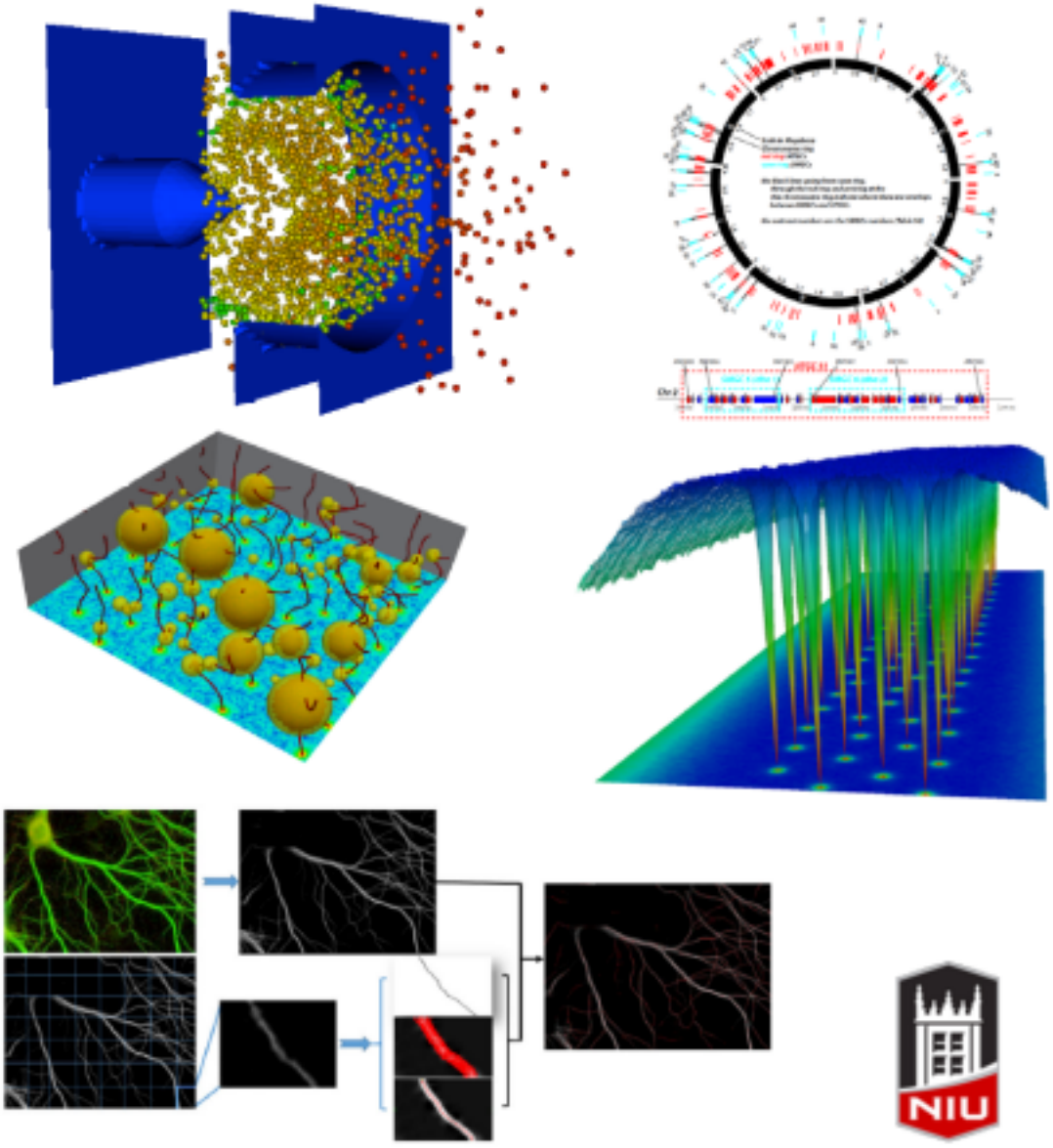
2019-2021 REPORT

CENTER FOR RESEARCH COMPUTING AND DATA

18/11/2021



Northern Illinois University
Division of Research and Innovative Partnership

Abstract

This document describes Center for Research and Computing and Data (CRCD) operations in FY2019-FY2021. Scholarly activities associated with the CRCD are also reported.

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1 EXECUTIVE SUMMARY

The Center for Research Computing and Data (CRCD) stewards computationally and data-intensive research at Northern Illinois University. In support of excellence and engagement in research, scholarship, and instruction, the Center's mission is to promote and strengthen the role of computation at NIU. The facilities and other resources are available to all NIU faculty, staff, students and their collaborators. The Center is a component of the Division of Research and Innovation Partnerships.

From 2018 through 2021 the center's resources were brought to bear on thirty-five research projects that span a broad range of disciplines (the relative usage of CRCD facilities in CPU-hours by discipline is illustrated in Figure 1). Those efforts produced more than seventy journal papers and more than thirty conference presentations and student research. Team leaders of supported research projects submitted fifty proposals requesting $20.5M in external research funding. Of those, twenty proposals were awarded a total of $6.2M and three proposals requesting $3.1M are still under review. Over the same period the Center's resources were used to complete ten doctoral dissertations with three in progress, to complete ten Masters theses with two in progress, and for thirteen other student engagement activities including undergraduate and graduate courses and numerous independent study courses. Finally, the Center's resources were used in collaborations between the university's faculty and scientists, doctors, engineers, and faculty at thirty-one institutions around the world including national laboratories, medical centers, other universities, and companies in the private sector, including one company in the Midwest region.

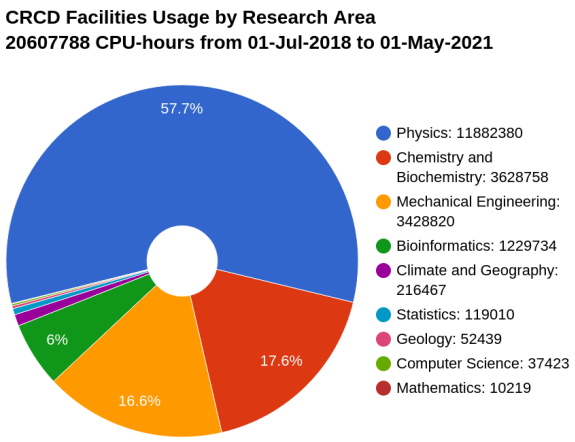


Figure 1. CRCD Facilities Usage by Research Area

2 HISTORY

The NIU Center for Research Computing and Data (CRCD) has its roots in two significant scientific projects. The years 2011-2013 saw the inception of the proton Computed Tomography (pCT) project at NIU aimed at developing a new medical imaging method, which required large amounts of computing power, utilizing emerging GPU technology. The Gaea hybrid compute cluster was commissioned with a grant from the Department of Defense augmented

by Department of Energy funds. After the pCT award period, Gaea was opened to the campus community, and the Center was established. Between 2009-2011 the Northern Illinois Center for Accelerator and Detector Development (NICADD) CPU compute cluster was built by Physics Department to analyze data of High Energy Experiments at FNAL and CERN and support CPU-intensive applications for advanced accelerator research and development. Today, Gaea remains the primary resource available to all CRCD users, while NICADD supports Physics Department applications and serves as a testbed for system development.

3 OPERATIONS

3.1 Facilities and use

In the reported period the Center operated two computing facilities: Gaea and NICADD. Both systems have 1 Gbit/s external connections. Gaea is the center's flagship computing facility, while NICADD serves specific Physics Department projects that need resources not available on GAEA (i.e. large memory nodes), for time-consuming workflows requiring no Infiniband connectivity. NICADD also serves as a test bed for Gaea OS and application upgrades.

Gaea is a 60-node CPU/GPU hybrid cluster. Each node is equipped with twelve 2.66 GHz compute cores (Intel X5650 processors), 72 GB RAM (6 GB/core), 4 x 500 GB drives in a RAID10 array (i.e., 1 TB effective storage space on each node), and 2 x NVIDIA M2070 FERMI GPUs, each with 6 GB RAM and connected via PCI-E. All 60 nodes are connected via Full 1:1 non-blocking 40 Gbit/s Infiniband and 1 Gbit/s Ethernet switch connectors. The cluster also has two storage servers providing disk storage array with 192 TB of effective storage space (RAID6). The storage array is connected to the storage servers via six Gigabit per second SAS connections. The system is located in the Swen Parson computer center, cooling and power is managed by NIU DoIT personnel.

The NICADD cluster provides 700 processor cores (Intel and AMD 1.9-2.6 GHz CPUs) with combined peak single precision compute performance of 6 teraflops, 1.5-10 GB RAM/core, 26-256 GB scratch/core and 200 TB of shared storage space. Nodes are connected via 1-4 Gbit Ethernet. The cluster is running under the HT CONDOR batch system allowing complex priority-based model of sharing resources between users. The system is located in Physics Department with power and cooling provided via NIU services.

3.2 Organizational Structure

In FY2019 (July 01, 2018 - June 30, 2019), Gaea was managed by the Computer Science department and staff from the Division of Information Technology (DoIT), while the Physics Department operated NICADD. Since 2019, both clusters have been managed by four CRCD staff members: Center Director (professor Bela Erdeliy), Application Engineer (senior research scientist Dr. Sergey Uzunyan @0.75 FTE) and the DoIT team (System Administrator Dave Ulrick @0.5 FTE and Operation Director Andrew Johnson @0.1 FTE). Since 2020, both Center Director and Application Engineer roles have been filled by Dr. Uzunyan as the Center Acting Director.

The reduction in operating personnel was possible due to the 2017 Gaea System OS upgrade (Uzunyan/Ulrick) that established similar OS and application stack layouts for both systems. Additionally, in FY2020, the new GAEA (`https://crcd.niu.edu`) and NICADD (`https://nicadd.niu.edu/nhpc`) websites were created (Erdeliy/Uzunyan) to focus on providing introductory and monitoring information for CRCD users, especially for the newcomers: most users (e.g., faculty

and students) are not computer programmers, and even fewer have knowledge in the computer science sub-disciplines of high-performance computing and data.

