

## iCER Director's News

*March // 2014*



### ***A word from our Director***

After completing my first six months at iCER, I want to give my thanks for such a warm Spartan welcome here at MSU. I can say it has been nothing but a wonderful experience thus far. Our office has been busy these last few months working to accomplish new goals and take on new initiatives, like this Director's Newsletter. As the iCER Director, I believe it is important to reach out and communicate with our users and supporters. In an effort to more effectively connect with you all, I will be sending out iCER updates and key information during the first week of each month. Our hope is that this will be a

helpful tool used to educate and inform, while building upon our relationship with iCER supporters.

We are pleased to announce members of our current team have taken on new positions within the iCER office. Kelly Osborn has been named Director of Business Operations, Dr. Dirk Colbry has been named the Director of HPCC, and Dr. Ben Ong has been named the Director of Outreach. With these recent transitions, we have seen great things happening already. We have hired four new team members in the last two months- you can check below for more info on that! With our team rapidly expanding, we are still looking to hire an iCER Director of Training. Further details can be found at [jobs.msu.edu](http://jobs.msu.edu), posting #9024.

The big buzz around the office is the installation of the Intel 14 cluster. This new hardware was installed in record time taking only one month from its arrival on campus to being put into production for beta users. This purchase includes 220 nodes with 4400 CPU cores and between 64 GB to 256 GB of memory per node. HPCC Director, Dr. Colbry comments, "I am excited simply due to the fact that everything is bigger, stronger, and faster, which significantly shortens time to discovery."

-Dr. Kennie Merz

### ***Meet our new team members!***

#### **Dr. Matthew Scholz // Research Specialist**

Matt traveled to MSU all the way from Santa Fe, New Mexico where he previously worked at Los Alamos National Laboratory - Genome Sciences working as a Postdoctoral Scientist. Matt earned his Ph. D. in Microbiology from the University of Tennessee. His major goal at iCER is to improve the ease of use of iCER's computational capacity for biological scientists by applying the most up to date software, assisting with training users, and implementing standardized pipelines wherever possible.

#### **Taylor Lundgren // Secretary**

A recent graduate from MSU, Taylor spent just over one year working at the Lansing Center as an Event Coordinator before joining our team. She will be helping to plan and coordinate upcoming iCER events and travel needs, assist with communication efforts, provide administrative support, and everything else in between!

#### **Jessy Howe // Communications Coordinator**

A recent graduate from Central Michigan University, Jessy joined iCER after working on the Strategic Communications team at Consumers Energy. She will be working to increase engagement and communication on behalf of iCER through new marketing materials, social media, news articles, event coordination and more.

#### **Xianxing (Adele) Han // Temporary Videographer Specialist**

Adele, a December 2013 graduate of MSU, is coming to iCER with her expertise in the exciting world of videography. She will be helping iCER ramp up our visual outreach with promotional videos, training videos, and more. Stay tuned to see what great new things iCER is doing!

### ***Introduction to the Intel 14 cluster***



Based on the next generation Intel Xeon Ivy Bridge E5-2670v2 processors, these new compute cores are up to 2-3 times faster than our existing system, significantly shortening time to discovery. All of the compute nodes are tied together with the latest low latency 56 Gb/s FDR Infiniband connections.

In addition to the more powerful CPUs and the high speed network interface, the new system includes 80 NVIDIA K20 GPUs and 56 Xeon Phi 5110P accelerator cards. Combined, this new hardware is theoretically 10 times more powerful than all previous HPCC systems combined, and would put the HPCC's overall compute capability within the top 500 fastest supercomputers in the world. This extra capacity will significantly improve throughput, and the scheduling system is being adjusted to allow for bigger jobs and shorter queue times. The updated HPCC system is specifically designed to target the following research workflows:

