MICHIGAN STATE UNIVERSITY | Institute for Cyber-Enabled Research

A letter from our Director | January 2015

After working at iCER for six years, first as a Domain Expert and then as Director of the High Performance Computing Center (HPCC), Dr. Dirk Colbry has decided to take a position in private industry. Effective February 2015, Dirk is taking on a new research and development position at Pixel Velocity in Ann Arbor where he will work on a range of image processing projects. In the interim, I will take over as Director of the HPCC while we conduct a national search to identify our new director. We want to thank Dirk for all his efforts on behalf of iCER and MSU.

A public reception will be held in his honor on **Wednesday, January 28 from 3–5pm** at iCER in the Biomedical & Physical Sciences Building, Room 1440. We encourage you to join us as we celebrate his future endeavors.

Happy New Year from everyone at iCER!

Go Sparty!

iCER Director, Kennie Merz

Dr. Kennie Merz

iCER Director,
Dr. Kennie Merz

February 2015

I'd like to welcome a new member to our Domain Expert team within iCER, Patrick Bills. Pat has nearly 20 years experience designing, integrating, building, and analyzing database systems for a range of research endeavors across campus. Pat has a BS in Mathematics and an MS in Entomology, both from MSU.

Pat has worked on projects in several programming languages, operating systems, statistical analyses, GIS systems, digital media, data management, and relational database systems. He has helped departments and labs on campus build and utilize network and server systems in all major operating systems for researchers and their students. Pat has also taught and mentored students in data modeling, SQL, HTML, and R. Additionally, he currently co-chairs the MSU Web Developer 'CAFE' and has built many web applications to augment research databases. Most recently he was affiliated with MSU Zoology Department. With iCER, he will support the database needs of MSU researchers and will participate in iCER based training in the area of database design and development. Please welcome Pat to our team and look for his upcoming workshops!

Recently, we had to bring the entire HPC system down due to concerns that we were being affected by the GHOST vulnerability. Luckily this was not the case, but it is important for everyone to be aware that while we do everything to protect our systems, attempts to hack computer systems is a modern fact of life. Please protect yourself by ensuring that important data on our systems is stored in our home or research spaces, which are backed up off-site, or back up your data independently off our systems. If you have any further questions about this issue, please contact Andy Keen or myself.

Wishing you a productive spring semester!

Go Sparty!

Kennie Merz

ICER

A LETTER FROM OUR DIRECTOR

iCER Director,
Dr. Kennie Merz

March 2015

With the deep freeze of winter settled into East Lansing, we are suffering our usual downtimes due to cooling issues associated with our server room. The cooling capacity actually decreases as the temperature decreases to when we get below ~0F we have to shut down a large swath of our computing capacity to protect the systems in the HPCC server room. By the end of the month we estimate that the HPCC clusters will have been unavailable to run jobs for ~5 days (122.5 hours). This is nearly 100 CPU-years of work that we will be unable to provide (~7,000 cores * 122.5 hrs. = 850,000 CPU-hours). There was an additional 16 hours in January that we were offline due to this cooling issue. Moreover, we've only been able to run weeklong jobs once this month due to

these issues. We ask that you remain patient as we get through this unusually cold patch.

Behind the scenes we are diligently working on improving the cooling capacity of the server room, while working on a longer-term solution involving the construction of a state-of-the-art server building.

All updates on the emergency cold weather system reservations can be found on the wiki update here. The next weather outage is scheduled for **12AM – 12 PM on 2/26** and from **7PM on 2/26 to 12 PM 2/27.**

Again, thank you for your patience. We hope you are having a productive spring semester!

Go Sparty!

Kennie Merz

ICER
A LETTER FROM OUR DIRECTOR

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April 2015

I frequently get asked about how to keep up with the latest happenings at iCER. At the moment we have 7+ outreach avenues where you can get the latest iCER news, which is summarized below. These various outreach mechanisms cover all the latest information on issues we might be having with the system including Lustre, Moab/Torque, outages due to extremes in temperatures, planned outages for system upgrades, etc. as well as detailed information on upcoming events and training workshops at iCER.

