# iCER Monthly Bulletin//March 2014



MICHIGAN STATE UNIVERSITY

# Institute for Cyber-Enabled Research

#### Intel 14 has arrived!

We are excited to announce and celebrate the launch of our latest computer cluster, the Intel 14. The Intel 14 cluster includes 220 nodes with 4400 CPU cores and stores between 64 GB to 256 GB of memory per node—enough power to run 110 homes or 330,000 iPhone 5S. <u>To read more,</u> <u>click here!</u>



#### **Upcoming iCER Events**

March 14         HPCC Cluster Opening Ceremony           8:30am - 10:00am in the Engineering Building, Room 3405A           Come enjoy a light breakfast, a few words from our Director, and a tour of the HPCC in celebration of the High Performance Computing Center's new cluster.	
March 14 RTSF Core Seminar Series- "Genomics" presented by Nick Beckloff 2:00pm - 3:00pm in the BPS Building, iCER Seminar Room Snacks and drinks provided for attendees!	
April 1 MathWorks MATLAB Seminar 10:00am - 2:30pm held in G030 Hubbard Hall This is an introductory seminar to MATLAB Software. A light lunch will be provided for attendees from 12:00pm - 12:30pm.	

#### **Upcoming Opportunities**

March 3	2014 ACM/IEEE-CS George Michael Memorial HPC Fellowship Submissions open from March 3 - May 1 For eligibility, selection, procedure, and award details, <u>see more here!</u>
March 10	Petascale Computing Resource Allocation (PRAC) Proposal deadline on March 10! For information or to apply, click here!
March	Data-Intensive Computing- Research Experience for Undergraduates This 8 week program from June 2 - July 25 is held in Clemson, South Carolina. Application review will begin early March and will continue until positions are filled. For more information, click here!
April 7	Computational Methods for Spatially Realistic Microphysiological Simulations 2014 3 day workshop in Pittsburgh, PA at the Pittsburgh Supercomputing Center. Applications due April 7th! <u>For details or to apply, click here!</u>



Do you know about an event, opportunity, job posting, or general news that would be of interest to our community? We would love to hear about it! Email icer@msu.edu and we will get the word out.

All submissions will be posted at the discretion of the iCER Communication Coordinator.



# iCER Monthly Bulletin//April 2014



MICHIGAN STATE UNIVERSITY

# Institute for Cyber-Enabled Research

#### Galaxy, coming soon to iCER

iCER is working hard to install and test Galaxy, a web-based bioinformatics workflow management system (to learn more, visit **usegalaxy.org**). Galaxy will decrease the time, effort, and computational expertise required for performing and repeating bioinformatics analyses. Galaxy will be directly integrated with the current HPCC resources allowing users to continue to use current workflows and data. To use Galaxy, all you will need is an HPCC account and you can be up and running!



### Traveling Road Shows

Do you have a group that would like to learn more about iCER and the HPCC? Contact us today to have a representative come present about iCER to learn more about the HPCC, how to use it to its full capability, and for an open Q&A. Road shows are a great opportunity to gain knowledge on the HPCC and how it can best benefit you. Contact us at icer@msu.edu today to schedule!



Dr. Dirk Colbry speaks with MSU Neuroimaging about the High Performance Computing Center.

#### **Upcoming iCER Events**

April 4	<u>MSU Science Festival: High Performance Computing</u> 11:00am - 12:00pm in the Engineering Building, Room 3300 Come enjoy tours of the HPCC, hands-on demonstrations, games, and deconstruct a hard drive! Suggested ages 9+, FREE to everyone! For the full Science Festival schedule, visit <u>sciencefestival.msu.edu</u> .
April 11	<u>RTSF Core Seminar Series- "Mass Spec" presented by Dan Jones</u> 2:00pm - 3:00pm in the BPS Building, iCER Seminar Room Snacks and drinks provided for attendees!
April 11	Special Guest Presenter: Carlile Lavor 1:30pm - 2:30pm held in the BPS Building, Room 1300 Discrete Distance Geometry and Molecular Structure Calculation Presented by Professor Carlile Lavor from the University of Campinas, Brazil. Please join us for this special SATE/iCER seminar. Snacks and beverages provided at this event!
April 24	Take Your Child to Work Day         8:30am - 2:30pm         This event is sponsored by the Women's Resource Center and Family Resource Center.         Give your child the opportunity to visit MSU, explore their futures, and have fun! iCER is happy to be a site option for tours and career exploration! For more information, visit         wrc.msu.edu.       A full list of tour sites, activities and details will be posted April 18.
May 6	<u>"Globus Online" presented by Dirk Colbry</u> 8:30am in Bessey Hall, Room 211 This event is part of Seminars in Research and Instructional Technology hosted by MSU IT Services. Only 25 seats open! Enrollment ends May 2, visit <u>tech.msu.edu</u> to register.