Support of routine CRCD operations is organized as follows:

- the Director is responsible for resource allocation for current and new projects, web sites maintenance, cluster usage accounting, budget, communications with NIU support services, and other administrative tasks.
- the DoIT team handles routine system-related tasks (implementing various system policies for user accounts, security, scheduling and back-up, hardware support and contracts, node rebuilds after failures, etc.).
- the Application Engineer is responsible for routine application-related tasks (primarily maintenance of locally installed applications and control of access to remote software repositories).

3.3 System and application support

Since 2017 both CRCD compute clusters are running custom installations of similar flavors of Linux operating system - Redhat Enterprise Linux 7.x (GAEA) and Scientific Linux 7.x (NICADD). System installations and rebuilds (when needed for repair) are automated. Security patches are applied only on public systems (login and service nodes of both clusters). Compute nodes use local frozen snapshots of proprietary and community-supported software repositories, allowing running stable and synchronized sets of system packages on all compute nodes of each cluster. The setup allows the use of NICADD-build user packages on GAEA and vice-versa. It also permits instant distribution of additional system packages to compute nodes when required with no downtime and without danger of breaking systems functionality.

Both clusters support three types of users applications:

- external software libraries accessible from all nodes via network file system
- locally build packages, installed and supported by CRCD personnel
- local packages (primarily Python applications) installed and supported by users

3.4 User support

CRCD provides documentation and tutorial pages for GAEA and NICADD systems on their websites as an entry support point. Both sites are equipped with "Search CRCD" functionality to find relevant information and with several monitors of system status helping users to schedule their job submissions. Additionally, several command-line monitor tools are available for users on login nodes.

For more complex cases, CRCD personnel account and process individual user requests using archived e-mail lists for group review: crcdhelpdesk@niu.edu at Gaea and system@nicadd.niu.edu at Nicadd. Beginning September 2019, a web-based "CRCD Helpdesk" application is available for Office365 NIU users for formal ticket submission (53 tickets are completed by May of 2021). All requests and tickets categorized by users as routine are processed on a "first in - first out" basis in the background to "high-priority" and emergency events. Expected processing times (logged) are one business day for account-related requests, three business days for help with the installed applications, and a week for a new package installation. CRCD personnel also provides in-person consultations when needed - typically an introductory meeting with PIs requesting a new project.

User's requests are divided into two major categories. The first category includes system-related requests - accounts, quotas, job scheduling, and reservations. The second category is

user's application support - choice, install, debug of applications required by research projects. The first category on Gaea is served by the System administrator and the second by the Application Engineer. The entire team handles a fraction of tasks requiring combined efforts (like installing system packages for a specific research project).

3.5 Workflow organization

Each project that uses the center's resources has a principal investigator (i.e., faculty leader). Projects typically include students, other faculty, and sometimes external collaborators. On occasion, system administrators also run jobs for routine maintenance and system checking.

On GAEA, users develop and/or test theirs applications on the login node and then submit their job to a batch system for execution by specifying the number of nodes (typically more than one node) and a duration (typically in minutes or hours, but sometimes hours that can last for days) that their program will run. The jobs then run with exclusive access on the number of requested nodes, all simultaneously, for a duration up to the time requested time.

NICADD has three capable login nodes and a more sophisticated queue system - users specify a combination of resources they needed for a job (the node-set, memory, number of cores, scratch size, e.t.c). Then the batch system provides job slots when they are available accounting priorities. The job preempting/eviction mechanism is configured to provide resources for jobs with the highest priority by evicting and re-queuing lower priority jobs when possible.

3.6 Budget

Support for the center comes almost entirely from the University. Table 1 shows CRCD budgets for FY2019-FY2021. Additionally, a modest support at a level of $2000/year was provided by Physics department for the NICADD cluster hardware.

Table 1. CRCD budget in FY2019-FY2021

Budget positions	FY19	FY20	FY21
Total Expenditures	$302,052	$215,286	$143,826
Facilities			
Hardware support	$44,786	$56,214	$34,968
Software	$10,000	$10,000	$16,000
Upgrade/replacement	$977	-	$5,597
Total Facilities	$55,763	$66,215	$56,565
Personnel			
Directors	N/A	$47,879	$41,261
Research Associates	$206,289	$36,652	-
Students	-	$18,540	-
External Funding, Personnel	-	-	-
DoIT Support	$20,000	$46,000	$46,000
Total Personnel	$226,289	$149,071	$87,261

4 USAGE ANALYSIS

While running, submitted jobs occupy one or several elementary compute elements, known as processor cores. We quantify Gaea's and NICADD's use by the time jobs occupy conventional (non-graphics) compute cores in the form of "CPU-hours" where a single CPU-hour represents a single CPU core running a program continuously for one hour. Batch systems in use do not allow to share graphics processors (GPUs) between jobs and correspondingly we count an entire multi-core graphics processor as an elementary compute element to count GPU-hours.

4.1 Supported research projects

For FY2019-2021, CRCD facilities supported 35 research projects as shown in Table 2. A total of ~12 billions CPU-hours (66% out of total available in the reported period) were used on Gaea and 9 billions CPU-hours (48%) were spent running Nicadd jobs. Six projects used outdated Gaea's GPUs at a level of 117000 GPU-hours (0.6%).

Figure 2 shows Gaea utilization in terms of percentage load per day and as a number of active users/PIs per month. Observed peak loads on Gaea are 90% and 28 users/month. Corresponding numbers for NICADD are 99% and nine users/month. The Gaea utilization is limited by the batch system configuration only allowing "per node" job scheduling, while the batch system at NICADD uses a more flexible "per core" mechanism.

For both systems usage by projects and users are shown in Figures 3 and 4. A wide range in the amount of consumed compute time was observed:

- five "power projects" continuously contribute ~90% to the consumed CPU time
- fourteen projects used a significant amount (>1%) of available CPU time;
- the majority of projects used a modest amount of CPU and GPU time

Such usage pattern can be interpreted as follows - CRCD has conventional CPU resources to support "power projects" while satisfying the requirements of occasional users for which the most important factor is the convenience of centrally-managed resources (software, disk space, accessibility) but not the computing power.

4.2 Software

To date, CRCD provides 67 unique (158, accounting for all supported versions) application packages locally installed on Gaea and NICADD systems. Those actively used in batch jobs in FY2021 are presented in Table 3. The majority of applications are open-source projects, and custom builds were performed to satisfy user needs. CRCD also allows and supports the purchase and installation of proprietary packages (Intel compiler suites, Gaussian Inc. software for chemical processes modeling, TRELIS for high-quality mesh generation) and supports user-controlled development and installations of Python modules and personal packages.

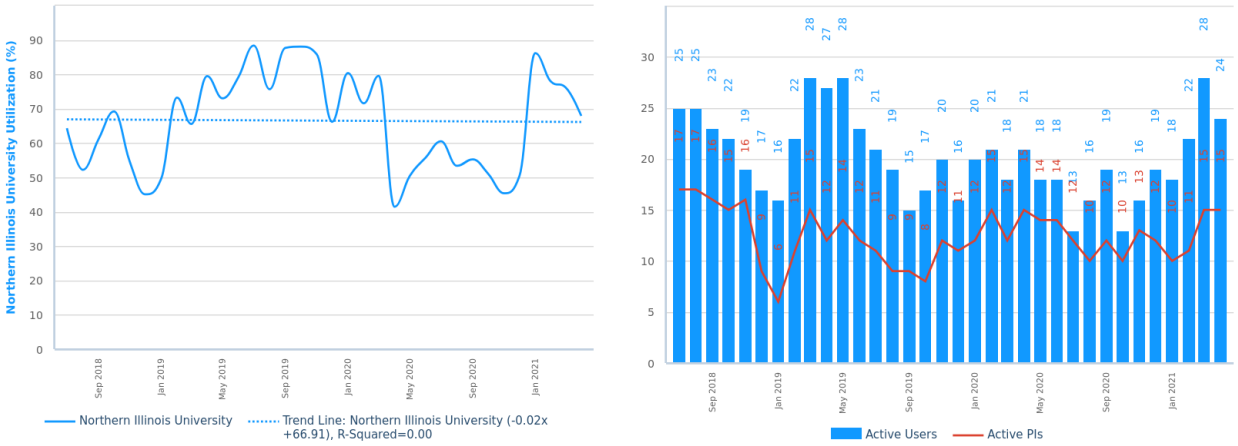


Figure 2. GAEA utilization: Cluster load (a) and Number of Active Users and PIs (b) as functions of time.

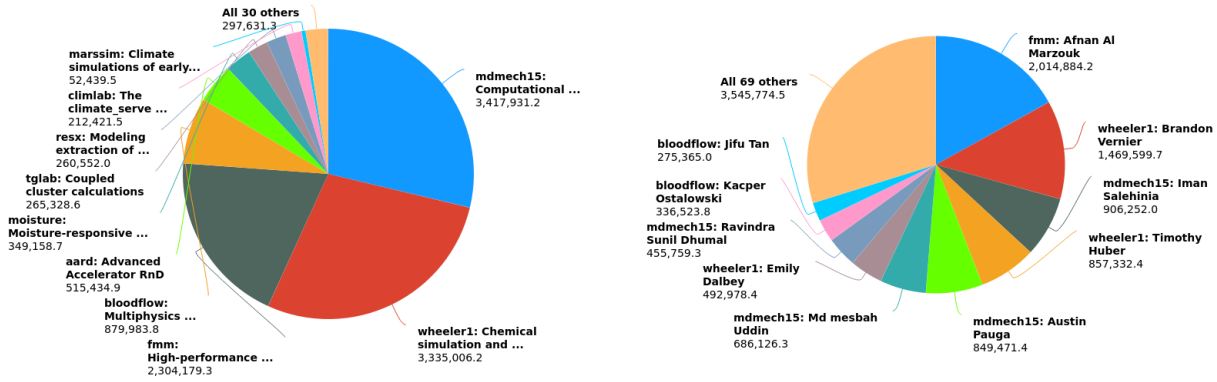
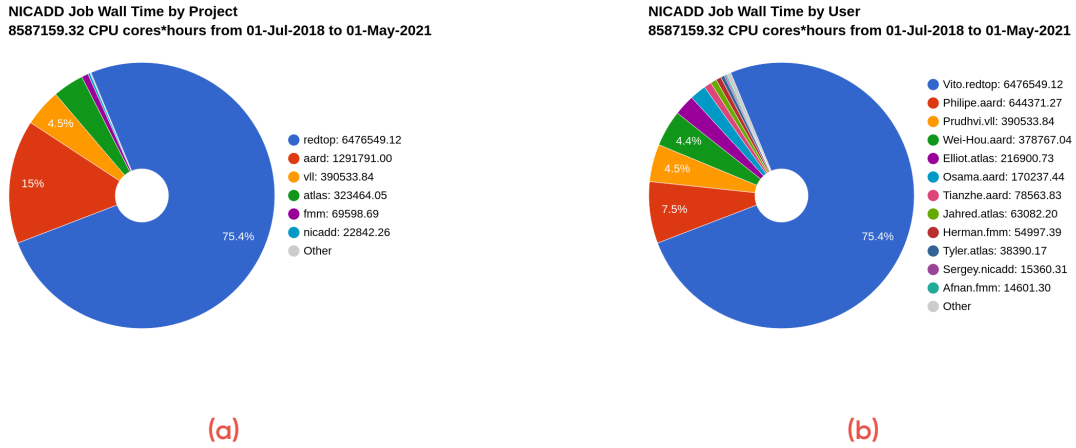


Figure 3. Gaea Wall Time Usage: (a)by Project; (b) by User.



