

## Case Research Computing Newsletter

### 28 November 2005

#### News from Case

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1. gridMathematica to be available on the Case pilot HPC cluster
2. MATLAB and Gaussian to be available on the Case pilot HPC cluster
3. R statistical software is available on the Case pilot HPC cluster
4. Case announces availability of Oracle HTML DB service

#### Funding News

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5. Microsoft funding opportunity
6. European Union funds computational systems biology
7. NSF announces grant awards in "cyber-enabled chemistry"

#### News of Conferences and Professional Societies

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8. SC|05 November 12-18 Seattle, WA
9. WSCG 2006 call for papers and participation
10. IEEE International Symposium on High Performance Distributed Computing - June 2006 - Paris, France - Call for Papers
11. Announcement and call for papers for the HPCS 2006 meeting.
12. Megaconference VII set for December 1

#### Other news

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13. UCSC and Los Alamos National Laboratory to form partnership
14. Materials scientists at North Dakota State University use high performance computing to study the strength of abalone shells
15. New supercomputers for nuclear weapons analysis
16. New HPC effort by Ferrari in aerodynamic simulations for Formula One racing
17. Virginia Tech to showcase supercomputing over National LambdaRail
18. UCSD dedicates new technology institute
19. Faster computation yields insight into genetic basis of disease
20. Largest computational biology simulation mimics life's most essential nanomachine
21. Gordon Bell Prize awarded to researchers at Lawrence Livermore Labs and IBM for "100+ TFlop Solidification Simulations on BlueGene/L"
22. New list of the top 500 supercomputers in the world is released

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**1. gridMathematica to be available on the Case pilot HPC cluster**  
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ITS has acquired the gridMathematica product from Wolfram Research for installation on the pilot HPC cluster. Installation of the package on the pilot cluster began on November 7 and it should be available for use very shortly. See <http://www.wolfram.com/products/gridmathematica/> for information on gridMathematica.

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**2. MATLAB and Gaussian to be available on the Case pilot HPC cluster**  
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ITS is planning to install the MATLAB and Gaussian software on the pilot HPC cluster. A timetable for this installation will be announced as soon as licensing is resolved.

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**3. R statistical software is available on the Case pilot HPC cluster**  
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The R statistical package was installed on the pilot cluster on November X and is available for use. See <http://www.r-project.org> for more information on R.

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**4. Case announces availability of Oracle HTML DB service**  
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ITS is now making available a hosting service for Oracle HTML DB. ITS hosts HTML DB on its servers and provides access via web browser to the research community for a small monthly fee. Please see <http://www.case.edu/its/researchcomputing/databasehosting.htm> for details.

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**5. Microsoft funding opportunity**  
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Microsoft Research anticipates making 15 to 20 awards in the range of \$20,000 to \$100,000 as part of its \$1.2 million "Digital Inclusion through Mobile and Wireless Technologies Research Funding Initiative" announced on October 20. Proposals must be submitted by January 13, 2006. See [http://research.microsoft.com/ur/us/fundingopps/RFPs/DigitalInclusion\\_2005\\_RFP.aspx](http://research.microsoft.com/ur/us/fundingopps/RFPs/DigitalInclusion_2005_RFP.aspx) for additional details on this opportunity.

For information on the broader set of research funding opportunities at Microsoft Research, see <http://research.microsoft.com/ur/us/fundingopps/default.aspx>.

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**6. European Union funds computational systems biology**  
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<http://www.supercomputingonline.com/article.php?sid=9665>

The Commission of the European Union has awarded €9 million over five years for a new Network of Excellence that will make computational systems biology accessible to bench scientists throughout Europe and beyond. ENFIN, which stands for "Experimental Network for Functional INtegration," brings together some of Europe's best computational and experimental biology labs - 20 groups across 17 institutions in 13 countries - to build a virtual institute that will put Europe at the center of the systems biology revolution.

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**7. NSF announces grant awards in "cyber-enabled chemistry"**  
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<http://www.scimag.com/ShowPR.aspx?PUBCODE=030&ACCT=3000000100&ISSUE=0511&Origreltype=iw&RELTYPE=pr&PRODCODE=00000000&PRODLETT=L>

The National Science Foundation (NSF) has announced the first round of grants in "cyber-enabled chemistry," a program developed by its chemistry division to explore how researchers and educators in that field can fully exploit the potential of cyberinfrastructure.

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**8. SC|05 November 12-18 Seattle, WA**  
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<http://sc05.supercomputing.org/>

The 18<sup>th</sup> annual supercomputing conference was held in Seattle earlier this month and was attended by a record 9777 people. For complete information, see [sc05.supercomputing.org](http://sc05.supercomputing.org).