May 7 Introduction to High Performance Computing at MSU 8:30am - 9:30am in 403 Computer Center This event is part of Seminars in Research and Instructional Technology hosted by MSU IT Services. Only 25 seats open! Enrollment ends May 2, visit tech.msu.edu to register.

#### May 7 Advanced Topics in HPCC: Making Your Research Go Faster

1:30pm - 4:30pm in 403 Computer Center This event is provided to continue to build off of the Introduction to High Performance Computing at MSU workshop. This event is part of Seminars in Research and Instructional Technology hosted by MSU IT Services. Only 25 seats open! Enrollment ends on May 2, visit tech.msu.edu to register.

#### **Upcoming Opportunities**

<ul> <li>April 7 Computational Methods for Spastically Realistic Micro Physical Simulations 2014 Workshop organized by MMBioS April 28 - April 30 in Pittsburgh, PA at the Pittsburgh Supercomputing Center. Applications due April 7! For details or to apply, click here.</li> <li>April 14/15 April in Montreal There are 5 parallel Software Carpentry events April 14 - April 15 Deadline to attend is the day before the event but limited space is available! Visit the bootcamp page here for the full list of Montreal events.</li> <li>May 1 ACM/IEEE-CS George Michael Memorial HPC Fellowship Honors exceptional PhD students whose research focus is on HPC applications, networking, storage, or large-scale data analysis. Submission deadline May 1! For details or to apply, click here.</li> <li>June 9 NSF Critical Techniques and Technologies for Advancing Big Data Science &amp; Engineering (BIGDATA) Applications due on June 9! For details or to apply, click here.</li> <li>June 19 NIH Big Data to Knowledge (BD2K) Grant Applications due June 19! For details or to apply, click here.</li> </ul>	April 4	Open Science Grid User School 2014 July 7 - July 10 at the University of Wisconsin–Madison. Applications due April 4! <u>For details or to apply, click here!</u>
There are 5 parallel Software Carpentry events April 14 - April 15         Deadline to attend is the day before the event but limited space is available!         Visit the bootcamp page here for the full list of Montreal events.         May 1       ACM/IEEE-CS George Michael Memorial HPC Fellowship         Honors exceptional PhD students whose research focus is on HPC applications, networking, storage, or large-scale data analysis. Submission deadline May 1!         For details or to apply, click here.         June 9       NSF Critical Techniques and Technologies for Advancing Big Data Science & Engineering (BIGDATA)         Applications due on June 9!       For details or to apply, click here.         June 19       NIH Big Data to Knowledge (BD2K) Grant	April 7	Workshop organized by MMBioS April 28 - April 30 in Pittsburgh, PA at the Pittsburgh
<ul> <li>Honors exceptional PhD students whose research focus is on HPC applications, networking, storage, or large-scale data analysis. Submission deadline May 1! For details or to apply, click here.</li> <li>June 9 NSF Critical Techniques and Technologies for Advancing Big Data Science &amp; Engineering (BIGDATA) Applications due on June 9! For details or to apply, click here.</li> <li>June 19 NIH Big Data to Knowledge (BD2K) Grant</li> </ul>	April 14/15	There are 5 parallel Software Carpentry events April 14 - April 15 Deadline to attend is the day before the event but limited space is available!
Engineering (BIGDATA) Applications due on June 9! <u>For details or to apply, click here</u> . June 19 NIH Big Data to Knowledge (BD2K) Grant	May 1	Honors exceptional PhD students whose research focus is on HPC applications, networking, storage, or large-scale data analysis. Submission deadline May 1!
5	June 9	Engineering (BIGDATA)
	June 19	

#### In need of assistance with grant opportunities?

iCER is happy to help coordinate the NIH Big Data to Knowledge Initiative and/or the NSF Critical Technique and Technologies for Advancing Big Data Science & Engineering grant opportunities. Please let us know if you are interested in being part of either of these BIGDATA proposals by filling out a ticket with your request at <u>contact.icer.msu.edu</u>.

Do you know about an event, opportunity, job posting, or general news that would be of interest to our community? We would love to hear about it! Email icer@msu.edu and we will get the word out. All submissions will be posted at the discretion of the iCER Communication Coordinator.



# iCER Monthly Bulletin / May 2014



MICHIGAN STATE UNIVERSITY

Institute for Cyber-Enabled Research

### HPCC Scheduled Maintenance Outage on May 8th

The HPCC will be unavailable to users on **Thursday, May 8th** due to our regularly scheduled biannual maintenance. No jobs will run during this time. Jobs that will not be completed before May 8th will not begin until after maintenance is complete. For example, if you submit a four-day job three days before the maintenance outage, your job will be postponed and will not begin to run until after maintenance is completed.