(a) (b)

Figure 4. Nicadd Wall Time Usage: (a) by Project; (b) by User.

Table 2. Supported projects in FY2019-FY2021

Project group	PI	Project title	Facility[1] FY 19-20-21	Usage CPUxHRS	Usage GPUxHRS
		Bioinformatics			
bloodflow	J. Tan	Blood Rheology Studies	G-G-G	879,983	0.0
moisture	B. Sinko	Moisture-Responsive Materials	G-G-G	349,159	0.0
cazyme	Y. Yin	cazyme	G-*-*	592	0.0
		Chemistry and Biochemistry			
wheeler1	R. Wheeler	Chemical Simulations and Analysis	G-G-G	3,335,006	0.0
tglab	T. Gilbert	Coupled Cluster Calculations	*-G-G	265,739	0.0
omlab	O. Malgonde	Health Data Analytics	*-G-G	28,013	0.0
		Computer Science			
buddha	N. Karonis	buddha	G-*-*	21,528	3,588
pct	N. Karonis	Proton Compute Tomography	G-G-G	5,086	4,961
prad	N. Karonis	Proton Radiography	G-*-*	3,500	79.5
datalab	H. Alhoori	datalab-ml	G-G-G	3,641	606.5
hqgroup	H. Alhoori	HQueue	G-*-*	3,556	592.5
potoftea	P. Giabbanelli	POlicy Testing On Fast-foods	G-*-*	112.0	5.0
		Climate and Geography			
climlab	V. Gensini	High-Resolution Numerical Weather Predictions	G-G-G	212,421	0.0
cogvis	T. Pingelx	spatialcogvis	G-*-*	4,046	0.0
		Geology			
marssim	W. Luo	Climate Simulations of Early Mars	G-G-G	52,439	0.1
		Mathematics			
bigcrunch	N. Krislock	bigcrunch	G-G-G	10,219	10.0
		Mechanical Engineering			
mdmech15	I. Salehinia	Computational Material Science	G-G-G	3,417,931	0.0
npems15	J. Shelton	Thermophysical Properties of Nanoscale Materials	*-G-*	10,889	0.3
		Physics			
redtop	C. Gatto	Detector Development for REDTOP experiment at FNAL	N-N-N	6,480,383	0.0
fmm,iota	B. Erdelyi	High-Performance Beam Dynamics	G-G-G	2,308,003	0.0
			N-N-*	69,598	0.0
aard	P. Piot	Advanced Accelerator R&D	G-G-G	515,434	0.0
			N-N-N	1,307,418	0.0
resx	M. Syphers	Modeling Proton Extraction in Non-Linear Accelerators	G-G-G	260,552	0.0
vll	S. Martin	Simulations of Particle Collisions at the LHC	G-G-*	48,611	8,091
			N-N-N	397,333	0.0
mu2e	V. Zutshi	Detector Development for MU2E experiment at FNAL	N-N-N	41,492	0.0
atlas	J. Adelman	Data analysys for ATLAS experiment at CERN	N-N-N	422,976	0.0
fast	P. Piot	Fermilab Accelerator Science and Technology	G-G-G	12,374	0.0
waveguide	P. Piot	xraywaveguide	G-*-*	13,168	0.0
rnntitles	J. Adelman	Recurrent Neural Networks	G-G-*	3,686	3,686
activesys	A. Glatz	Cell Migration in a 3D computational model	G-G-G	1,352	0.0
		Statistics			
dmr	D. Ryu	Differentially Methylated DN	G-G-G	49,647	0.0
cutpoint	S. Basu	Bayesian Methods for Optimal Cancer Treatment	G-G-*	38,411	0.0
mdep	L. Hua	Statistical and Machine Learning Techniques	G-*-*	30,952	0.0
		Miscellaneous			
hpc-admin	D. Ulrick	hpc-admin	G-G-G	150	1.1
hpc-apps	S. Uzunyan	hpc-apps	GN-GN-GN	5,388	1.5
		Projects Summary			
	FY2019	**FY2020**	**FY2021**		
N Projects	28	24	19	11,910,840	17,969
N Areas	9	9	8	11,910,840	17,969

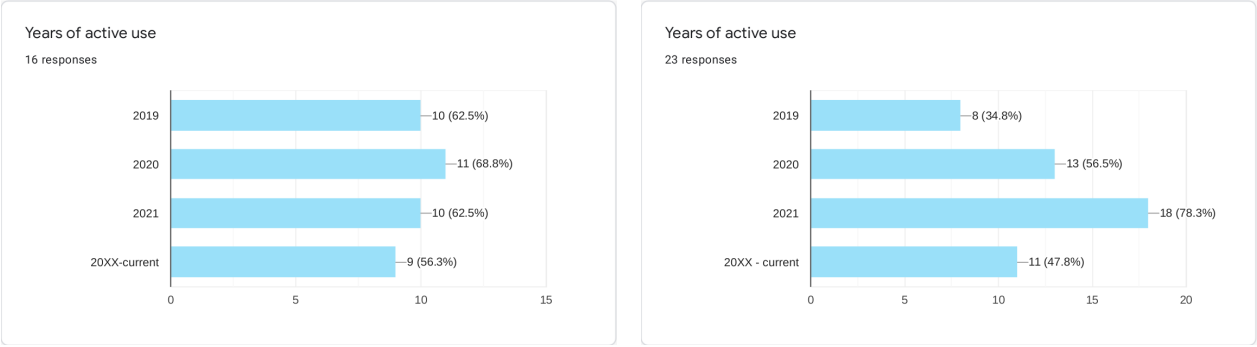
[1] "G" denotes GAEA, "N" - NICADD.

5 USERS ACTIVITY SURVEY

A users activity survey was conducted in September-October of 2021. All GAEA and NICADD registered users were asked to respond to the Google questionnaire available at https://-forms.gle/K7KQUHjvzbXG6mT67. We obtained 16 responses from Project Investigators and 23 from staff and students, that cover the most active projects shown in Table 2.

Table 3. CRCD supported software, FY2021

Module	Description	License/cost	Projects
cm1r20.1	Atmospheric Research	MIT/free	climlab
cuda,v6.0-7.5	NVIDIA GPU Libraries	NVIDIA/free	prad, wheeler, marssim,pct,iota
g16-rA03sse4	Chemical processes modeling	Gaussian/$$	wheeler1,tglab
GEANT4	Physics Detectors simulations	CERN/free	redtop,mu2e,atlas
gcc, v4.8.5-9.3.0	GNU Compiler Collections	GPL/free	all
intel-13.0.1	Intel Compiler Collection	Intel/$$	wheeler1
intel-2015	Intel Compiler Collection	Intel/$$	prad, fmm, wheeler1
lammps-20181218	Molecular dynamics simulator	GPL/free	wheeler1
namd-2.12	Parallel molecular dynamics	UIUC/free	moisture, wheeler1
netcdf-4.4.1	Scientific data format library	UNIDATA/free	marssim, climlab, aard
openmpi, v1.8.1-4.0.2	OpenMPI libraries	GPL/free	blodflow, wheeler1, aard
opal-2.0	Parallel Accelerator Library	GPL/free	aard,fast
orca-4.2.1	Quantum chemistry program	Academic/free	tglab
PYTHIA,MADGRAPH	Particle collisions simulations	GPL/free	redtop, atlas,vll
ROOT	Physics Analysis	GPL/free	redtop,mu2e,atlas,vll
trelis-16.5	High-quality mesh generation	Coreform/$$	aard,fast
qmcpack-3.9.2	Quantum chemistry Monte-Carlo package	Academic/free	wheeler1
qp2-2.1.2	Quantum chemistry, wave function methods	Academic/free	wheeler1
richdem-0.0.3	Hydrologic analysis tools	Academic/free	marssim
wwrf-4.1.3	Weather Research and Forecasting Model	Academic/free	climlab



(a) (b)

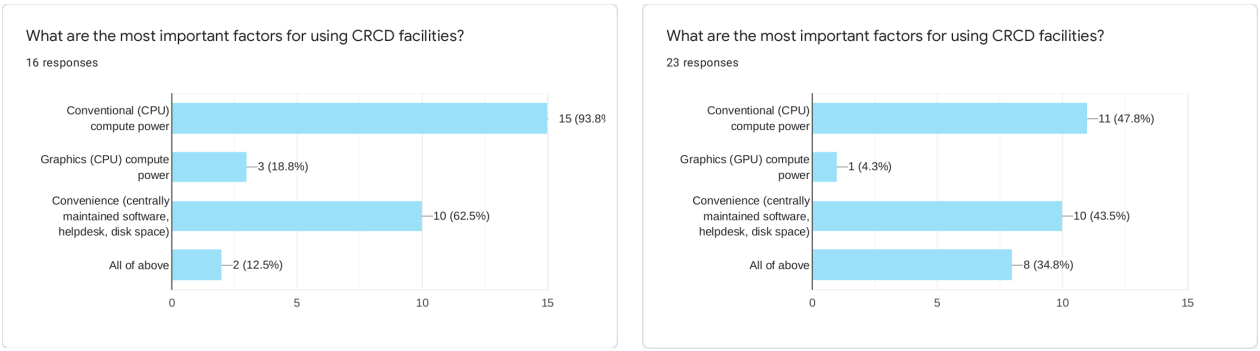
Figure 5. GAEA and NICADD projects by year: (a) by PIs; (b) by Team Members.