Catch up with us in any of the following ways:

- iCER Website
- Our Wiki, the Wiki Announcements Blog in particular. Important updates such as the Lustre issues that are currently being worked on may be found here.
- iCER Directors Letter and the iCER Monthly Bulletin – 1,976 subscribers and counting! To join our newsletter mailing list, please email icer@msu.edu. All past newsletters can be found on our website.
- Let's connect! You can find us on Twitter, Facebook, and YouTube.
- Message of the Day: Important information can be seen when first logging into the HPCC through our Message of the Day.

We are currently in the process of completely redesigning our website to further enhance our outreach. With this project, we have a number of goals aimed at further improving iCER's communication to our user community. Specifically, we will be adding:

- Systems status page
- Systems utilization page
- A more prominent area for announcements

We very much look forward to rolling out our new website in the fall of 2015, which will continue to increase our commitment to the computing community at MSU. We strive to keep our user community up-to-date on all events at iCER and we always welcome feedback on how we can better keep our users in the loop.

Everyone at iCER hopes you are having a productive spring semester!

Go Sparty, beat Duke!

Kennie Merz

ICER
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May 2015

Over the past thirty years, researchers have seen the role of the computational sciences evolve from being the realm of the cognoscenti to being an essential tool for experts and non-experts alike. Today, researchers from all disciplines want to benefit from the insights provided by the "third leg" of science (the other legs being experimentation and theory). This has led to a wide range of new innovative computational approaches that address a range of contemporary problems in a broad range of disciplines. While most of us sense that having a local supercomputer has benefits, the return on investment for university purchases of relatively expensive supercomputing hardware and support has not been quantified.

To address this issue, the National Science Foundation (NSF) has supported a project to attempt to better establish the impact of local supercomputing resources on the host institution. What the authors found is that institutions with TOP500 supercomputers, ranked according to the LINPACK benchmark, experienced a significant increase in efficiency in the production of research and related outputs. Some disciplines experienced greater increases in efficiency than others. For example, my research field of Chemistry received the greatest benefit.

Please take a moment to review the article, as it proves, yet again, how crucial investment in high performance computing is for cutting-edge research universities. With MSU's existing resources, the formation of the new [Department of Computational Mathematics, Science and Engineering](), and hopefully the realization of a new data center for the university, we are well positioned to benefit from the rapid increase in both the interest and use of computational tools to address important scientific and societal challenges.

Wishing you a productive summer!

Go Green!

Kennie Merz

ICER
A LETTER FROM OUR DIRECTOR

iCER Director,
Dr. Kennie Merz

June 2015

I'd like to welcome a new member to our Domain Expert team within iCER, Xiaoge Wang. Before joining MSU, Xiaoge worked at Tsinghua University in Beijing, China for nearly 20 years. She has her BS and MS in Computer Science from Tsinghua University, and a Ph.D in Computer Science from UIUC.

Xiaoge has over 20 years of experience in scientific computing, especially in the development of parallel algorithms for various science and engineering applications. She has collaborated with faculty members in various academic disciplines, in China and elsewhere, on a wide range of challenging problems including: the design of parallel algorithms for the acceleration of numerical simulations; studies on the infrastructure needed for pervasive computing; and more recent research on machine learning methods for the analysis of signal noise artifacts. Additionally, her extensive experience in international research collaborations, teaching and guidance of students adds strength and diversity to iCER.

Within iCER, Xiaoge will support the needs of MSU researchers in computing algorithms and will participate in iCER based training in the area of parallel algorithm design and development. Please welcome Xiaoge to our team and look for her upcoming workshops!

Our existing scratch file system has reached the end of its useful life and I am pleased to announce that it will be replaced over the next couple of months with a significantly improved file system. The current ~350TB scratch file system will be replaced with a 1700TB (1.7PB) system with i/o speeds 4-fold better over our existing hardware. The new file system will enhance the stability of our scratch storage while providing the ability to temporarily store large data sets for analysis or temporary scratch files for running programs. We are excited to be installing this new file system and expect it to significantly enhance our ability to host large scale calculations.