#### New software available

iCER is pleased to provide a suite of Allinea software products (DDT, MAP, and Performance Report) for helping researchers debug, profile (up to 512 processes!), and optimize their software. We hope that the user interface and feature set (support of advanced architectures such as GPUs and Intel Phis) will significantly reduce the mean-time-to-science for many research groups on campus. To use Allinea on HPCC systems, please type module load Allinea. A brief demo will be demonstrated at the Lightening Talk on May 19th. (See below for details.)

iCER is also purchasing several seats for COMSOL, a multi-physics software package for simulating complex engineering or multi-physics problems. The software provides modeling, meshing, and a slew of different solvers depending on the type of PDE that the user is trying to solve. The software suite is commonly used in industry. iCER's license will enable researchers to do parametric studies at scale. The acquisition is in process, we anticipate having the software installed and configured by the end of May.

### 2014 Large Memory Buy-In Opportunity

We are excited to announce the Large Memory 2014 buy-in options for MSU researchers and partners. Buy-in users enjoy priority access to purchased cluster resources for their research group. iCER provides the support infrastructure of racks, network switches, cabling and support servers, as well as the cooling and power infrastructure. Users may purchase priority access to four node configurations that you can further <u>explore here</u>. If you are interested in participating, please <u>contact the HPCC staff</u> as soon as possible. The first order will go out early May.

Summer 2014- Virtual School of Computational Science and Engineering iCER is excited to announce we will be hosting two multi-day VSCSE courses this upcoming summer!

♦ Harness the Power of GPU's: Introduction to GPGPU Programming June 16 – 20, 2014

Harness the Power of GPU's: Introduction to GPGPU Programming is a mixture of lectures and labs that introduces all levels of parallelism as well as common approaches for parallelization in order to achieve the following goals:

Better utilization of the GPUs by enabling more scientists to use them

· Better understanding of the efficiency in the GPU utilization by the application developers

· Higher job throughput by enabling more resources and shortening job runtimes

In addition, participants will understand and avoid the common pitfalls of parallel computing, learn CUDA and OpenACC, understand the basic principles of data parallel computing, tap into enormous computing power, even on a laptop, and speedup research.

#### Data Intensive Summer School June 30 – July 2, 2014

The Data Intensive Summer School focuses on the skills needed to manage, process, and gain insight from large mounts of data. It is targeted at researchers from the physical, biological, economic, and social sciences that are beginning to drown in the data. We will cover the nuts and bolts of data intensive

computing, common tools and software, predictive analytics algorithms, data management, and nonrelational database models. Given the short duration of the summer school, the emphasis will be on providing a solid foundation that the attendees can use as a starting point for advanced topics of particular relevance for their work.

For more details or to register, please visit here.

#### Upcoming iCER Events

### May 6 – Introduction to High Performance Computing at MSU

8:30am - 9:30am in 403 Computer Center This event is part of Seminars in Research and Instructional Technology. Only 25 seats open! Enrollment ends May 2, visit <u>tech.msu.edu</u> to register. If past May 2 and you would still like to enroll, please contact Dirk Colbry at colbrydi@msu.edu

#### May 7 - "Managing, Sharing, and Moving Big Data"

8:30am - 9:30am in 403 Computer Center

Learn how to set up and use shared research spaces on the HPCC, transfer moderate sized files using FileDepot and large datasets (greater than 900 MB) using Globus. Enrollment ends May 2, visit <u>tech.msu.edu</u> to register. If past May 2 and you would still like to enroll, please contact Greg Mason at gmason@msu.edu

#### **May 7 – <u>Advanced Topics in HPCC: Making Your Research Go Faster</u> 1:30pm - 4:30pm in 403 Computer Center**

This event is provided to continue to build off of the Introduction to High Performance Computing at MSU workshop. This event is part of Seminars in Research and Instructional Technology. Only 25 seats open! Enrollment ends on May 2, visit <u>tech.msu.edu</u> to register. If past May 2 and you would still like to enroll, contact Dirk Colbry at colbrydi@msu.edu

May 8 – <u>HPCC Regularly Scheduled Biannual Maintenance Outage</u> The HPCC will be unavailable at this time due to our regularly scheduled biannual maintenance.

#### May 9 - RTSF Core Seminar Series- "iCER"

2:30pm - 3:30pm in BPS 1440, iCER Seminar Room Take this opportunity to learn how iCER capabilities and services can help you, specifically related to tools provided for bioinformatics research. Snacks and drinks provided!