5.1 Response analysis

The responses are summarized in Figures 5-8. As shown in Figure 5 , GAEA and NICADD facility use is uniform in time for PIs, with new users joining in 2021. Both PIs and team members value the convenience of cluster use and the conventional CPU power of the machines, but outdated GPUs provide limited options, Figure 6. Figure 7 shows that all available sources of support (web pages, helpdesk application, CRCD helpdesk e-mail) are in use. The support satisfaction is rated higher among PIs but overall gained high grades among all users, Figure 8. User feedback on the CRCD compute clusters importance and convenience is presented in Sections 5.2-5.3.

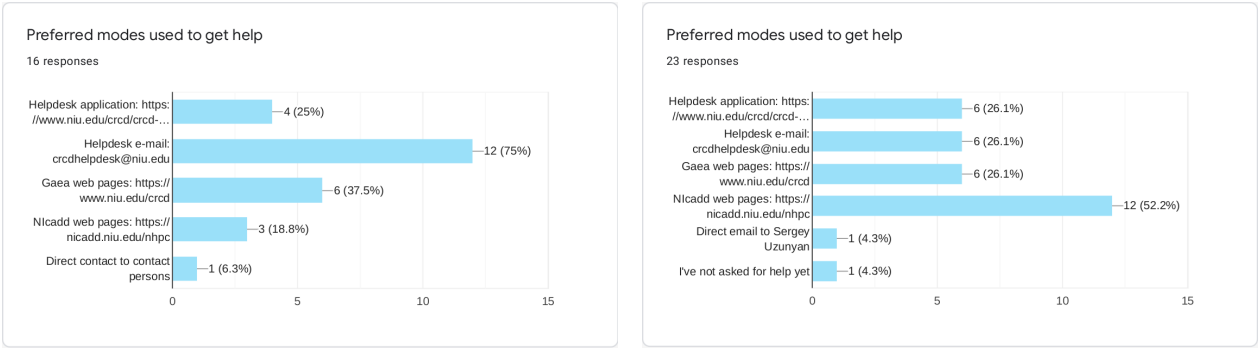
Some of the activity questions were designed to collect information about the outcome of research conducted with GAEA and NICADD clusters starting from July 2019. A full list of results are provided in Sections 6-8, but a numeric summary follows:

1. Submitted research proposals: 50 requesting $20.5M
2. Funded research: 20 totaling $6.2M
3. Proposals still under review 3 totaling $3.1M
4. Journal papers: 71
5. Ph.D. thesis: 13 (10 completed/3 in progress)



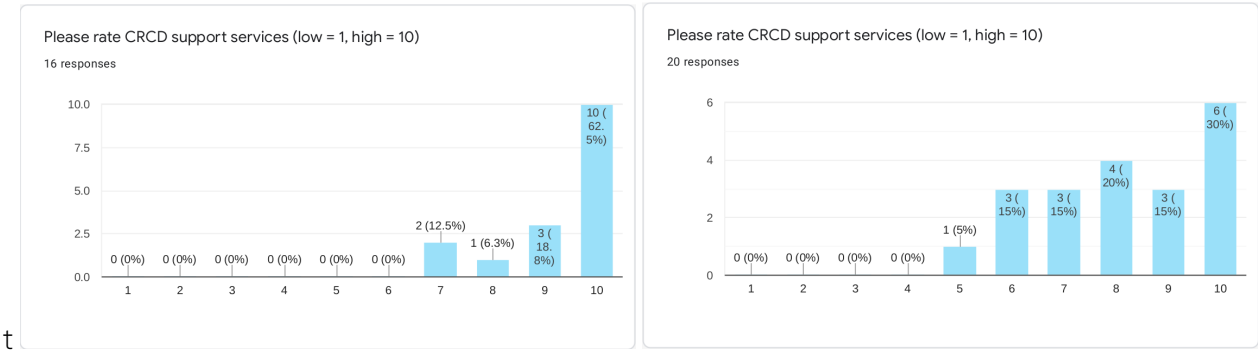
(a) (b)

Figure 6. Reasons for use of CRCD compute clusters: (a) PIs; (b) Team Members.



(a) (b)

Figure 7. Preferred modes of help: (a) PIs; (b) Team Members.



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(a) (b)

Figure 8. Support services score (1-low,10-high): (a) PIs; (b) Team Members.

6. Master thesis: 12 (10 completed/2 in progress)
7. Conference presentations: 38
8. External collaborations: 25

5.2 PI feedback

Prof. Thomas Gilbert, "Gaea allows for large, time-consuming electronic structure calculations I could not perform elsewhere. Sergey and Dave have installed all the software I need in timely fashion. they have been extremely helpful with access setup, and my occasional brain lapses"

Prof. Philippe Piot, "CRCD gives us access to computing capabilities to perform simulations of the dynamics of bright-electron beams, the interaction of electron beams with external field (lasers) to support compact accelerator-based light sources. Likewise, it has been used to support simulation of novel acceleration technique based on wakefields. All these projects are part of funded grants, and the work are essentially performed by students."

Prof. Jahred Adelman, "Sergey has worked closely with my group to help us when we destroy the NICADD batch system, to make sure the interactive nodes are running well, etc. I think this has supported all of my ATLAS group's research, which is too numerous to list"

Prof. Vector Gensini, "CRCD's facilities have a significant impact on the scholarship, student engagement, and grantsmanship of the Weather, Climate, Society (https://wcs.niu.edu) research group at NIU. Over the past few years, Surgey Uzunyan, Kirk Duffin, and Dave Ulrick have greatly assisted us with software installation and user onboarding. CRCD has allowed us to pilot research experiments in the weather and climate modeling space that have turned into significant external awards through the federal government and private companies. These award have netted a significant number of referred articles and scholarly presentations at conferences, including those led by students. Finally, student engagement in the form of independent studies have become important for our curriculum. We are examining ways to integrate CRCD into our upper-level undergraduate and graduate courses (e.g., GEOG 493/593 Programming for the Geosciences) to expose a wider student body to CRCD. We recognize the important role that CRCD will play in our future scholarship, grantsmanship, and student engagement."

Prof. Bela Erdeliy, "(GAEA is used) for large scale, high-fidelity, high-performance particle dynamics modeling and simulations"

Prof. Jifu Tan, "CRCD's facilities and technical support from the staff shaped my research profile after joining NIU. All my research work is based on the computing facilities such as Gaea. The computational work also helped me collaborate with both internal and external colleagues. Gaea also helped me training both undergraduate and graduate students through independent studies and thesis. I also used Gaea to demonstrate high performance computing in both undergraduate and graduate classes (e.g., MEE 380 numerical methods, MEE 480/580/615 finite element, MEE 658 computational fluid dynamics). "

Prof. Mike Eads, "The NICADD cluster is an important tool for faculty, staff, and students. It is important to the completion of particle physics research."

Prof. Stephen Martin, "CRCD's high performance computing facilities were indispensable in generating Monte Carlo samples (simultaneously using multiple cores and CPUs) and analyzing the data needed for our research publications. Sergey A. Uzunyan, Nicholas T. Karonis, John Winans and the entire CRCD staff were very helpful in setting up and using the necessary software packages required for our research."

Dr. Corrado Gatto, "REDTOP collaboration has participated in the Physics beyond Collider Study Group at CERN, the European Strategy for Particle Physics and is engaged in the Snowmass-2022 Community Study. All studies have required extended computing simulations.

About 20% of the computing power used was from NICADD cluster"

Prof. Wei Luo, "CRCD facilities and staff help played an important role in my PhD student's Mars work, without Gaea, he would not be able to complete the Optimal Channel Network simulation in time. He has successfully defended his dissertation and is now a postdoctoral researcher at University of Maryland at Baltimore County. CRCD is also critical in my success in obtaining the most recent NASA grant. I anticipate to use CRCD facilities and staff help even more in the coming 3 years on the new NASA grant. This is a critically important service to the NIU research community. Thank you for the great service and please keep it going!"

Prof. Michael Cyphers, "The CRCD's facilities have allowed for NIU students to perform high quality research that prepared them for next steps to be followed at national laboratories and at other high performance computing facilities associated with those laboratories. Their initial preparations through the use of CRCD facilities put them ahead of the curve, providing them with local resources that led to papers, presentations, and theses which would not have been available to them otherwise at their particular phases of their academic careers. The CRCD staff have always been approachable and extremely supportive in all aspects of the students' experiences."

Dr. Nicholas Karonis "Gaea was a critical facility in the early development of our software that reconstructs tomographic images from protons."

Prof. Robert Sinko. "CRCD's computational resources have been incredibly valuable as a new faculty member trying to get their research program established. John Winans was incredibly helpful when my first graduate student was trying to get molecular simulations running on the system and helped get the simulations working and troubleshoot errors we encountered. Rather than just fixing the errors himself, he made a point to educate us on the functionalities of GAEA so that we were better prepared to handle issues that came up in the future. I believe CRCD facilities will be incredibly valuable to my future work as they provide a computing platform for my students to perform their computational research and I look forward to having more of them use their resources in the future."

Prof. Ralph Wheeler, "As a computational chemist, I use the CRCD's facilities as my research group's primary computational resource. My work would be impossible without it, as i would have no computing resources and no "on ramp" to apply for computer time at large national centers. My research, grantsmanship, and student engagement would stop."

Prof. Iman Salehinia, "All Gaea staff are very helpful, the results of my student's current research will be used to help me write a proposal for external funding. I am also planning to submit a proposal on the research several students in my research team have worked on for some time."

5.3 User comments

Prof. Thomas Gilbert, "I contributed to the proposal for a replacement supercomputer on the strength of what i accomplished on Gaea. Even if that supercomputer is funded, i will still use Gaea for many calculations."

Prof. Jifu Tan, "HPC training for students such as summer camp. Maybe in the future we can have a one day symposium on campus-wide computational research."

Dr. Corrado Gatto, "Staff was excellent in all respects. More disk storage would be extremely welcome."