Wishing you a productive summer!

Go Green!

Kennie Merz

ICER
A LETTER FROM OUR DIRECTOR

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September 2015

I'd like to welcome Dr. Dhruva Chakravorty to the iCER team. Dhruva will be the new Associate Director of iCER who will oversee our team of Research Consultants. Before joining MSU, Dhruva was on the faculty at the University of New Orleans. He has his BS and MS in Chemistry from St. Stephen's College (Delhi University), and a Ph.D. in Chemistry from the Pennsylvania State University.

Dhruva's research interests lie in using and developing computational chemistry methods to understand protein-graphene, protein-ligand, protein-complex and protein-aggregate chemistry. He aims to broaden our understanding of protein-protein interactions from a pre-dominantly sequence based view to a more encompassing dynamical perspective that accounts for conformational changes within the protein environment. Findings from his work have helped identify the driving forces and the molecular origins of the specificity in the assembly of protein complexes. In addition to teaching and training efforts, his experience in administering REU and RET programs, sustaining research collaborations with industry, grant proposal development and building on diversity efforts will help strengthen iCER and its ability to serve the MSU community. Please feel free to stop by and say hello to Dhruva!
Here's to a productive fall semester!

Go Green!

Kennie Merz

ICER
A LETTER FROM OUR DIRECTOR

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July 2015

I'd like to welcome two new members to the iCER team– Elizabeth Ivkovich and Dharanya Sampath. Elizabeth Ivkovich is joining the Business team within iCER. Before beginning at MSU, Elizabeth worked at VCS for three years as an Administrative Assistant. She has a BS in Family Community Services from MSU. We are excited to have this new addition to our Business office.

Dharanya Sampath joins the Research Consultant team at iCER with over three years of experience working as a Scientific Programmer for the Barley Genome Sequencing project. Dharanya has an MSc in Bioinformatics from the University of Edinburgh, UK and her B.Tech in Bioinformatics from VIT University, India. Dharanya was employed at The Genome Analysis Centre in UK where she was handling the sequence assembly and lead the sequence integration efforts for the Barley Genome Sequencing project. She has been involved in projects based on genomic, transcriptomic and exome capture data from crops such as Wheat and Barley. Dharanya's major areas of interest are on genome mapping and assemblies, variant calling and RNASeq data analysis.

Please feel free to stop by and say hello to Elizabeth and Dharanya!

Summer tends to be a slow time where faculty and staff catch up after a busy school year. However, things at iCER are moving apace as we have many ongoing projects that we are continuing to work on over the summer months.

In my previous update, I discussed our new file system and I am happy to report as I write this that it is being built and is expected to be on campus in the coming weeks. We are also preparing for a major cluster purchase in the next academic year and have started the process with MSU purchasing. Concomitant with this new cluster purchase there continues to be a lot of discussion about a modern data center for MSU. In addition, our Communication Team continues to prepare for the fourth annual [Cyberinfrastructure (CI) Forum](), previously known as CI Days, on October 22, 2015 in the MSU Union. This year we debut the new conference name, location, as well as a new one-day format. Registration will open in early August– we look forward to seeing you there! Dr. Matt Scholz and Camille Archer continue to work with Dr. Steven Hsu's office to expand bioinformatics training offerings at MSU, along with working beside the new [Computational Mathematics, Science and Engineering (CMSE)]() department to develop a NSF Research Experience for Undergraduates (REU) program in computational sciences.

As progress continues on our many projects, I will update the MSU community with more details in future newsletters.

MSU, in collaboration with the University of Michigan (U-M), will have a major presence at [Supercomputing (SC) 2015]() in Austin, Texas this November. For the past three years we have enjoyed a cordial and collaborative interaction with U-M ARC and have had small joint booths at SC. This year, both MSU and U-M thought it was time to take things to the next level. This involves the creation of a larger "house-divided" booth with half representing MSU in green and half representing U-M in blue. This is an exciting opportunity for our two schools to get the word out about supercomputing in the great state of Michigan! If anyone has an interest in participating in this event or in presenting a workshop at our joint booth, please let us know!