#### May 19 - Lightening Talk

10:00am - 11:30am in BPS 1440, iCER Seminar Room An exciting and intriguing fast paced seminar covering 9 topics in quick 10 minute presentations. Topics include Virtual Compute Laboratory, DDT, MAP/Performance Report, MKL, Condor, Globus Plus, Hadoop-ondemand, Galaxy, and Navigating iCER's Resources. Snacks and drinks provided!

# May 29 – Facundo Gomez - Statistically Probing the Merger History of the Milky Way

2:30pm - 3:30pm in BPS 1440, iCER Seminar Room During this talk, we will discuss how semi-analytic models of Galaxy formation, coupled to cosmological N-body simulations, can allow us to constrain the Milky Way merger history.

#### **Upcoming Opportunities**

June 9 – NSF Critical Techniques and Technologies for Advancing Big Data Science & Engineering (BIGDATA). Applications due on June 9! <u>For</u> details or to apply, click here.

June 15 – Experiencing HPC for Undergraduates Program. Applications due June 15! For Details or to apply, click here.

June 19 – NIH Big Data to Knowledge (BD2K) Grant. Applications due June 19! For details or to apply, click here.

#### In need of assistance with grant opportunities?

iCER is happy to help coordinate the NIH Big Data to Knowledge Initiative and/or the NSF Critical Technique and Technologies for Advancing Big Data Science & Engineering grant opportunities. Please let us know if you are interested in being part of either of these BIGDATA proposals by filling out a ticket with your request at <u>contact.icer.msu.edu</u>.



Catch the full video recap of iCER at the 2014 MSU Science Festival!

You can also find us on Twitter and YouTube



Do you know about an event, opportunity, job posting, or general news that would be of interest to our community? We would love to hear about it! Email icer@msu.edu and we will get the word out. All submissions will be posted at the discretion of the iCER Communication Coordinator.

# iCER Monthly Bulletin / June 2014



MICHIGAN STATE UNIVERSITY

### Institute for Cyber-Enabled Research

#### Investigating Marek's Disease with Hans Cheng: An iCER Research Highlight

If you're like most people, you've recently eaten chicken. This is because poultry is the most popular meat consumed in the U.S., and this trend is projected to grow to 2020 and beyond. Primarily due to advanced poultry breeding programs, tremendous progress in producing chickens has been made to meet the growing demands of consumers.

Several major issues confront the poultry industry today. With high-density chicken rearing, controlling infectious diseases are critical for sustaining economic viability, maintaining public confidence, and enhancing animal welfare. Among poultry diseases, Marek's disease (MD), a T cell cancer caused by the Marek's disease virus



The long-term focus of Dr. Hans Cheng and his lab has been to increase genetic resistance to Marek's disease in chickens.

(MDV), continues to be at or near the top of the list of concerns. Alarm about MD is enhanced by the unpredictable and spontaneous vaccine breaks that result in devastating losses to poultry farms... Continue reading this story



# Don't forget to register for one, or both, of the VSCSE Summer School courses!

iCER is excited to host two VSCSE Summer School courses beginning this month at MSU! Introduction to GPGPU Programming is a mixture of lectures and labs and introduces all levels of parallelism as well as common approaches for parallelization. Data Intensive Summer School focuses on the skills needed to manage, process and gain insight from large mounts of data. It is targeted at researchers from the physical, biological, economic and social sciences that are beginning to drown in the data. Registration is an

easy 2-step process and we encourage you to sign-up now to secure a place, as classes are beginning to fill and seating is limited. Lunches will be provided to all attendees. An iCER sponsored reduced rate and "hardship fellowship grants" are available. *Continue for more details and registration* 



#### Take Your Child to Work Day: Video Recap

Each year iCER participates in the MSU Take Your Child to Work Day, a campus wide event. This year's theme was "Plant a Seed: Grow a Future." The program focuses on children ages 8 through 14 with the goal in mind that we want to expose girls and boys to their future careers along with family and community responsibilities. It gives them a hands-on, fun opportunity to view career choices at MSU and think about their futures in a new and exciting way.



#### **Upcoming iCER Events**

June 13 – <u>RTSF Core Seminar Series-</u> "Proteomics and Bioinformatics" 2:00pm - 3:00pm in BPS 1440, iCER Seminar Room

Take this opportunity to sit in on "Proteomics and Bioinformatics" presented by Curtis Wilkerson. Snacks and drinks provided for attendees!