Prof. Wei Luo, "I participated in a workshop organized by Bridge-2 at PSC this summer. It was very helpful and informative to me. Please keep letting us know such opportunities. Thanks!"

Ph.D. Student Michael Hood, "Some downtime of nodes in the past happened, but was

always taken care of quickly. Some confusion on allotted wall time for jobs, as people have been submitting many jobs with over 2 days of wall time recently. Overall services have been very good, and all supported software is easy to access and use."

Ph.D. Aakaash Narayanan, "Is it possible to use select number of cores (less than 10 cores) at a time instead of using one full node (which consists of 10 cores)? If yes, great! If not, this could be useful since a job that doesn't need as much computation needn't consume one full node."

Resources that would be useful in future:

1. Wei Hou Tan, Ph.D. Student: "New graphics cards"
2. Tianzhe Xu, Tianzhe Xu: "Dedicated nodes to run Jupyter server"

6 GRANTSMANSHIP

6.1 Funded Research

1. P. Piot, Department of Energy, submitted 2018 and funded up to 2021: Phase-space tailoring and cooling of charged-particle beams for energy- and intensity-frontier applications; total $330k
2. P. Piot, National Science Foundation | Center for Bright Beams, submitted 2019 and funded up to 2026: R&D on Optical Stochastic Cooling / supplemented with research on Coherent Synchrotron Radiation (October, effective 2021); accumulated total as of 08/2021: $220k
3. P. Piot, Department of Energy, submitted 2020 and funded up to 2023: High-Gradient High-efficiency Wakefield Acceleration; total $330k
4. P. Piot, DOE/NNSA w. Euclid Tech LLC, submitted 2021 funded for one year: Design of a compact Electron brachytherapy system $42k
5. J. Adelman, NSF grant "Searches for New Phenomena in the Higgs Sector at the LHC" awarded for $1.05 million (Total for 3 years), had requested $1.4 million
6. J. Adelman,US ATLAS Postdoc support funded for 3 years for $70,000
7. J. Adelman, co-PI, "U.S. ATLAS Operations: Discovery and Measurement at the Energy Frontier" award for $307,000
8. V. Gensini, National Science Foundation, Advancing our understanding of intraseasonal U.S. severe convective storm variability.2021–2023, Role: PI. ($474,682) Awarded.
9. V. Gensini, American Family Insurance, Inc., Weather/Climate Modeling, Data Science and Analytics2020–2023, Role: Co-PI. PI: W. Ashley (NIU), Co-PI: A. Michaelis (NIU) ($475,000) Awarded.
10. V. Gensini, Metlife, Inc., Creation of automated severe weather guidance for operations.2019–2020, Role: PI. ($20,000) Awarded.
11. B. Erdelyi, Department of Energy (HEP, NP) total of $495K awarded
12. J. Tan, PI, Bioinspired microfluidics design for circulating tumor cell separation learned from pulmonary capillary vessel networks, Division of Research and Innovative Partnerships, $15,000, NIU, 2021.
13. J. Tan, PI, Multiscale modeling of circulating tumor cell transport and adhesion in blood flow, Division of Research and Innovative Partnerships (RIPS), $14,500, NIU, 05/01/2018 - 06/30/2019
14. J. Tan, PI, Predictive Modeling of Blood Clotting with Experimental Validations, Great journeys assistantship program, NIU, $15,970, 08/16/2018 - 05/15/2019
15. J. Tan, PI, Multiscale modeling of circulating tumor cell transport and adhesion in blood flow, undergraduate research program, Illinois Space Grant Consortium, $9,000, 2018.
16. D. Ryu, NIH R15 at 2018, NIH R20 at 2019, NSF at 2019

17. Luo, W., PI, NASA Mars Data Analysis Program grant, "Testing early Mars climate from global spatial distribution of valley network geomorphology," submitted in 11/2020, $335,069 requested, awarded!
18. N. Karonis, "A Proton Tomography System for Optimization of Proton Therapy," National Institutes of Health, co-PI, $1,989,510, April 1, 2020 – March 31, 2022. awarded
19. N. Karonis, "A Proton Radiography System for Optimization of Proton Therapy," National Institutes of Health, consortium PI, $1,983,562, September 23, 2016 – February 28, 2019. awarded
20. R. Sinco, "NIU/ISGC Nasa Internships, Fellowships. and Scholarships, STEM Engagement, Institutional Engagement, Educator Professional Development Project", Illinois Space Grant Consortium/NASA, $39,000, Awarded

6.2 Declined Proposals

1. V. Gensini, National Oceanic and Atmospheric Administration, Improving extended range severe weather forecasts.2021–2023, Role: PI. Co-PI: R. Adams-Selin (AER), Co-PI: A. Haberlie (LSU). ($527,765) Declined.
2. V. Gensini, National Oceanic and Atmospheric Administration, Developing severe weather guidance for weeks 3–4.2020–2022, Role: PI ($498,571) Declined.
3. V. Gensini, National Oceanic and Atmospheric Administration, Improving severe weather forecasts for days 4–8. 2020–2022, Role: PI. ($582,025) Declined.
4. V. Gensini, National Science Foundation, Collaborative Research: Advancing our understanding of intraseasonal variability in U.S. severe convective storms.2020–2023, Role: PI. ($477,076) Declined.
5. V. Gensini, National Science Foundation, CAREER: Improving our understanding of climatic controls on hazardous convective weather2020–2025, Role: PI. ($797,627) Declined.
6. PI: Michael Papka, Co-PI: Jifu Tan, Christine Nguyen, Vittorio Gensini, Joseph Insley, NSF, MRI: Acquisition of a Computational Instrument to Enable Research and Training in Simulation, Data, and Learning, submitted 01/19/2021, $959,349.
7. PI: Tan, NIH, Multiscale modeling of particle transport and adhesion in nasal airways, submitted 02-25-2020, $426,752.07, 08/15/2020-08/14/2023
8. PI:Tan, NSF, CAREER: A scalable multiphysics simulation framework for biological flows with complex suspensions and adhesion, $610,782.43, submitted 08/10/2020 03/01/2021-02/28/2026
9. PI: Tan, BSSw Fellow: improve scientific software performance and training students in high performance computing, submitted 09/30/2020, $25,000 , 01/01/2021-09/30/2021
10. PI: Venumadhav Korampally, Co-PI: Pallavi Singh,Robert Sinko, Jifu Tan, NSF, Meeting the demands for effective personal protection equipment (PPE): Investigation of Nano Cellulose based filter electrets for the production of PPE, $421,980 , submitted 12/21/2020
11. PI: Niechen Chen, Co-PI: Jifu Tan, Geometric Variation Prediction for Additive Manufacturing Through a New Physics Modeling and Simulation Approach, $549,295, submitted 10/21/2020
12. PI, Tan, Illinois Space Grant Consortium, Modeling of Fluid Structure Interactions for Biological Flows, May, 6th, 2019, $9,750
13. Co-PI: Federico, Nguyen, Tan, The Materials informatics for Sustainable Digital Manufacturing and Design (MSDMD), NSF NRT, Feb. 6th, 2019, $499,929.
14. PI: Tan, Collaborative Research: ISS: Isolation and Molecular Profiling of Extracellular Vesicles Derived from Glioma Cells in Microgravity, NSF, Feb. 28th, 2019, $48,615
15. PI:Tan, Clot growth modeling and uncertainty quantification using the Azure platform:

an integrated research and teaching approach, Microsoft corporation, Aug. 16th, 2019, $200,000.

16. Co-PI: Tan, A reliable device for rapid efficient isolation of pure extracellular vesicles derived from cancer cells in microgravity for comprehensive molecular analyses, Binghamton University, State University of New York, Sep. 27th, 2019, $268,991
17. PI: Tan, Food & Drug Administration, Multiscale modeling of drug particle transport and clearance in nasal cavity using a massively parallel fluid solid coupling tool, $278,834. June 7, 2018
18. "Probing the Standard Model and Beyond with the CMS and DUNE Experiments", DOE OHEP proposal. M. Eads is co-PI and V. Zutshi is PI. Jul 1, 2020 – Jun 30, 2023. $610,267 (submitted Jan 2020, declined)
19. "Probing the Standard Model and Beyond with the CMS and DUNE Experiments", NSF EPP proposal. M. Eads is PI and V. Zutshi is co-PI. Jul 1, 2020 – Jun 30, 2023. $610,267 (declined)
20. "Probing the Standard Model and Beyond with the CMS and DUNE Experiments", grant proposal through the NSF experimental particle physics program. V. Zutshi PI, M. Eads co-PI. Submitted Dec 2018, to cover the period July 2019 – June 2022. $612,771. (declined)
21. Luo, W., PI, NASA Mars Data Analysis Program grant, "Testing early Mars climate from global spatial distribution of valley network geomorphology," submitted in 10/2018, $270,584.00 requested, declined
22. Luo, W., PI, NASA Mars Data Analysis Program grant, "Testing early Mars climate from global spatial distribution of valley network geomorphology," submitted in 11/2019, $302,685.00 requested, declined
23. R. Sinco, "Meeting the demands for effective personal protection equipment (PPE): Investigation of Cellulose based filter electrets for the production of PPE", NSF, $421,980, Rejected
24. R. Wheeler, NSF; $418,974; "Atomic contributions to calculated structure factor peaks for ionic liquids"; Submitted 9/18; rejected.
25. R. Wheeler, NSF/REU; $330,267; "REU Site: Integrated Experimental/Computational REU Site at Northern Illinois University"; Submitted 8/19; rejected
26. R. Wheeler, NSF/REU; approximately $350,000; "REU Site: Integrated Experimental/Computational REU Site at Northern Illinois University"; Submitted 8/20; rejected.
27. R. Wheeler, American Chemical Society/Petroleum Research Fund; $110,000; "Approximate nanoscale size of polar aggregates in chloroaluminate ionic liquids for isobutane alkylation"; Submitted 3/21; rejected.

6.3 Under Review

1. J. Adelmah, DOE grant "Chicagoland HEP Instrumentation Traineeship Program" pending for $2.42 million (total for 5 years)
2. Corrado Gatto "2021 - DOE - Physics and detector studies of a propose h/h' factory in the US" - $280K (pending)
3. R. Wheeler, NSF; $370,224; "Collaborative Research: Molecular Modeling and Experimental Investigations of Structure and Dynamics of Nanoscale Structural Inhomogeneities in Room Temperature Ionic Liquids"; Submitted 9/21; under review.