We hope that everyone is a having a productive and invigorating summer!

Go Green!

Kennie Merz

ICER
A LETTER FROM OUR DIRECTOR

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October 2015

I'd like to welcome Sharan Kalwani to the iCER team. Sharan is the new iCER HPCC Director, and I am absolutely thrilled to have such a qualified and experienced addition to our team! Before joining MSU, Sharan was part of the Scientific Computing Division at Fermi National Accelerator Lab. He has his Bachelors in Mechanical Engineering from the Delhi College of Engineering (University of Delhi, India) and Masters in Computer Science from Wayne State University, in Detroit, Michigan.

Sharan's HPC experience is varied and extensive. Before FermiLab, he was the Subject Matter Expert/Project lead at a startup venture - the UberCloud project, working on helping to realize HPC in the cloud. He has worked for various HPC industry leaders, including Cray Research and Silicon Graphics. At General Motors, he managed the global engineering HPC centers. He was on the leadership team of the King Abdullah University of Science & Technology (KAUST) near Jeddah, Saudia Arabia, where he built and led the new university's HPC.

Sharan is a member of the ACM, senior member of IEEE/Computer Society, USENIX/LISA (formerly SAGE), AAAS and the Union of Concerned Scientists. He was one of the original founders of the open source michigan!/usr/group (mug.org). He also runs the popular discussion group 'Innovative Uses of HPC' on LinkedIn.com, besides numerous other social media in which he is actively engaged.

In addition to his expertise in HPC, Sharan is a teacher, having done adjunct stints as with Loyola University in Chicago, the Illinois Institute of Technology on the South Side of Chicago, Oakland University in Rochester, University of Michigan@Dearborn and recently at KAUST. He is active with CSinparallel.org, which is an NSF program aimed at encouraging inclusion of parallel computing concepts in Computer Science curricula. Furthermore, his experience in fostering industry collaboration projects will help raise the profile of iCER and its ability to serve the MSU community.

Besides taking over leadership of the HPCC group, Sharan, will also spearhead the purchase of our next generation machine in the coming months. Please feel free to stop by and say hello to Sharan and share your thoughts on the future of the HPCC!

We also have some exciting news on the technical side of things here at iCER! In collaboration with the University of Michigan, Wayne State University and the Van Andel Institute a joint proposal was funded by the NSF CC*DNI program entitled "Multi-Institutional Open Storage Research InfraStructure" or MI-OSiRIS. The goal of the MI-OSiRIS project is to build a replicable model for a high speed, multidisciplinary, multi-institution research storage platform, http://msutoday.msu.edu/news/2015/msu-nets-part-of-5m-big-data-grant-from-national-science-foundation/. In addition to funding for hardware and networking, the grant will support a storage engineer at MSU whose responsibility will be to integrate the MI-OSiRIS platform with MSU's research resources, working with MSU researchers to use object-based storage in their workflows, and participation in the development of the MI-OSiRIS platform. This is an exciting in-state collaborative project that will broadly improve networking infrastructure for research applications both within the state of Michigan and beyond. Please contact me if you have any questions about how MI-OSiRIS can facilitate your research workflow!

Go Green!
Kennie Merz

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ICER

A LETTER FROM OUR DIRECTOR

iCER Director,
Dr. Kennie Merz

November 2015

I write this as the beautiful month of October comes to a close. We enjoyed some amazing weather and lovely fall colors this year, along with an improbable victory against our friends in Ann Arbor. At iCER, we had a very exciting month. In addition to finalizing the replacement of our scratch storage with a new system, we've also started to plan for the purchase of the most powerful supercomputer to grace the banks of the Red Cedar. I'll touch more on this in upcoming newsletters.

The main event for iCER in October was the CI Forum, and was it ever stimulating! This year, we followed a one-day format consisting of three keynote speakers supplemented by multiple smaller lectures led by staff and scientists at MSU who discussed how they make use of iCER and its HPCC resources.