June 16 - 20 – <u>Harness the Power of GPU's:</u> Introduction to GPGPU Programming

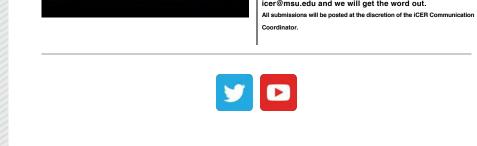
June 30 - July 2 - Data Intensive Summer School

#### Research Opportunities

June 9 – NSF Critical Techniques and Technologies for Advancing Big Data Science & Engineering (BIGDATA) Applications due June 9! Details here.

June 15 – SC14 Experiencing HPC for Undergraduates Program Applications due June 15! <u>Details here</u>.

June 19 – NIH Big Data to Knowledge (BD2K) Grant Applications due June 19! Details here.



#### <u>www.icer.msu.edu</u> | 517.884.3600

# iCER Monthly Bulletin / July 2014



MICHIGAN STATE UNIVERSITY

# Institute for Cyber-Enabled Research

# *Connecting Chemistry and Mechanics via Multi-scale Simulation Methods*

At the Materials Simulation for Clean Energy (MSCE) Lab, Yue Qi and her group develop multiscale simulation methods to design materials atom by atom. They screen materials chemistry by solving quantum mechanical equations to predict the properties that are difficult to measure experimentally. They also work to simulate deformation and reaction processes that involve millions of atoms using molecular dynamics with faster and... <u>Continue reading this article</u>



Yue Qi, Associate Professor, MSU Department of Chemical Science and Material Engineering

### In a Galaxy Not So Far Away

iCER is pleased to announce that we have installed and tested a working instance of the Galaxy Bioinformatics web



service. There are currently tools for SNP discovery, RNASeg Analysis,

The Galaxy team is a part of BX of from State, and the Bulloux of In other based partners for out a relation to provide a relation. The Calaxy Transit I Computer Science Adjustments at Ensury Environments. The Calaxy Project is in The Institute for CyberCommon at Penn States, and Ensure University.

Read-mapping, and other miscellaneous tools. If you are not familiar with Galaxy and would like more background information on the Galaxy project, see *galaxyproject.org*. If you are interested in using Galaxy at MSU, contact us via our *web-contact form* so that we may set up your account.

# 2014 Virtual School of Computational Science and Engineering Recap

This summer, Michigan State University joined with a national group of geographically dispersed, prominent universities as host sites for advanced computational workshops organized by the Virtual School of Computational Science and Engineering (VSCSE). The VSCSE is a virtual organization that delivers computational science curriculum to accelerate the ability of researchers to leverage emerging computational resources to advance science and engi... *Continue reading this article* 



The seminar room fills up with participants ready for the VSCSE "Data Intensive" Summer School course



priority access to purchased cluster resources support infrastructure of racks network switches cabling/support servers cooling and power infrastructure

### Learn more

# Quantum Chemistry Package Gaussian 09 now available at iCER

# Upcoming iCER Events

### July 14 - 18, 8am - 12pm – <u>Lady Spartans:</u> Women in Engineering (WIE)

This event is aimed at young women and is hosted by the College of Engineering/Women in Engineering. Take this opportunity to attend university tours and gain exposure to various engineering majors! <u>Details here</u>

### August 23, 10am - 12pm – <u>Graduate School</u> Welcome and Resource Fair

This event is sponsored by The Graduate School and is hosted for new and returning graduate students of MSU. iCER will be present at the resource fair to provide information to all attendees. <u>Details here</u>



Do you know about an event, opportunity, job posting, or general news that would be of interest to our community? We would love to hear about it! Email us at icer@msu.edu and we will get the word out.

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MICHIGAN STATE UNIVERSITY

### Institute for Cyber-Enabled Research

#### Software Updates

iCER will be updating the default versions of MATLAB, PGI, CUDA, and the MKL software titles on August 12th. All users that use compiled MATLAB codes will be affected. For more information on the upcoming software updates, please visit the *full post here*.

#### New Large Memory Cluster

iCER is finalizing installation of the Intel14-XL cluster, which has 48 or 96 cores and 1-6 TB of RAM per node. The first set of nodes are now available to buy-in users, and will be available to the general community later this week. If interested, see *further details here*.

#### New Remote Desktop Gateway

The new RDP Gateway provides a faster and easier to use interface for programs that use remote graphics. For more information, please visit the *<u>full post here</u>*.

#### **MSU Global Portal**

Users can now connect to Globus Online with their MSU NetID credentials: <u>globus.msu.edu</u>. For further information about Globus Online, please visit the <u>full post here</u>.

#### New Hardware Evaluation Gateway

iCER is please to announce the launch of eval.hpcc.msu.edu, which provides access to development nodes that are not part of our main cluster for benchmarking and debugging. Multiple alternative architectures and accelerators are currently available, and more are on the way. More information is available in the Announcements blog and can be seen by visiting the <u>full post here</u>.