7 SCHOLARSHIP AND INNOVATIONS

7.1 Journal papers

1. "MoCl3(dme)" Revisited: Improved Synthesis, Characterization, and X-ray and Electronic Structures. Shaw, Thomas E.; Diethrich, Timothy J.; Scott, Brian L.; Gilbert, Thomas M.; Sattelberger, Alfred P.; Jurca, Titel, Inorganic Chemistry (2021), 60(16), 12218-12225.
2. Additivity of Diene Substituent Gibbs Free Energy Contributions for Diels-Alder Reactions between (F3C)2B = NMe2 and Substituted Cyclopentadienes. Strominger, Abbygale M.; Sutherland, Brooke L.; Flemming, Austin S.; Dutmer, Brendan C.; Gilbert, Thomas M. Journal of Physical Chemistry A (2021), 125(24), 5456-5469.
3. Computational studies of cis- and trans-isomer preferences of low-spin d6 [M(DABF)2A2]+ and [M(CO)4A2]+ complexes (M = Co, Rh, Ir; A = anionic ligand): spectator ligand π-backbonding and DFT exchange. Bacchi, Samantha M.; Waters, Cara M.; Agunoye Jones, Oreoluwa A.; Becker, Greg; Bryan, Alexander P.; Easter, Tyler D.; Evans, Mykayla G.; Farace, Jessica M.; Johnson, Kristopher D.; Kasse, Julian M.; et al. Computational & Theoretical Chemistry (2021), 1200, 113235.
4. T. Gilbert:: "I have three more manuscripts under review that acknowledge my use of Gaea"
5. Tan, et al., https://doi.org/10.1103/PhysRevAccelBeams.24.051303
6. Mohsen, et al., https://doi.org/10.1016/j.nima.2021.165414
7. Andorf, et al. https://doi.org/10.1364/CLEO_AT.2017.JW2A.90
8. Halavanau, et al., https://doi.org/10.1103/PhysRevAccelBeams.22.114401
9. Lemery, et al., https://doi.org/10.1103/PhysRevLett.122.044801
10. Andorf, et al. https://doi.org/10.1103/PhysRevAccelBeams.21.100702
11. Fritzen, R., V. Lang, and V. A. Gensini, 2021: Trends and variability of North American cool-season extratropical cyclones: 1979–2019. J. Appl. Meteor. Climatol. DOI: 10.1175/JAMC-D-20-0276.1 [in-press] [Fritzen and Lang are students]
12. Haberlie, A. M., W. S. Ashley, V. A. Gensini, and M. Karpinski, 2021: SVRIMG: Radar Reflectivity Images Centered on Severe Weather Reports.11th Symposium on Advances in Modeling and Analysis Using Python, Virtual Meeting, American Meteorological Society, P1037.[Karpinski is a student]
13. Haberlie, A. M., W. S. Ashley, V. A. Gensini, and C. Battisto, 2021: Performance of Continental-Scale Regional Climate Simulations for High-Impact Weather Events.34th Conference on Climate Variability and Change, Virtual Meeting, American Meteorological Society, 14B.10. [Battisto is a student]
14. Gensini, V. A.and B. M. Boustead, 2021: A Modern Look at the 28 August 1884 Tornado Outbreak.19thHistory Symposium, Virtual Meeting, American Meteorological Society, 11.8.
15. Ashley W. S., A. M. Haberlie, and V. A. Gensini, 2020: Reduced frequency and size of late twenty-first-century snowstorms over North America. Nat. Clim. Chang., 10, 539–544, DOI: 10.1038/s41558-020-0774-4
16. Gensini V. A. , A. M. Haberlie, and P. T. Marsh, 2020: Practically perfect hindcasts of severe convective storms. Bull. Amer. Meteor. Soc., 101, E1259–E1278, DOI: 10.1175/BAMS-D-19-0321.1
17. Fritzen, R. C.,V. A. Gensini, S. Collis, and R. Jackson, 2020: Distributed Workflow for WRF Processes and Visualization Using WRF-Python and Dask.30th Conference on Weather Analysis and Forecasting (WAF)/26thConference on Numerical Weather Prediction (NWP), Boston, MA, American Meteorological Society, J68.4. [Fritzen is a student]
18. Gensini, V. A., A. M. Haberlie, W. S. Ashley, and R. S. Schumacher, 2020: Sensitivity of Simulated Summer MCS Activity to Select WRF Parameters. Severe Local Storms Symposium,

Boston, MA, American Meteorological Society, P967.
19. Ungar, M., G. Izzi, E. Lenning, V. A. Gensini, W. S. Ashley, and A. M. Haberlie, 2020: An Environmental Climatology of Quasi-Linear Convective System Mesovortices around Northern Illinois.25th Conference on Applied Climatology, Boston, MA, American Meteorological Society, 2.6. [Ungar is a student]
20. Converse C. M., K. Pittman, L. R. Bundy, B. Brock, and V. A. Gensini, 2020: Environmental Discriminators for Significant Tornadoes and Hail in the Midwestern United States.19th Annual Student Conference, Boston, MA, American Meteorological Society, S159. [Converse, Pittman, Bundy, and Brock are students]
21. Gensini, V. A., D. Gold, J. T. Allen, and B. S. Barrett, 2019: Extended U.S. tornado outbreak during late May 2019: A forecast of opportunity. Geophys. Res. Lett., 46. DOI: 10.1029/2019GL084470
22. Gensini, V. A., and M. K. Tippett, 2019: GEFS predictions of day 1–15 tornado and hail activity.23rd Severe Storms and Doppler RADAR Conference, Des Moines, IA, National Weather Association.
23. Changnon, D., and V. A. Gensini, 2019: Changing spatiotemporal patterns of 5- and 10-day Illinois heavy precipitation amounts, 1900-2018. J. Appl. Meteor. Climatol., 58, 1523–1533. DOI: 10.1175/JAMC-D-18-0335.1
24. Gensini, V. A., and M. K. Tippett, 2019: Global Ensemble Forecast System (GEFS) predictions of days 1–15 U.S. tornado and hail frequencies. Geophys. Res. Lett., 46, 2922–2930. DOI: 10.1029/2018GL081724
25. Gensini, V. A., and H. E. Brooks, 2018: Spatial trends in United States tornado activity. npj Climate and Atmos. Science., 1, 1–5. DOI: 10.1038/s41612-018-0048-2
26. Gensini, V. A., and H. E. Brooks, 2018: Spatial trends in United States tornado frequency.29th Conference on Severe Local Storms, Stowe, VT, American Meteorological Society, 10B.1.
27. Tencate, A. J. and Gee, A. and Erdelyi, B. *Differential algebraic fast multipole-accelerated boundary element method for nonlinear beam dynamics in arbitrary enclosures*, Phys. Rev. Accel. Beams 24, 054601 (2021)
28. A. Al Marzouk, H. D. Schaumburg, S. Abeyratne, and B. Erdelyi, *Efficient algorithm for high fidelity collisional charged particle beam dynamics*, Phys. Rev. Accel. Beams 24, 074601
29. A. Tencate and B. Erdelyi, "A high-precision emission computational model for ultracold electron sources," Proceedings of NA-PAC2019, East Lansing, September 1-6, 2019.
30. S. Abeyratne, A. Gee and B. Erdelyi, "An adaptive Fast Multipole Method in Cartesian basis, enabled by algorithmic differentiation," Communications in Nonlinear Science and Numerical Simulation 72, 294-317 (2019)
31. A. al-Marzouk and B. Erdelyi, "Collisional N-Body Numerical Integrator with Applications to Charged Particle Dynamics, SIAM Journal on Scientific Computing," 40:6, B1517-B1540 (2018)
32. S. Rexford and B. Erdelyi, "Numerical discretization of completely integrable nonlinear Hamiltonian systems," Phys. Rev. Accel. Beams 21(11), 114601 (20 pp.) – Published 14 November 2018
33. H. D. Schaumburg and B. Erdelyi, "A Study on a New Method of Dynamic Aperture Enlargement," arXiv: 1809.03418, pp. 68 (2018)
34. H. Schaumburg, A. al Marzouk and B. Erdelyi, "Picard Iteration-Based Variable-Order Integrator with Dense Output Employing Algorithmic Differentiation," Numerical Algorithms, 80(2), 377-396 (2019).
35. H. Higgins, M. Roeing-Donna, K. Krupiarz, R. O'Connor, J. Tan, N. A. Pohlman, "Granular flow behavior in a conveyor system: From local velocity profiles to mass flow rates", Powder