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**9. WSCG 2006 Call for Papers and Participation**  
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W S C G ' 2006 (formerly the Winter School of Computer Graphics)

14th International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision 2006 in co-operation with EUROGRAPHICS. University of West Bohemia, Plzen, Czech Republic, January 30 - February 3, 2006

Topics include computer graphics and visualization, computer vision, image processing and pattern recognition, fundamental algorithms, graphical human computer interfaces, geometric modeling and computer aided geometric design, computational geometry, rendering and virtual reality, animation and multimedia, medical imaging, graphical interaction, object\_oriented graphics, parallel and distributed graphics, WWW technologies, CAD/CAM, DTP and GIS systems and others.

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**10. IEEE International Symposium on High Performance Distributed Computing - June 2006 - Paris, France - Call for Papers**  
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HPDC'15 - The 15th IEEE International Symposium on High Performance Distributed Computing June 19-23 2006 Paris, France → [www.hpdc.org](http://www.hpdc.org)

The Fifteenth IEEE International Symposium on High-Performance Distributed Computing (HPDC) will be a forum for presenting the latest research findings on the design and use of parallel and distributed systems for high end computing, collaboration, data analysis, and other innovative applications. Submissions are welcomed covering all aspects of high-performance distributed computing, Grids, and global computing ensembles. New scholarly research emphasizing empirical and reproducible results as well as investigative expositions of successful application and deployment efforts are particularly encouraged.

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**11. Announcement and call for papers for the HPCS 2006 meeting**  
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<http://www.ace-net.ca/events/hpcs2006/>

The 20<sup>th</sup> International Symposium on High Performance Computing Systems and Applications will be held May 14-17, 2006 at Memorial University of Newfoundland in conjunction with OSCAR'06. The deadline for submission of papers is December 15, 2005. See <http://www.ace-net.ca/events/hpcs2006> for more information. See <http://www.csm.ornl.gov/oscar06/> for information on OSCAR'06.

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**12. Megaconference VII set for December 1**  
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The Ohio Supercomputer Center, in conjunction with The Ohio State University and Internet2, will jointly host the seventh annual Megaconference on December 1, 2005. Megaconference is the world's largest

simultaneous connection of Internet videoconferencing communication devices.

Please see [www.osc.edu/press/releases/2005/megaVII.shtml](http://www.osc.edu/press/releases/2005/megaVII.shtml) for the OSC press release and the Megaconference site [www.megaconference.org](http://www.megaconference.org) for more information.

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**13. UCSC and Los Alamos National Laboratory to form partnership**

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<http://www.supercomputingonline.com/article.php?sid=9670>

The University of California, Santa Cruz, and Los Alamos National Laboratory have agreed to establish a new collaborative institute for research and education.

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**14. Materials scientists at North Dakota State University use high performance computing to study the strength of abalone shells**

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<http://www.supercomputingonline.com/article.php?sid=9668>

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**15. New supercomputers for nuclear weapons analysis**

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<http://www.supercomputingonline.com/article.php?sid=9648>

On October 27 the National Nuclear Security Administration (NNSA) officially dedicated two new supercomputers, housed at Lawrence Livermore National Laboratory, for use in nuclear weapons analysis.

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**16. New HPC effort by Ferrari in aerodynamic simulations for Formula One racing**

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<http://www.supercomputingonline.com/article.php?sid=9656>

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**17. Virginia Tech to showcase supercomputing over National LambdaRail**  
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<http://www.supercomputingonline.com/article.php?sid=9660>

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**18. UCSD dedicates new technology institute**  
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<http://www.supercomputingonline.com/article.php?sid=9658>

The University of California, San Diego, dedicated its high-tech research home for the California Institute for Telecommunications and Information Technology (Calit2) recently and unveiled a \$1.5 million gift to the institute from QUALCOMM Incorporated.

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**19. Faster computation at UCSD yields insight into genetic basis of disease**  
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<http://www.supercomputingonline.com/article.php?sid=9641>

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**20. Largest computational biology simulation mimics life's most essential nanomachine**  
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<http://www.scimag.com/ShowPR.aspx?PUBCODE=030&ACCT=3000000100&ISSUE=0511&origreltype=iw&RELTYPE=pr&PRODCODE=00000000&PRODLTT=K>

Researchers at Los Alamos National Laboratory have set a new world's record by performing the first million-atom computer simulation in biology. Using the "Q Machine" supercomputer, Los Alamos computer scientists have created a molecular simulation of the cell's protein-making structure, the ribosome. The project, simulating 2.64 million atoms in motion, is more than six times larger than any biological simulations performed to date.

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**21. Gordon Bell Prize awarded to researchers at Lawrence Livermore Labs and IBM for "100+ TFlop Solidification Simulations on BlueGene/L"**

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[http://home.businesswire.com/portal/site/google/index.jsp?ndmViewId=news\\_view&newsId=20051117005981&newsLang=en](http://home.businesswire.com/portal/site/google/index.jsp?ndmViewId=news_view&newsId=20051117005981&newsLang=en)

This year's Gordon Bell Prize, announced at Supercomputing 2005, was awarded for "100+ TFlop Solidification Simulations on BlueGene/L" by authors Frederick H. Streitz, James N. Glosli, Mehul V. Patel, Bor Chan, Robert K. Yates, Bronis R. de Supinski (Lawrence Livermore National Laboratory), and James Sexton, John A. Gunnels (IBM). The Gordon Bell Prize, awarded each year at the annual [Supercomputing Conference](#), was established in 1988 by [Gordon Bell](#), a pioneer in computer architecture who taught engineering and computer science at Carnegie Mellon from 1966 to 1972. Bell, who spent 23 years at Digital Equipment Corp. as vice president of research and development, is a senior researcher in Microsoft's Media Presence Research Group, part of the San Francisco-Bay Area Research Center which maintains an interest in startup ventures.