- **Large Memory Jobs (Bioinformatics, Big Data Analytics)** - Augmenting the HPCC's existing set of 2TB compute nodes, all nodes in the new Intel 14 cluster will have at least 64 GBs of memory. In fact, there are 24 nodes that have 256 GBs of memory and 64 nodes that have 128 GBs of memory.
- **CPU Intensive Jobs** - The new Intel Xeon Ivy Bridge processors support the AVX instruction set which allow for significant improvements in vectorization of compiled code. It is not uncommon to see 2-3 times speedups over intel10 hardware with just a recompile of a program. Additionally, the new cluster more than doubles the total number of cores available on the HPCC.
- **Large Shared Memory Jobs (ex. OpenMP)** - Each new node has 20 CPU cores, allowing for higher core count shared memory jobs. Additionally, users familiar with OpenMP may also be able to take advantage of offloading some of the work to the new Intel Xeon Phi accelerator cards.
- **Large Shared Network Jobs (ex. MPI)** - The low latency 56 Gb/s FDR Infiniband connections enables faster inter-node communications. Also with the larger total number of CPUs on the system, the HPCC is increasing the maximum number of computing cores that an HPC user can utilize from 144 cores to 384 cores. Priority is given to larger jobs that can take full advantage of the new hardware that are not easily run on other systems.
- **General Purpose Graphical Processing Unit (GPGPU) jobs** - The new NVIDIA K20 cards are significantly faster than the NVIDIA C1060 that are still available in the gfx10 hardware. These new cards offer over 16 times faster double precision performance.
- **Hybrid parallelization** - For the first time the HPCC can accommodate our most advanced users that want to run hybrid jobs that include accelerators, shared memory and/or shared network parallelization. This type of software is on the cutting edge of research and will likely be required for all research code to take advantage of the worlds biggest computers now and into the future.

In 2010, Central Michigan University was the first institution to invest in the Michigan State University HPCC, establishing iCER as a regional center in scientific computing. With this current hardware purchase, iCER has established partnerships with two additional institutions; Kettering University and the USDA. All three institutions contribute funds to the HPCC, which allows us to construct a larger system that is more efficient than any individual organization effort. iCER is in negotiations with two other investor institutions and is actively seeking other partnerships to expand our regional influence and research capabilities.

## iCER Director's News

April 2014

### ***Cluster ceremony attracts attention***

On March 14, the Engineering Deans Conference Room was abuzz with excitement by several folks joining iCER in celebration of the High Performance Computing Center's new cluster. As guests enjoyed breakfast pastries and coffee, friends and supporters mingled with one another around the room.

iCER Director, Kennie Merz, took the podium for a brief presentation noting past leaders, milestones made, and the direction we are continually working to see iCER go towards in the future. "Down the line, we want to collaborate with other schools in the state to really continue to build the computational resources in the state of Michigan," he expressed.

Following a round of applause, the crowd poured down the hall and made way to the High Performance Computing Center for tours by our HPCC staff. Many of the attendees were engaged asking questions and snapping photos. HPCC tours created an environment that sparked great conversations amongst guests. The State News was also present at the event interviewing. View the [published article here!](#)



### ***Joseph Zichis Endowed Chair in Chemistry***

iCER Director, Kennie Merz, was honored and named the Joseph Zichis Endowed Chair in Chemistry at his investiture ceremony held March 14th in the Christman Lounge of the Wharton Center for Performing Arts.

Rob Maleczka, Department of Chemistry Chairperson, commented, "It is exciting to have been able to recruit a nationally recognized scholar such as Kennie to occupy the Zichis Chair."

The Joseph Zichis Endowed Chair in Chemistry was created to recognize Joseph Zichis's passion for research and his many contributions as a scientist and inventor.



*Rob Maleczka and Kennie Merz pose for a photo after Merz was presented the chair medallion.*

### ***Meet our new team member!***

Please help us welcome Anthony Parker who has joined the iCER team as our newest System Administrator. He earned his Bachelor of Science in Informatics from Indiana University where he also worked for the Department of Telecommunications for the previous 10 years. We are excited to have Anthony join our office!



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## A letter from our Director | June 2014

### *A look at summer 2014*

As summer has finally arrived at Michigan State University, we have transitioned into our new seasonal items at the iCER office and we have never been busier. With the installation of [Intel14](#), the last few months have been very exciting as we have brought this machine into full service. It is satisfying to see that the MSU community has rapidly begun carrying out their science on the new cluster - this has happened so rapidly that we have already reached full capacity!



*iCER Director, Dr. Kennie Merz*

We are still continuing to build up the iCER team to better serve our users as well as the MSU community. This summer we will be welcoming Dr. Yongjun Choi, our newest Research Specialist with emphasis on software development. In the near future, we will also introduce a Director of Training, whose main responsibility will be expanding our ability to reach out to our user community with the various workshops and classes hosted by iCER.

Currently, we are preparing the final details of the Virtual School of Computational Science and

Engineering (VSCSE) Summer School beginning this month featuring two separate course options. I encourage you to think about attending one, or both, of these educational summer schools. More details on VSCSE can be found on the iCER website under “[events & workshops](#)”. Furthermore, we have been working hard to plan the third annual MSU Cyberinfrastructure (CI) Days this fall! We are happy to announce that CI Days will take place on October 23 - 24, 2014. Keep an eye out for upcoming news on this event.