Technology 382, 263-273, 2021 (M Roeing-Donna is a graduate student in the group).
36. Tan, J., Ding, Z., Hood, M., Li, W. Simulation of circulating tumor cell transport and adhesion in cell suspensions in microfluidic devices, Biomicrofluidics 13 (6), 064105, 2019 (Note, Hood Michael is a graduate student in the group.)
37. Tan, J., Sohrabi, S., He, R. and Liu, Y., Numerical simulation of cell squeezing through a micropore by the immersed boundary method. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, pp. 502–514, 232(3), 2018
38. Tan, J., Sinno, T., Diamond, S., A parallel fluid–solid coupling model using LAMMPS and Palabos based on the immersed boundary method, Journal of computational science, 25, p89-100, 2018
39. P. N. Bhattiprolu and S. P. Martin, "Prospects for vectorlike leptons at future proton-proton colliders," Phys. Rev. D **100**, no.1, 015033 (2019) [arXiv:1905.00498 [hep-ph]].
40. P. N. Bhattiprolu and S. P. Martin, "Signal-background interference for digluon resonances at the Large Hadron Collider," Phys. Rev. D 102, no.1, 015016 (2020) [arXiv:2004.06181 [hep-ph]].
41. P. N. Bhattiprolu, S. P. Martin and J. D. Wells, "Criteria for projected discovery and exclusion sensitivities of counting experiments," Eur. Phys. J. C 81, no.2, 123 (2021) [arXiv:2009.07249 [physics.data-an]].
42. P. N. Bhattiprolu and S. P. Martin, "High-quality axions in solutions to the mu problem," Phys. Rev. D 104, no.5, 055014 (2021) [arXiv:2106.14964 [hep-ph]].
43. J. Adelman and ATLAS collaboration, 273 papers 2018-2023
44. D. Ryu et al., "Identification of Differential Methylated Region" (presented in ASA and submitted to journal).
45. D. Ryu et al., "Shape Analysis", (under preparation)
46. D. Ryu et al., "Outcome-Dependent Follow-Up model", (under preparation)
47. C. Gatto et.al, The REDTOP experiment. e-Print: arXiv:1910.0 (2019).
48. Physics Beyond Colliders at CERN: Beyond the Standard Model Working Group Report , J. Beacham(Duke U. (main)), C. Burrage(U. Nottingham), D. Curtin(Toronto U.), A. De Roeck(CERN), J. Evans(Cincinnati U.) et al. (Jan 20, 2019) : J.Phys.G 47 (2020) 1, 010501
49. J. Beacham et.al, Physics beyond colliders at CERN: beyond the Standard Model working group report. Journal of Physics G: Nuclear and Particle Physics, Volume 47, Number 1 (2019)
50. B. Fabela, C. Gatto, I. Pedraza Morales. The REDTOP experiment: Rare Eta Decays with a TPC for Optical Photons, presented at the International Conference on high Energy Physics (ICHEP16), Chicago, (2016). To be published.
51. Cang, X. & Luo W. , under review, The Maturity of Martian Watersheds, submitted to Earth and Space Science
52. "Particle-Tracking Proton Computed Tomography - Data Acquistion, Preprocessing, and Preconditioning," B. Schultze, P. Karbasi, C. Sarosiek*, G. Coutrakon, C.E. Ordoñez, N.T. Karonis, K.L. Duffin, V.A. Bashkirov, R.P. Johnson, K.E. Schubert, and R.W. Schulte, IEEE Access, 2021, Vol 9, pp. 25946-25958, doi:10.1109/ACCESS.2021.3057760. Refereed.
53. "Analysis of Characteristics of Images Acquired With a Prototype Clinical Proton Radiography System," C. Sarosiek, E.A. DeJongh, G. Coutrakon, D.F. DeJongh, K.L. Duffin, N. Karonis, C. Ordoñez, M. Pankuch, J.R. Winans, and J.S. Welsh, Medical Physics, 2021, Vol 48, Issue 2, doi:10.1002/mp.14801. Refereed.
54. "Clinical Sensitivity of a Prototype Proton Radiography System," M. Pankuch, E. DeJongh, C. Sarosiek*, D. DeJongh, G. Coutrakon, J. Welsh, V. Rykalin, N. Karonis, C. Ordoñez, J. Winans, R.Schulte, W. Hartsell, International Journal of Particle Therapy, 2019, Vol 6, Issue 3, pp. 50, DOI 10.14338/IJPT.19-PTCOG-NA-6.1. Refereed.
55. "Fast In Situ Image Reconstruction for Proton Radiography," C.E. Ordoñez, N.T. Karonis,

K.L. Duffin, J.R. Winans, E.A. DeJongh, D.F. DeJongh, G. Coutrakon, N.F. Myers, M. Pankuch, and J.S. Welsh, Journal of Radiation Oncology, 2019, DOI 10.1007/s13566-019-00387-x. Refereed.

56. "Reconstructed and Real Proton Radiographs for Image-guidance in Proton Beam Therapy," C. Miller, B. Altoos, E.A. DeJongh, M. Pankuch, D.F. DeJongh, V. Rykalin, C.E. Ordoñez, N.T. Karonis, J.R. Winans, G. Coutrakon, and J.S. Welsh, Journal of Radiation Oncology, 2019, Vol. 8, Issue 1, pp. 97-101, DOI 10.1007/s13566-019-00376-0. Refereed.
57. "Comparison of Proton Stopping Power Measurements of Animal Tissues from Proton CT and X-Ray CT Systems," D. DeJongh, E. DeJongh, V. Rykalin, M. Pnakuck, G. DeFillippo, J. Welsh, R. Schulte, N. Karonis, C. Ordoñez, and G. Coutrakon, PTCOG 2020, September 13-14, 2020, virtual. Refereed.
58. "Image Reconstruction with a Fast Monolithic Proton Radiography System," D. DeJongh, E. DeJongh, V. Rykalin, J Welsh, M. Pankuch, N. Karonis, C. Ordoñez, K. Duffin, J. Winans, G. Coutrakon, and C. Sarosiek, APPM '18, Nashville, TN, July 20-August 2, 2018. Refereed.
59. "A Quantification of the Accuracy of Proton Radiography for Patient Alignment of Intracranial Targets," M. Pankuch, E. DeJongh, A. Panchal, S. Boyer, D. Alexandar, N. Kammes, A. Pruneuau, M. Weirich, D. DeJongh, V. Rykalin, G. Coutrakon, C. Sarosiek* , N. Karonis, C. Ordoñez, J. Winans, K. Duffin, R. Schulte, J. Welsh, and W. Hartsell, APPM '18, Nashville, TN, July 20-August 2, 2018. Refereed.
60. Sinko, R.; Breen-Lyles, M (NIU Student Author)..; Tailoring Thermomechanical Properties and Moisture Responsiveness of Cellulose-Based Nanocomposites Using Direct Polymer Grafting. 56th Annual Technical Meeting of the Society of Engineering Science (SES 2019). October 13 – 15, 2019, Washington University, St. Louis, MO, USA
61. Breen-Lyles, M. (NIU Student Author).; Sinko, R.; Modifying the Moisture Adsorption of Cellulose Nanocrystal by Direct Polymer Grafting. (In Preparation)
62. Wohler, P. (NIU Student Author); Sinko, R; Filler/Matrix Interfacial Dynamics of Polymer-Grafted Cellulose Nanocrystal (In Preparation)
63. Wheeler, R.A.; Dalbey, Emily E.#; "Structure factor lineshape model gives approximate nanoscale size of polar aggregates in the ionic liquid N-methyl-N-propylpyrrolidinium bis(trifluormethylsulfonyl)imide"; Phys. Chem. Chem. Phys. 2021; 23, 9061-9064.
64. Mackoy, Travis#; Kale, Bharat#; Papka, Michael E.; Wheeler, R.A.; "viewSq, a Visual Molecular Dynamics (VMD) module for calculating, analyzing, and visualizing X-ray and neutron structure factors from atomistic simulations"; Comput. Phys. Commun. 2021; 264, 107881-/1-11.
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66. A. Snyder, I. Salehinia, Study of Nanoscale Deformation Mechanisms in Bulk Hexagonal Hydroxyapatite under Uniaxial Loading using Molecular Dynamics, Journal of the Mechanical Behavior of Biomedical Materials, 2020, 110, 103894.
67. R.S. Dhumal, D. Bommidi, and I. Salehinia, Thermal conductivity of Metal-Coated Tri-Walled Carbon Nanotubes in the Presence of Vacancies- Molecular Dynamics Simulations, Nanomaterials, 2019, 9 (6), 809.
68. D. Bommidi (student), R.S. Dhumal (student), and I. Salehinia, Study of the thermal conductivity of a metal-coated multi-walled carbon nanotube using molecular dynamics atomistic simulations, MRS Advances, 2019, 4 (8), 507-513.
69. W. Yang (postdoc), G. Ayoub (collaborator), I. Salehinia, B. Mansoor (collaborator), H. Zbib (collaborator), The effect of layer thickness ratio on the plastic deformation mechanisms of

nanoindented Ti/TiN nanolayered composite, Computational Materials Science, 2018, 154, 488-498.
70. G. Blazey, J. Colston, A. Dyshkant, K. Francis, J. Kalnins, S. A. Uzunyan, V. Zutshi, S. Hansen, P. Rubinov and E. C. Dukes, *et al.* "Radiation Tests of Hamamatsu Multi-Pixel Photon Counters," Nucl. Instrum. Meth. A **927**, 463-470 (2019) doi:10.1016/j.nima.2018.12.050 [arXiv:1906.07237 [physics.ins-det]].
71. A. Belloni, Y.M. Chen, A. Dyshkant, T. K. Edberg, S. Eno, V. Zutshi, J. Freeman, M. Krohn, Y. Lai, D. Lincoln, S. Los, J. Mans, G. Reichenbach, L. Uplegger, S. A. Uzunyan "Test beam study of SiPM-on-tile configurations," JINST **16**, no.07, P07022 (2021) doi:10.1088/1748-0221/16/07/P07022 [arXiv:2102.08499 [physics.ins-det]].

7.2 Conference presentations

1. Clot growth modeling considering physical interactions between flow and blood cell components, Jifu Tan, 16th U.S. National Congress on Computational Mechanics, Chicago, July 25-29, 2021
2. Microfluidics Layout Design for Improved Circulating Tumor Cell Capture Efficiency, Michael C. Hood, Jifu Tan, Summer Bioengineering Conference, online, June 14 - June 18, 2021
3. Modeling Granular Flow with Heterogeneous Mixtures Under a Movable Gate, M Roeing-Donna, N Pohlman, J Tan, Bulletin of the American Physical Society, November 22-24, 2020, Chicago, IL
4. Red Blood Cell Deformation Index and Simulation Performance in Lattice-Boltzmann Method and Dissipative Particle Dynamics, K Ostalowski, M Hood, J Tan, Bulletin of the American Physical Society, November 22-24, 2020, Chicago, IL
5. Effects of Shear Rate, Blood Hematocrit, and Cell Stiffness on Circulating Tumor Cell Transport in a Microfluidic Device, M Hood, J Tan, Bulletin of the American Physical Society, November 22-24, 2020, Chicago, IL
6. Simulation Of Clot Mechanics Consisting Of Blood Cells And Fibrin Network, K Ostalowski, J Tan, Summer Bioengineering Conference, online, June 17 - June 20, 2020
7. Simulation of thrombus growth considering platelet activation and red blood cell collision, J Tan, Summer Bioengineering Conference, online, June 17 - June 20, 2020
8. Modeling Cell Interior Viscosity: Continuum And Molecular Approaches, M Hood, J Tan, Summer Bioengineering Conference, online, June 17 - June 20, 2020
9. modeling particle transport in mucus layer with flow driven by beating slender structure, M Roeing-Donna, J Tan, Summer Bioengineering Conference, online, June 17 - June 20, 2020
10. Visualization of Flow of Circulating Tumor Cells and Blood Cell Suspensions in Microfluidics, Joseph A. Insley, Michael Hood, Jifu Tan, Silvio Rizzi, Janet Knowles, Michael Papka, SC20, online, Nov. 18, 2020
11. Multi-physics modeling and parallel computing in complex fluids, invited seminar, July 09, 2020, Texas Tech.
12. Circulating tumor cell transport and adhesion in microfluidic devices, Summer Biomechanics, Jifu Tan, Zhenya Ding, Wei Li, Bioengineering and Biotransport Conference, June 25 -28, 2019, Seven Springs, PA, USA,
13. Circulating tumor cell transport, adhesion, and capture efficiency prediction in cell suspensions in microfluidic devices, Jifu Tan, Zhenya Ding, Wei Li, 56th Annual Technical Meeting of the Society of Engineering Science, October 13 - 15, 2019, Washington University, St. Louis, MO, USA
14. Cell transport and adhesion in microfluidic devices under flow, Jifu Tan, Zhenya Ding, Wei Li,

20th International Conference on Fluid Flow Problems, March 31 – April 3, 2019, in Chicago, USA.