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**22. New list of the top 500 supercomputers in the world released**

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[http://www.top500.org/news/articles/article\\_80.php](http://www.top500.org/news/articles/article_80.php)

The 26th edition of the semiannual TOP500 list of the world's fastest supercomputers was released on November 14, 2005 at the Supercomputing Conference (SC05) in Seattle, WA. The new TOP500 list can be found at <http://www.top500.org/lists/2005/11>. Complete information on the TOP500 effort can be found at <http://www.top500.org>.

On the latest list, the top position was again claimed by the BlueGene/L System, a joint development of IBM and DOE's National Nuclear Security Administration (NNSA) and installed at DOE's Lawrence Livermore National Laboratory in Livermore, CA. BlueGene/L also occupied the top position on the previous two TOP500 lists. However, the system was doubled in size to 131,072 processors during the last six months and has reached a new record LINPACK benchmark performance of 280.6 TFlop/s ("teraflops" or trillions of calculations per second). No other system had previously exceeded the level of 100 TFlop/s and this system is expected to remain in the top position for the next few editions of the list. The pace of innovation and performance improvements seen at the very high end of scientific computing shows no sign of slowing down. Four of top ten systems on the previous June 2005 TOP500 list were displaced by newly installed systems, and 221 of the systems on the June 2005 list failed to make the latest list.

A LINPACK benchmark of 1.64 TFlop/s was required to make the bottom position on the latest list, compared to 0.8506 TFlop/s one year ago. The last system on the latest list would have been listed at position 173 just one year ago. The entry level for the top ten positions on the new list exceeds 20 TFlop/s and the entry point for the top 100 moved from 2.026 TFlop/s one year ago to 3.98 TFlop/s. Total combined performance of all 500 systems on the list is now 2.30 PFlop/s ("petaflops" or thousand teraflops), compared to 1.127 PFlop/s one year ago.

Of the 500 systems on the list, 266 are classified as "industry", 121 as "research", and 70 as "academic". Among vendors, IBM leads with 219 systems, followed by Hewlett-Packard with 169, Cray and SGI with 18 each, and Dell with 17. Among processor types, Intel 32-bit processors lead with 206, followed by Intel 64-bit Xeon EM64T with 81, IBM Power with 73, AMD Opteron with 55, and Intel Itanium2 with 46.

There are 360 systems now labeled as clusters, making this the most common architecture in the TOP500. Of these, 249 cluster systems are connected using Gigabit Ethernet, 101 use the proprietary Myrinet product from Myricom, and 27 use the new Infiniband standard.

Among the top 100 supercomputers, U.S. universities occupied the following positions:

- 20 Virginia Tech
- 27 NCSA / University of Illinois
- 34 UCSD / San Diego Supercomputer Center
- 40 Caltech
- 43 Pittsburgh Supercomputing Center

- 48 University of Southern California
- 49 NCSA / University of Illinois
- 59 NCSA / University of Illinois
- 60 NCSA / University of Illinois
- 66 Brigham Young University
- 67 University of Oklahoma
- 74 Boston University
- 79 Princeton
- 80 UCSD / San Diego Supercomputer Center
- 85 University of Illinois
- 87 Pittsburgh Supercomputing Center
- 90 University of Tennessee
- 92 Caltech / Jet Propulsion Laboratory
- 95 University of Texas.

How does Case stack up? Our ITS pilot cluster has 36 Pentium 4 Xeon EM64T 3.2 GHz processors. Increasing its size to approximately 400 processors would land this cluster in the top 500. Approximately 550 processors would be required to enter the top 300. Approximately 1000 processors would be required to make the top 100 overall and place among the top 20 U.S. universities.

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**About the newsletter**  
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The Case Research Computing Newsletter is distributed on the last Thursday of each month and is intended to provide information of interest to researchers in the areas of high performance computing, high bandwidth networking, grid computing, visualization, and other uses of computation in research. To manage your subscription to the newsletter (or to unsubscribe), please visit <https://lists.case.edu/> and select the "RC-newsletter" mailing list. For comments about the newsletter or more information about research computing at Case in general, please contact [Roger.Bielefeld@case.edu](mailto:Roger.Bielefeld@case.edu) or see [www.case.edu/its/researchcomputing](http://www.case.edu/its/researchcomputing). Old issues of the newsletter are archived at [www.case.edu/its/researchcomputing/newsletter](http://www.case.edu/its/researchcomputing/newsletter).