As always, my door is open to the MSU community to discuss iCER and its role in the computational sciences at MSU. I wish you a fantastic and productive summer!

Dr. Kennie Merz

[www.icer.msu.edu](http://www.icer.msu.edu)



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## A letter from our Director | July 2014

I hope everyone is having a wonderful and productive summer! In the coming monthly updates, I will be highlighting recent happenings at iCER and luckily I have many to choose from.

iCER has an extensive software “stack” that supports researchers from biology to the social sciences, but a missing title has been Gaussian 09. We have had many requests for this title from researchers interested in studying molecular structure. This is an *ab initio* quantum mechanics package originally developed in the late John Pople’s laboratory (1998 Nobel Prize in Chemistry) at Carnegie Mellon University. We recently acquired the rights to use this program at the HPCC and details of how to gain access can be found by [clicking here for instructions](#).



*iCER Director, Dr. Kennie Merz*

I’d also like to take this opportunity to welcome Dr. Yongjun Choi to the iCER team. He brings extensive experience in software development and code optimization/parallelization along with research expertise in the modeling and simulation of gas, particle and fluids, as well as plasma surface interactions using Monte Carlo/PIC/CFD/hybrid codes. Yonjun’s role will be to facilitate the development and optimization of codes supported by iCER. Please stop by the iCER offices to welcome Yongjun to MSU and explore possible

collaborative projects with him.

Finally, I'd like to wish everyone a happy and healthy 4th of July!

Dr. Kennie Merz

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## A letter from our Director | August 2014

It's hard to believe, but the dog days of summer are here and the Fall 2014 semester is less than a month away. Summer has been a very busy time for all of us at iCER with new staff searches underway and several new hires coming on board. In particular, iCER has had a strong commitment to training in the computational sciences since its inception. To take our training efforts to the next level, we have been actively seeking out a Director of Training. I am happy to report in this newsletter that we have successfully filled this position.

I'd like to take this opportunity to welcome our new Director of Training, Ms. Camille Archer, to the iCER team. Camille is an MSU graduate and has worked as a data analyst in the healthcare industry, as well as an educator. She will be responsible for organizing and participating in training courses aimed at helping MSU researchers make effective use of high-performance computing (HPC) resources. Quoting Camille, "I am a big believer in user-focused training. For this reason I'm invested in meeting with researchers across campus to better understand their HPC training needs and the ways in which iCER can come alongside to provide opportunities for purposeful learning." Please take Camille up on her offer and stop by the iCER offices to both welcome and explore training needs with her.



*iCER Director, Dr. Kennie Merz*



Finally, I'd like to wish everyone a happy and healthy end of summer!

Dr. Kennie Merz

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## A letter from our Director | September 2014

The excitement of the fall semester is upon us, with new friends to be made, new classes to teach and attend, and a highly ranked football team to cheer on to victory! At iCER, we continue to be very busy on many fronts aimed at expanding our ability to positively impact the teaching and research efforts of faculty and students at MSU. Along these lines we have two openings for Research Specialists within iCER, which will expand our ability to support the computational and bioinformatics communities at MSU. The full descriptions of these positions can be found at [icer.msu.edu/employment](http://icer.msu.edu/employment). If you have any questions regarding these positions, we encourage you to please contact iCER. If you know of qualified candidates, please alert them to these openings!

Every year, we co-sponsor of MSU's Cyberinfrastructure Days (CI Days) and this year we have an exciting slate of events associated with this event. This two-day free event, held on October 23–24, offers workshops to hone or improve your computational bag-of-tricks, talks from nationally recognized speakers on digital humanities and bioinformatics, a poster session for students and faculty to highlight their computational research efforts with the chance to win cash prizes, a resource fair, and finally several social events. Full details of the program can be found by visiting [vprgs.msu.edu/ci-days](http://vprgs.msu.edu/ci-days). Registration closes on October 17, so please register today so you can enjoy the events of CI days.



*iCER Director, Dr. Kennie Merz*

I wish you a fun and productive semester!

Go Sparty!