#### Upgrading to NSF v4

Currently, iCER is in the process of changing the protocol that provides home directories to the cluster from NFS version 3 to 4, to improve security, reliability, and usability. It will be transparent to users and no action is required. For further information about this migration, please see the <u>full post here</u>.

#### Swelling of the human airway

Professor Thomas Pence and Dr. Kun Gou in the Department of Mechanical Engineering at Michigan State University are working on a research project entitled "New mathematical models for the large strain swelling response of biological tissues." This is an international project sponsored by the Qatar National Research Foundation in collaboration with Carnegie Mellon University in... <u>Continue reading</u>



Dr. Kun Gou and Professor Tom Pence share their research focused on the swelling of the human trachea

#### Lady Spartans: Women in Engineering!

During the month of July, a of enthusiastic group of young women visited the High Performance Computing Center while participating in "Lady Spartans: Women in Engineering", a week long camp held on the MSU campus. Throughout the week, the group had the opportunity to explore engineering on a deeper level by gaining knowledge and being exposed to hands-on experiences. Take a look at the video to hear from participants!





#### **Research Opportunities**

#### August 14, 8:30am - 4pm – Intel Phi Coprocessor Developer Training

This one-day training will provide software developers the foundation needed for modernizing their code to take advantage of parallel architectures found in both the Intel Xeon processor and Intel Xeon Phi coprocessor. **Details here** 

#### Parallel Processing Course: Fall semester

CSE 891 Section 1: Parallel Computing: Fundamentals and Applications. Fall 2014, 3 credits, M/W 3:00pm – 4:20pm. <u>Details here</u>



#### Upcoming iCER Events

August 14, 1pm - 3pm - "iCER-Cream Social Series" kickoff! Topic: RNAseq

#### August 23, 10am - 12pm – Graduate School Welcome and Resource Fair

This event is sponsored by The Graduate School and is hosted for new and returning graduate students of MSU. iCER will be present at the resource fair to provide information to all attendees. **Details here** 

#### October 23 & 24, Cyberinfrastructure Days

This free two-day conference brings faculty and students together to understand the benefits that cyberinfrastructure can bring their scholarly pursuits, to see what others are doing with cyberinfrastructure, and to learn what resources are available on campus, across institutions, and nationally. Features: special guest speaker presentations, interactive workshops, poster session contest, a resource fair, and plenty of free food and networking opportunities. **Details here** 



#### Contribute to the newsletter!

Do you know about an event, opportunity, job posting, or general news that would be of interest to our community? We would love to hear about it! Email us at <u>icer@msu.edu</u> and we will get the word out.

All submissions will be posted at the discretion of the iCER Communications Coordinator.



# iCER Monthly Bulletin / September 2014



MICHIGAN STATE UNIVERSITY

# Institute for Cyber-Enabled Research

## Account Renewals

HPCC will be sending an email alert to expiring accounts (of graduated Spartans and non-MSU users) in the next couple of weeks.

- Expiring accounts will have 30 days to get their account re-sponsored to maintain access.
- Data in deactivated accounts will be stored for six months.
- Instructions for renewal will be provided in the email.
- \*\* Some MSU students will also need to renew their accounts if they delisted themselves from the MSU public search completely.

## Acknowledgements

MSU has generously sponsored the Institute for Cyber Enabled Research (iCER) as a campuswide resource for MSU researchers. For continued support, we need evidence that iCER is contributing to research. We would appreciate if you please contact us at <u>http://contact.icer.msu.edu</u> to share information about new research software, publications, and/or grant awards that benefited from MSU's HPCC and/or iCER resources.

- Software (<u>http://icer.msu.edu/software)</u> highlights research software that has been developed by Michigan State University researchers
- Publications (<u>http://icer.msu.edu/publications</u>) highlights recent iCER-related research at MSU. We accept bulleted list, BibTeX and EndNote entries.
- Funding Awards (<u>http://icer.msu.edu/funding-highlights</u>) highlights research awards related to iCER and HPCC resources.

 Other announcements (<u>http://wiki.hpcc.msu.edu/x/QAGQ</u>) relating to scientific computing and the MSU community.

Thank you for your help in ensuring that iCER and the HPCC remain a valuable resource in the MSU community!