15. Jifu Tan, High performance computing in fluid solid interaction with applications to biological flow problems, The Midwest Numerical Analysis Day, Illinois Institute of Technology (IIT), Chicago, on Sat. April 20, 2019
16. B. Fabela, C. Gatto, I. Pedraza Morales. The REDTOP experiment: Rare Eta Decays with a TPC for Optical Photons, presented at the International Conference on high Energy Physics (ICHEP16), Chicago, (2016). To be published.
17. Chintalapati: MS Thesis, presentation at New Perspectives 2019;
18. Narayanan: presentation at April APS Meeting 2020, IPAC2021 (paper and poster)
19. Wheeler, R.A., St. Norbert College Department of Physics; De Pere, WI; October 14, 2021; "Disordered nanocrystallite model for the structures of ionic liquids for battery electrolytes".
20. Wheeler, R.A., Lawrence University Department of Chemistry; Appleton, WI; October 13, 2021; "Disordered nanocrystallite model for the structures of ionic liquids for battery electrolytes".
21. Wheeler, R.A., American Chemical Society 258th National Meeting; San Diego, CA; August 26, 2019; "Quantitation and visualization of static structure factor peaks for a phosphonium-based ionic liquid"; ENFL 0116; Mackoy, Travis#; Wheeler, R.A.
22. Wheeler, R.A., Argonne National Laboratory; Lemont, IL; April 10, 2019; "Temperature dependence of nanoscale ordering in a pyrrolidinium-based ionic liquid".
23. Wheeler, R.A., North Central College; Department of Chemistry and Physics; Naperville, IL; April 1, 2019; "Temperature dependence of nanoscale ordering in a pyrrolidinium-based ionic liquid".
24. Wheeler, R.A., Western Illinois University; Department of Chemistry; Macomb, IL; January 26, 2018; "Protonation states of histidine ligands to the oxidized Rieske iron-sulfur cluster of cytochrome bc1: Implications for coupled electron and proton transfer".
25. I. Salehinia (invited speaker), Mesbah Uddin, Aaron McKeown, Michael Zawadzki, On Scratching Behavior of Ceramic/Metal Nanolaminates, Materials Science & Technology 2019, symposium: Nanostructured Materials under Extreme Environments, Portland, Oregon, Sep 29-Oct 3, 2019.

7.3 External collaborations

1. T. Gilbert, Dr Alfred P. Sattelberger, Argonne National Labs and U Central Florida, Orlando, FL USA
2. T. Gilbert, Prof Titel Jurca, U Central Florida, Orlando, FL USA
3. T. Gilbert, Dr Brian Scott, Los Alamos National Labs
4. T. Gilbert, Prof Brendan Dutmer, Highland Community College
5. T. Gilbert, Prof Marc Adler, Ryerson University, Toronto, Ontario, Canada
6. T. Gilbert, Prof Dale Wilger, Samford University, Birmingham, AL USA
7. P. Piot, Collaboration with Fermilab/IOTA (optical stochastic cooling modeling)
8. P. Piot, Collaboration with Argonne/Argonne Wakefield Accelerator (wakefield acceleration modeling)
9. P. Piot, Collaboration with DESY-Hamburg (FlashForward facility): modeling on bunch shaping
10. V. Gensini, Fall 2018, Maria Molina, Central Michigan University Ph.D. Candidate, collaboration complete
11. J. Tan, Wei Li, Ph.D., Texas Tech
12. J. Tan, Yuan Wan, Ph.D. Binghamton University

13. J. Tan, Silvio Rizzi, Ph.D. Argonne National Lab
14. J. Tan, Victor Mateevitsi , Ph.D. Argonne National Lab
15. C. Gatto, RedTop collaboration, https://redtop.fnal.gov/collaboration/
16. W. Luo, Alan Howard, Planetary Science Institute
17. W. Luo, Bob Craddock, Center for Earth and Planetary Studies, Smithsonian Institution
18. N. Karonis, Fritz DeJongh, Ethan DeJongh, Victor Rykalin, ProtonVDA.
19. N. Karonis, Jim Welsh Hines, VA Hospital.
20. N. Karonis, Reinhard Schulte, Loma Linda Hospital.
21. N. Karonis, Mark Pankuch, NW Proton Center
22. R. Wheeler, Prof. Nicholas Mauro; St. Norbert College; De Pere, WI.
23. I. Salehinia, G. Ayoub (University of Michigan-Dearborn),
24. I. Salehinia, B. Mansoor (Texas A-M, Qatar)
25. I. Salehinia, H. Zbib (Washington State University)

8 STUDENT ENGAGEMENT

8.1 Doctoral Dissertations

1. Alex Pixler, PhD, Scheduled 2023, Advisor: Thomas Gilbert.
2. Osama Mohesen, PhD, August 2021, Design and Optimization of Superconducting Radio-Frequency Electron Sources, Advisror: Philippe Piot.
3. Tyler Burch, Physics, PhD, Advisor Jahred Adelman, March 2020, A Search for Resonant and Non-Resonant Di-Higgs Production in the $b\bar{b}b\bar{b}$ Channel Using the ATLAS Detector.
4. Afnan al Marzouk (Ph.D. 2021) Collisional Methods in Beam Dynamics, (B. Erdelyi advisor)
5. Prudhvi Bhattiprolu, Ph.D., title "", Physics Department, completed August 2021, advisor Stephen Martin
6. Suvo Chatterji, Ph.D., June 2019, Bayesian Functional Data Analysis Over Dependent Regions and its Applications for Identification of Differentially Methylated Regions, advisor Duchwan Ryu
7. Hao Shen, Ph.D., Oct 2019, Applications of Bayesian Functional Data Analysis, advisor Duchwan Ryu
8. Yang Zhang, Ph.D., In progress, advisor Duchwan Ryu
9. Zhexuan Yang, Ph.D., In progress, advisor Duchwan Ryu
10. Cang, Xuezhi, Ph.D., "A Warm or Cold Early Mars: Evidence from Valley Networks", Department of Geographic and Atmospheric Sciences, May 2021, advisor Wei Luo
11. Christina Sarosiek, Physics 2021, Ph.D., advisor George Coutrakon, completed
12. Mollie Breen-Lyles, "Direct Polymer Grafting as A method of Maintaining the Mechanical Properties of Cellulose Nanocrystals in the Presence of Mositure", Mechanical Engineering, June 2019, Dr. Robert Sinko
13. Paul Wohler, "Enhancing the Mechanical Performance of Cellulose-Reinforced Nanocomposites by Direct Polymer Grafting", Mechanical Engineering, date still TBD (Spring 2022 tentative), Dr. Robert Sinko
14. Jill Belluomini; "The Structure and Aggregation of βB-Crystallin Protein and its R120G Mutant: A Molecular Dynamics Study"; Department of Chemistry and Biochemistry; Spring 2020; Honors thesis; Advisor: Ralph A. Wheeler

8.2 Master Thesis

1. Aaron Fetterman, MS, May 2021, Photoinjector Generation of high-charge magnetized beam for electron-cooling applications, Advisor: Philippe Piot.
2. Christopher Marshall, MS, August 2020, Development of an electron-beam diagnostics. Advisor: Philippe Piot.
3. Anusorn Lueangaramwong, Ph.D., June 2019, Study of Electron Beam Emitted from Nano-Structured Cathode. Advisor: Philippe Piot.
4. Cody Converse, M.S. Thesis, "Environmental Discriminators for significant tornadoes and hail in the U.S. using Proximity Soundings", Geographic and Atmospheric Science, August 2020, Advisor: V. Gensini
5. Summer 2021, Michael Roeing-Donna, thesis, Mechanical engineering, Simulation of Particle Transport in a Multi-component Flow with a High Viscosity Ratio Driven by Slender Structures, Master of Science, Advisor: Jifu Tan
6. Fall 2021(Expected), Michael Hood, thesis, Mechanical engineering, Microfluidics design considering hyperuniformity and cell transport in flow for improved circulating tumor cell capture efficiency, Master of Science, Advisor: Jifu Tan
7. Fall 2021(Expected), Kacper Ostalowski, thesis, Mechanical engineering, blood flow simulation in a microvascular network, Master of Science, Advisor: Jifu Tan
8. Prudhvi Chintalapati, thesis, "Resonant Extraction for Mu2e", PHYSICS, June 2019, Prof. M.J. Syphers
9. Ravindra Sunil Dhumal, effect of defects on the thermal conductivity of metal-coated carbon nanotubes, Mechanical Engineering, Spring 2019, Master of Science, Advisor: Iman Salehinia
10. Austin Pauga, Molecular Dynamic Simulations of Mechanical Properties in Nb-NbC Core-Shell Nanowires and Nodes, Mechanical Engineering, Spring 2020,Master of Science, Advisor: Iman Salehinia
11. Mesbah Uddin, Studying the Scratching Behavior of Nb/NbC Nanolaminate using Molecular Dynamics Atomistic Simulations, Mechanical Engineering, Spring 2020, Master of Science, Advisor: Iman Salehinia
12. Michael Zawadzki, MD Simulation of Femtosecond Laser-Controlled Melting of Core-Shell Nanoparticles, Mechanical Engineering, current, