from classroom to lab to clinic.

## Web sites

- For the scientific description of the project: <http://www.chem.ox.ac.uk/smallpox/>
- For more information about grid computing: [www.ibm.com/grid](http://www.ibm.com/grid) and [www.ud.com](http://www.ud.com)

## Global computational grid ...

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everyone against the disease, preventative vaccinations no longer take place making everyone susceptible to an outbreak. What the world needs urgently is an anti-smallpox drug in the event of an outbreak.

Achieving this requires millions of potential anti-smallpox molecules to be screened against the virus in as short a period of time as possible. That's where the computational challenges surfaced. In a truly global response to this problem, the computing power of millions of personal computers was volunteered to this effort by individuals in more than 190 countries. A virtual supercomputer capable of analyzing millions of molecules in a fraction of the time it would take in a laboratory was created by combining idle computing resources.

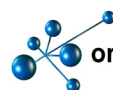
The computational grid achieved over 39,000 years of computing time in less than six months. The project used specialized computational software to screen 35 million potential anti-smallpox drugs against portions of the protein structure of the smallpox virus in the search for good drug targets. The results of the project, a ranked list of drug candidates, were delivered to the U.S. Department of Defense in September 2003.

"What we have managed to do is narrow that huge number to a few thousand potential molecules that can be considered lead candidates for the next phase of research," said McFadden. "The next step will be to test these potential drugs in the lab for the ability to inhibit the viral enzyme, called topoisomerase, which was the target of the screen. Once this screen is complete, the short list of drug candidates that remains then needs to be tested in animals for the ability to inhibit the virus."

McFadden's lab studies how these viruses that weaken the immune system's defenses carry out their attack. McFadden was a member of the 1999 Institute of Medicine committee in the United States that evaluated future uses of the smallpox virus for research purposes, and is a member of the current World Health Organization's committee deliberating the fate of the declared variola stocks, the virus that causes smallpox.

In addition to researchers at the U.S. Army Medical Research Institute of Infectious Diseases, which funded the project, essential technologies and services were provided by the University of Western Ontario, Robarts Research Institute, IBM, United Devices, Accelrys, Evotec OAI, University of Oxford, Memorial Sloan Kettering Cancer Research and Essex University.

Dr. McFadden's presentation is available at <http://www.orion.on.ca/pdf/mcfadden.pdf>



## Workshops emphasize urgency in adapting to new networking technology



A series of ORION-CA\*net 4 Advanced Networking workshops, held throughout Ontario in the last few weeks, emphasized the urgency of adapting to new networking and collaborative technology in the field of advanced research and education.

Presented by ORION and CANARIE and their host institutions, the workshops are part of a series that took presenters to five locations in Sudbury, Hamilton, London and Toronto (York and the U of T).

Well over 250 researchers and senior educators from a wide spectrum of institutions and organizations gathered to hear experts from ORION and CANARIE, as well as scientists and senior researchers from their institutions in several fields describe the benefits of advanced networking over high-speed networks.

While the events presented a comprehensive snap-shot of some of the most advanced research activities in Canada, presenters also made the case for a greater use of advanced networking technology and applications.

"Ontario has a distinct competitive advantage right now," said ORION President and CEO Phil Baker. "Ontario has at least an 18-month head start over other jurisdictions in North America with a network of this scale and capacity, but others are moving to establish similar networks," he said.

"Ontario colleges, universities, teaching hospitals and research labs have a wonderful R&E network infrastructure that is second to none in the world right now. Our challenge is to adapt quickly to this new technology and take advantage of it as soon as possible."

ORION Senior Manager of Strategic Partnerships Randy Neals sees these events as ideal outreach opportunities for potential users of the new network. "We are giving people basic information about research and education networks, and how these networks inter-connect here in Ontario, in Canada and throughout the world."

CANARIE, which celebrates its 10th anniversary this year, gave participants a broad overview of the evolution of R&E networking in Canada and outlined many of the successful projects that have been enabled over the CA\*net networks over recent years.

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### *"High bandwidth networking creates limitless possibilities" - Dr. J. Challis*

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CANARIE presenters, which included President and CEO Andrew Bjerring, also discussed "Third Wave" applications and technologies which will re-design business processes and relationships across organizational boundaries, part of a longer-term convergence of networks and IT, which will lead to an entirely new form of shared "infrastructure".

CANARIE also outlined details of its new \$4 million Advanced Applications funding program. Workshop presentations ranged from advancements in new collaborative technologies, to the latest news on university research activities.

Among the highlights were illustrations of the use of networks to develop new learning environments in 3-D space, geospatial information systems, and bioinformatics and computational biology, and grid computing in high-energy particle physics.

At York, a live demo illustrated immersive environments with the use of 3D graphics, avatars and collaborative virtual reality tools. Participants also learned about advanced networking and the arts and the Ontario Digital Library and Scholars Portal.

At both the York and University of Toronto sessions, participants learned about GTAnet, the new consortium of institutions that is collaborating with ORION to bring the new network to universities, colleges and teaching hospitals in the Greater Toronto Area.

York, the UofT and Ryerson University, which also participated in the presentations, are part of the consortium, which is receiving ORION local loop and connectivity funding.

"Enhanced networking technology is a crucial element of increased collaboration between U of T researchers and their colleagues around the world," said Dr. John Challis, Vice-President, Research and Associate Provost for the U of T, where \$2 million worth of research is conducted every day.

"High bandwidth networking creates limitless possibilities for university research – not just in science and engineering but across the disciplines."

ORION expects to stage more workshops in the next several months. Details are being finalized for events at the University of Waterloo and Queen's University in Kingston. Events will also be scheduled at a number of colleges, including Confederation College in Thunder Bay.

Over 40 of the workshop presentations are now available to download at [www.orion.on.ca/orioncanet4days.html](http://www.orion.on.ca/orioncanet4days.html)



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## Loyalist and Bioniche partner in botanical medicine research



Belleville's Loyalist College has partnered with Bioniche Life Sciences Inc. in a multi-year research project involving the use of high-pressure carbon dioxide extraction technology to produce high quality botanical medicines.

"This is the first scientific research project to be developed and delivered by the College," explained Loyalist President Doug Auld.

"Loyalist has a strong background in the delivery of applied science programs in the Bio-Sciences field," he said. The project grew out of the development of the college's cluster of Bioscience programs as well as the recognition of the need for biotechnology research in Ontario.

Other research partners include the University of Ottawa and the Canadian College of Naturopathic Medicine. Research will focus on

the identification, extraction, production and evaluation of botanical extracts. Identical extractor technology at Loyalist and the University of Ottawa will allow duplication of laboratory results. The Canadian College of Naturopathic Medicine will provide clinical assessment of the extractions and controlled trials to validate product efficacy. Bioniche will assess the study results to determine the commercialization potential of any of the products.

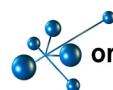
"We are delighted that Bioniche has joined in this project as an industrial partner, and we certainly look forward to the results over the next four years," said Auld. "We are very pleased to be involved in this innovative research project with Loyalist College and our other institutional partners," said Graeme McRae, Bioniche President and CEO.

"There is great potential here to develop high

quality natural health products for a rapidly growing marketplace, and also to build on the strengths that exist in the Quinte area to help develop a stronger regional economy."

Bioniche Life Sciences Inc., Loyalist and the Ontario Government are contributing a total of \$459,300 towards the project, which includes a new research laboratory at Loyalist that will be suitable for nutraceutical extraction. The installation will house testing equipment including a pilot plant extractor, believed to be the only one available in Ontario.

The University of Ottawa will perform primary research and develop protocols. Kari Kramp, a professor in Applied Science at Loyalist, is the primary researcher for the project. She has begun her doctoral studies at the University and will work with Dr. John Arnason, a pre-eminent Canadian researcher in nutraceutical extraction technology.





## ORION News Briefs

### Drilling complete for UOIT geothermal well field

The drilling of a geothermal well field, one of the largest in North America, has just been completed on the campus of Canada's newest university, the University of Ontario Institute of Technology. Some 380 holes, each drilled 213 metres (700 feet) into the earth will be linked to mechanical systems that will provide eight new university buildings with a highly efficient and environmentally friendly heating and cooling system. The drilling is just the first step in the development of a thermal energy storage system that uses the earth's relatively constant temperature to provide a stable, low maintenance and efficient energy source. In winter, fluid circulating through tubing extended into the wells will collect heat from the earth and carry it into the buildings. In summer, the system will reverse to pull heat from the building and place it in the ground. The ground source thermal system will be ready in May 2004.