### Intel14-xl Buy-in Opportunity

Intel14-xl (extra large) buy-in round 2 – This is your last chance to be included on the intel14-xl buy-in opportunity. Investors can also still buy into the existing main intel14 cluster. Prices include:

- intel14 Option 1 (20 core, 64GB base node): \$3805.82\*
- intel14 Option 2 (20 core, 256GB large memory node): \$5338.46\*
- intel14 Option 3 (20 core, 128GB NVIDIA K20 GPU node): \$7899.15\*
- intel14 Option 4 (20 core, 128GB Intel Xeon Phi 5115p node): \$9042.91\*
- intel14-xl Option 1 (1TB RAM, 48 cores): \$29,979
- intel14-xl Option 2 (1.5 TB RAM, 48 cores): \$34,989
- intel14-xl Option 3 (3 TB RAM, 48 cores): \$60,995
- intel14-xl Option 4 (6 TB RAM, 96 cores): \$142,772

\* Some funding agencies require that principal investigators purchase "fully working nodes" which can be removed from the cluster. Since the intel14 nodes are blade components, users purchasing intel14 nodes may also need to purchase an intel14 Chassis (\$1216.44). If you are interested in this opportunity, please **contact us**.

## **Upcoming Trainings**

iCER offers a variety of training in High Performance Computing (HPC). Workshops provide hands-on training in programming principles and techniques in HPC. Many of these events are free for MSU students and researchers but registration is required. Visit <u>iCER Events</u> for full course descriptions and registration details.

- 9/30 10/1: Software Carpentry Workshop
- 10/2-10/3: RNAseq Tools Workshop



#### 10/7: XSEDE OpenMP Workshop

#### 10/23: CI Days Training Opportunities

- Introduction to HPC at MSU
- Introduction to Python
- Top 10 Productivity Tools in MATLAB/ Programming with MATLAB
- Advanced Topics in HPC: Making Your Research Go Faster
- Advanced Python
- Optimizing Your MATLAB Code

### 11/3 – 11/6: <u>Computational Chemoinformatics</u> and Docking Studies

The third annual Cyberinfrastructure Days will be October 23 & 24, right here on campus! Don't miss your opportunity to attend this <u>free event</u>!

## Contribute to the newsletter!

Do you know about an event, opportunity, job posting, or general news that would be of interest to our community? We would love to hear about it! Email us at <u>icer@msu.edu</u> and we will get the word out.

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# *iCER Monthly Bulletin*

# October 2014

MICHIGAN STATE UNIVERSITY

# Institute for Cyber-Enabled Research

## Cyberinfrastructure Days is right around the corner!

The third annual Michigan State University **Cyberinfrastructure (CI) Days** event will be held on October 23–24, 2014. CI Days presents an opportunity for faculty and students to understand the benefits that cyberinfrastructure can bring their scholarly pursuits, to see what others are doing with cyberinfrastructure, and to learn what resources are available on campus, across institutions, and nationally. The free, two-day event features six interactive workshops, four breakout sessions, special guest speaker presentations, panel discussion, a resource fair featuring various CI resources, networking opportunities, as well as a poster session with the chance to win **cash prizes** up to **\$200!** 

CI Days registration will be closed on *Friday, October 17th*. Space is limited! Be sure to **register now** to ensure your space.

Posters and abstracts are due on **Tuesday, October 14th**. To participate, send these items to <u>cidays@msu.edu</u>. 1st place will be **awarded \$200**, 2nd place will be **awarded \$150**, and 3rd place will be **awarded \$100**! Full poster session details and judging criteria may be <u>seen here</u>.

# Additional Office Hours

In addition to our regularly scheduled open office hours each Monday from 1pm - 2pm, we will also begin hosting Thursday office hours from 1pm - 2pm. Office hours are held in the Biomedical and Physical Sciences (BPS) Building, Room 1455a.

# Dr. Benjamin Ong Leaves iCER

Please join us in wishing Dr. Benjamin Ong, Director of Research, well in his future endeavors and to thank him for his service and many contributions to the Institute for Cyber-Enabled Research over the past four years. Dr. Ong is taking on a new position as Assistant Professor in the Department of Mathematics at Michigan Technological University in January 2015. A public farewell reception will be held in honor of Dr. Ong on **Monday**, **November 24 from 4:00-7:00pm** in the Red Cedar Room of the Kellogg Center. Food, drinks, and good times will be served. If you wish to attend, please RSVP to **byerrumc@msu.edu**.



# Photonic Devices for Sensing and Communication

Dr. Adam Mock, Electrical Engineering Professor at Central Michigan University, an iCER affiliate institution, sits down to share his research focus with us. Take a look at his <u>Research</u> <u>Highlights video</u> to learn about how he performs computational electromagnetic modeling of micrometer and nanometer scale photonic devices or read the **full article here**.