Two of the keynote speakers are well known leaders in the supercomputing field: Dr. Craig Stewart heads up University of Indiana's supercomputer facilities as the Associate Dean of Research Technologies, and Dr. John Towns is the project director of the Extreme Science and Engineering Discovery Environment (XSEDE) project headquartered at The University of Illinois, Champaign-Urbana. Craig gave a very timely talk for iCER on how IU built up its supercomputing capacity to support both its local and national user base. He highlighted the role of hardware, and stressed how important it is to have relevant training and research to ensure the effective use of sophisticated compute hardware. In his speech, John discussed how XSEDE intends to support supercomputing at the national level, and how it will advance the skills and capacity of the U.S. to utilize sophisticated modeling and simulation techniques so that it can address a wide range of problems, from manufacturing to the discovery of novel therapeutics.

The final plenary lecture was delivered by Arthur Lupia, who presented a wide-ranging tableau on efforts toward broader sharing of primary data in the social sciences. He highlighted the Data Access & Research Transparency Joint Statement

and how it was fomenting broader sharing of information by primary data sources. The enthusiastic discussion after his lecture touched on a wide range of issues from data sharing to the politics of science funding in the United States.

Last but not least, I would like to welcome Allan Ross, who is iCER's new Communications Coordinator. Before joining MSU, Allan was the Arts Culture Editor at Lansing City Pulse newspaper. He has a Bachelors Degree in Journalism from Michigan State University, and has filled a number of writing, editing, and media relations roles in his career. He also spent more than 15 years in the hospitality industry. Beyond that, Allan is also an experienced public speaker, actor, and filmmaker. Stop on by and welcome Allan to iCER!

Go Green!

Kennie Merz

ICER
A LETTER FROM OUR DIRECTOR

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Dr. Kennie Merz

December 2015

Dear MSU community,

In the world of high-performance computing (HPC), no meeting is more important than the annual International Conference for High Performance Computing, Networking, Storage and Analysis, also known as the Supercomputing (SC) Conference Series — or SC15 this year, for short. Each year, hundreds of companies show off their HPC-related wares, and an equal number of government- and university-based HPC groups present the groundbreaking advances they've made in science and information technology using their HPC resources.

SC15 was held in Austin, Texas, from November 15-20. As per tradition, iCER shared a booth with our colleagues in Ann Arbor. This year we expanded our booth to better represent the exciting things going on at MSU and the state of Michigan vis-à-vis HPC. We had hundreds of visitors to our shared booth, which adopted a "house divided" theme: Half of the booth was MSU green and the other half was Michigan blue (see photo below). Many serious discussions about the current status of HPC at MSU occurred, but several visitors liked the fact that they could be in both "camps" at the same time — or taunt two rival schools at once. (Note: Buckeye fans were the worst offenders.)
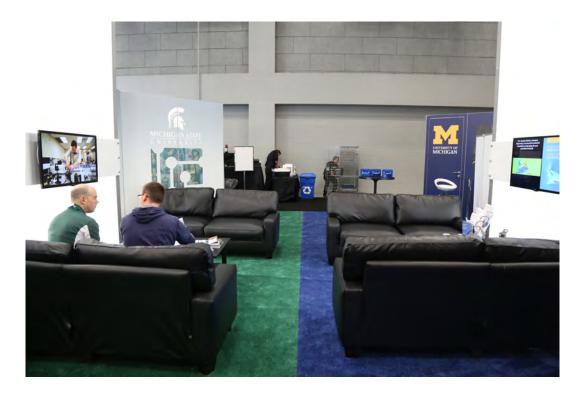
One of the main missions for iCER at SC15 was to hold meetings with the top HPC vendors to assess the technology available for the next supercomputer to be installed at MSU. We had many productive meetings giving a clear picture of the technology available for iCER's next machine, which will likely vault MSU into the upper half of the top 500 supercomputer list, while at the same time delivering much needed compute cycles to our ever-growing computational sciences community. Stay tuned for updates on this.

Finally, all of us at iCER wish you and the rest of the MSU community all the best for

the upcoming holiday season!

Go Green!

Kennie Merz

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