### Mining camp to house first on-site VRL

Laurentian University's Mining Innovation, Rehabilitation and Applied Research Corporation (MIRARCO) has teamed up with Goldcorp Inc. and Placer Dome Canada to build the first virtual reality laboratory (VRL) in an active mining camp. The new facility, to be

built at the Red Lake Mine located at Red Lake in Northwestern Ontario, will provide a state-of-the-art research and development facility that will help with ongoing mining and exploration.

VRLs offer high-end projection and viewing technologies using a large screen "immersive 3D" format. MIRARCO designed and manages Laurentian University's \$1.25 million VRL, the first virtual reality facility in the world designed to support mining and mineral exploration. Placer Dome Canada is one of the first companies to use virtual reality technology in mining exploration. For more information about virtual reality in the mining industry, visit [www.mirarco.org](http://www.mirarco.org).

### New head of strategic computing at UofT

The University of Toronto has appointed a director of strategic computing. Marden Paul, who has worked in the information systems field for the past 18 years, will assume the position on Jan. 5 2004.

The directorship is a redefinition of the position of provost's adviser on information technology, a position held by the late Jack Gorrie, a member of the ORANO Board of Directors. The position's broader mandate includes providing co-ordination, direction and guidance to the provost and U of T's computing divisions in

implementing administrative and academic computing systems. He will also advise on the strategic use of information technology resources in fulfilling U of T's research and teaching mission. Most recently, he served as client services manager in the Department of Administrative Management Systems.

### SNOLAB gets green light

The Sudbury Neutrino Observatory is receiving \$50 million to expand the facility and support a new project - SNOLAB - to conduct experiments that build on the success of the original SNO project. The Canada Foundation for Innovation (CFI) recently announced a \$39 million contribution towards the project. The CFI's investment will cover the cost of excavation of a new underground experimental cavern, surface support, new labs at Laurentian University, experimental equipment as well as operational support for the next five years. The Government of Ontario has already announced a \$10 million contribution for surface buildings to support researchers working on experiments. SNOLAB project brings together a consortium of researchers from six Canadian universities. The administrative centre will be located at Carleton University where the project leader, Dr. David Sinclair, is a Professor of Physics (College of Natural Sciences at Carleton University). Other Ontario-based participating researchers are from Queen's, Guelph, and Laurentian.



## orion research and discovery news

THE OFFICIAL NEWSLETTER OF THE ONTARIO RESEARCH AND INNOVATION OPTICAL NETWORK

### About ORION

ORION is an advanced high-speed fibre optic network that connects research and education institutions to each other and to colleagues around the world. Spanning 3,700-kilometre to 21 cities throughout the Province of Ontario, ORION was created to bring leading-edge network capability to Ontario's publicly funded R&E community and to become a catalyst for creative and innovative next generation Internet applications.

### For more information

ORION is owned and operated by the Optical Regional Advanced Network of Ontario (ORANO). For more information, visit our web site at <http://www.orion.on.ca>. Communicate directly with the Editor of the ORION Newsletter at [info@orano.on.ca](mailto:info@orano.on.ca).

To subscribe to the electronic version of this newsletter, visit this web site. <http://www.orano.on.ca/newsletter/subscribe.html>

### Network on track for connected users

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The colleges currently connected include Confederation (Thunder Bay), Cambrian (Sudbury), Durham (Oshawa), Fanshawe (London), Lambton (Sarnia), Seneca (Toronto) and Sheridan (Oakville).

Confederation's new director of Computer Services Paul Inkila, for one, is very pleased with the network's performance. "It's been smooth sailing, not a single hiccup," he said. The college has been connected since September. He noted the college is looking forward to exploring full use of the network and connectivity to CA\*net 4 and other networks.

ORION is also finalizing its agreement with GTAnet, a consortium of institutions that came together to connect to ORION, which includes four additional colleges that will connect to ORION. York University, Ryerson University and the University of Toronto are part of GTAnet's 12 founding members. The group also includes Baycrest Centre for Geriatric Care, Centennial College, George Brown College, Hospital for Sick Children, Humber College, Sunnyside and Women's College Health Sciences Centre, the University Health Network and the Ontario College of Arts and Design. GTAnet hopes to have all members connected by mid-2004.

Other organizations throughout Ontario are expected to sign on to ORION in the next several weeks and months. "We're confident of achieving our target of 60 users by March 31," said Quenneville.