# **Upcoming Trainings**

Details of upcoming trainings may be seen by clicking the title of the workshop or by visiting **icer.msu.edu/events** 

- 10/13 Workshop Series 2014: Data Analytic Tools for Social Science
- 10/15 Essential CUDA Optimization Techniques Webinar
- 10/17 Analyzing Amplicon Sequence Data With mothur
- 10/23 Intro/Advanced HPC, Python, & MATLAB Workshops (CI Days

#### Event)

- 10/29 Optimizing LAAMPS for Intel Xeon Phi Coprocessors Webinar
- 11/3 Computational Chemoinformatics and Docking Studies
- 11/5 XSEDE MPI Workshop











# *iCER Monthly Bulletin*

# November 2014

MICHIGAN STATE UNIVERSITY

Institute for Cyber-Enabled Research

# iCER Travels to SC14

We're off to New Orleans, LA to attend <u>SC14</u> once again during November 16–21. As the event website shares, "For over two decades, the SC Conference has been the place to build and share the innovations that are making life changing discoveries possible." iCER will be exhibiting in a shared booth collaborating with Advanced Research Computing (ARC)



from the University of Michigan to enhance Michigan's national and international presence and competitive edge in advanced computing. In addition to the many items on the **SC14 schedule**, iCER will be hosting a **Spartan Social** on Tuesday, November 18 from 5p–7p. If you're in the area, come check us out! Appetizers and party favors provided!

# Regional Climate Modeling – Nathan Moore

Dr. Nathan Moore, Assistant Professor in the College of Geography, shares with us that his research interests lie within: Regional climate modeling and climate variability; measuring and modeling impacts of human activity on the hydrologic cycle and surface-atmosphere interactions; regional and global land use/land cover change. Watch his **Research Highlights Video** to learn more or read the <u>full</u> <u>article here</u>.



# Working Hard to Increase Training

This has been an exciting semester for training at iCER! Thus far, iCER has offered a dozen hands-on workshops for researchers. Workshops ranged from multi-day domain specific training in mothur for sequence analysis and computational chemoinformatics, to basic computational training in the Linux command line, high performance computing, parallel programming languages, MATLAB and Python. Workshop participants included faculty, staff and graduate students from 5 colleges, over 26 departments and domains ranging from Engineering and Life Sciences to Social Sciences. In all, approximately 200 MSU researchers have participated in iCER training this semester. Continue to **full article here**.

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# Upcoming Trainings

Details of upcoming trainings may be seen by clicking the title of the workshop or by visiting **icer.msu.edu/events** 

# 12/4 - XSEDE Open ACC Workshop

farewell reception will be held **Monday, November 24 from 4:00-7:00pm** in the Red Cedar Room of the Kellogg Center. Food, drinks, and good times will be served. If you wish to attend, please RSVP to **byerrumc@msu.edu** by November 18th.





517-353-9309



# *iCER Monthly Bulletin*

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### Important! System maintenance outage; scratch space moving

The HPCC will be unavailable on Tuesday, January 6th for our regularly scheduled biannual maintenance. Jobs that would normally run during the maintenance window will start after the system work is completed. Jobs that will be able to complete before the maintenance window begins will still run.

As part of this scheduled maintenance, the HPCC staff will be moving the current Scratch file system to make room for a new one to be installed later this year. There is a 2% chance of scratch losing all data as part of this move, please make sure you back up and data on the scratch space before the outage.

If you have any questions about this planned outage, or anything else related to the HPCC in general, please contact HPCC staff at via the **web form**.

## **Origin of Electric Organs - Jason Gallant**

MSU Zoology Professor, Jason Gallant, is broadly interested in the genomics basis of phenotypic evolution and diversification, particularly in animal phenotypes that are related to communication behavior. Currently, Dr. Gallant's laboratory focuses on two main projects; The origin of electric organs and the evolution of communication diversity. Watch his full **Research Highlights Video** to learn more or read the **full article.** 



## **Upcoming Trainings**

Details of upcoming trainings may be seen by clicking the title of the workshop or by visiting icer.msu.edu/events

### 12/16 - Intro to HPC at MSU

- 12/16 HPCC Advanced: Making Research Go Faster
- 12/17 Manage, Share and Move Big Data

# Share vour thoughts!

In the coming year, we will be doing a complete web redesign and would appreciate your feedback! By taking a short survey, you will contribute invaluable information on how we may better serve you. Take website survey!



# **Blue Waters** Graduate Fellowship

The application period for the Blue Waters Graduate Fellowship is now open. Fellowship recipients will receive a stipend of \$38,000 for the year-long fellowship and up to a \$12.000 tuition allowance. Applicants should be in the second or third year of their PhD program and engaged in research that can take advantage of the Blue Waters supercomputer. Deadline to apply is February 4th. **Details** here.







517-353-9309