Dr. Kennie Merz

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MICHIGAN STATE UNIVERSITY

Institute for Cyber-Enabled Research

## A letter from our Director | October 2014

The High-Performance Computing Center (HPCC), within the Institute for Cyber-Enabled Research (iCER), is celebrating its 10th year of existence. In 2005, the HPCC was formed via a grassroots effort by a coterie of faculty at MSU with a strong interest in computational sciences. The HPCC facility was established to solidify the existence of high-performance computing at MSU and led to the formation of iCER in 2009. The HPCC has grown steadily in size, compute power and is staffed by an accomplished and skilled support group that works behind the scenes maintaining and updating our hardware palette. In the coming year, we will begin plans to acquire a new machine that will singularly increase our available compute power at MSU. With MSU's continuing commitment to iCER, the HPCC, the creation of a new department focused on the computational sciences and a new Datacenter on the horizon, the future of high-performance computing at MSU is, indeed, bright. This important milestone will be celebrated at the upcoming Cyberinfrastructure Days (CI Days). If you have not registered yet, full details can be found at [vprgs.msu.edu/ci-days](http://vprgs.msu.edu/ci-days). I hope to see you there.



*iCER Director, Kennie Merz*

The HPCC and iCER continue to enjoy strong support from The Office of the Vice President for

Research and Graduate Studies (VPRGS), The Vice Provost for Libraries, Computing and Technology (VPLCT), the National Superconducting Cyclotron Laboratory (NSCL), The Office of the Provost, The College of Social Science, The College of Engineering and The College of Natural Science. Through these groups, MSU has generously sponsored the Institute for Cyber-Enabled Research (iCER) as a campus-wide resource for MSU researchers. For continued support, we need evidence that iCER is contributing to the ongoing research effort of the university. We would appreciate if you please contact us at [contact.icer.msu.edu](mailto:contact.icer.msu.edu) to share information about new research software, publications, and/or grant awards that benefited from MSU's HPCC and/or iCER resources.

- Software ([icer.msu.edu/software](http://icer.msu.edu/software)) highlights research software that has been developed by Michigan State University researchers.
- Publications ([icer.msu.edu/publications](http://icer.msu.edu/publications)) highlights recent iCER-related research at MSU. We accept bulleted list, BibTeX and EndNote entries.
- Funding Awards ([icer.msu.edu/funding-highlights](http://icer.msu.edu/funding-highlights)) highlights research awards related to iCER and HPCC resources.
- Other announcements ([wiki.hpcc.msu.edu/x/QAGQ](http://wiki.hpcc.msu.edu/x/QAGQ)) 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!

I hope you are enjoying the beautiful Fall season!

Go Sparty!

Dr. Kennie Merz



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## A letter from our Director | December 2014

It's hard to believe that 2014 is almost behind us. It has been an incredibly busy year for iCER as we have extensively expanded our team to better serve the MSU research community in our three core areas of high-performance computing (HPC), training, and HPC-based research project support. The year kicked off with the installation of our latest computer cluster, [intel14](#), which is theoretically 10 times more powerful than all of the previous HPCC systems combined.

We have also been very busy increasing our [training opportunities](#) with the hiring of our Training Director, Camille Archer. We have hosted a number of workshops, webinars, and summer schools focused on effective utilization of HPC resources.

To better support bioinformatics research and training on campus, Dr. Matthew Scholz established the [Bioinformatics Center for Education and Productivity \(BiCEP\)](#) within iCER to serve as a core facility providing expertise and analysis to researchers.

In keeping with iCER's commitment to outreach, we were excited to be a tour site for the [MSU Science Festival](#), [Take Your Child to Work Day](#), and [Women in Engineering Summer Camp](#). Roughly 300 young men and women, ages 8-17, were introduced to computing at MSU and had the opportunity to begin career exploration in this field.

We plan on continuing to expand our research support, training efforts and outreach in the coming year, so we encourage you to stay tuned.



*iCER Director, Kennie Merz*



As mentioned, we have had several additions to our team in 2014. We began with a group of 10 and have grown to 19 team members. New team members include Camille Archer, Training Director; Carey Byerrum, Admin. Assistant to Director; Chun-Min Chang, Research Specialist; Yongjun Choi, Research Specialist; Xiaoxing (Adele) Han, Communications Coordinator; Jessie Howe, Communications Coordinator; Steven Lundback, Information Technician; Taylor Bates, Secretary II; and Anthony Parker, HPC Admin.

We are already in the planning stages for the purchase of another cluster for late 2015/2016 and as part of this process the iCER team attended Supercomputing '14 in New Orleans. This venue allowed us the chance to find out what new technologies are on the horizon and what various vendors are offering in the upcoming year.

Having been in this business now for several decades it still amazes me how far computational resources have progressed. The processor speeds and the expansion of data storage is mind-boggling. We can now purchase 1Pb of data storage for what it would have cost to purchase 25Gb of storage twenty years ago! We look forward to bringing a new cluster to campus and to further expand the available computational resources at MSU to enable cutting-edge science.

Happy Holidays from everyone at iCER!

Go Sparty!

Dr. Kennie Merz

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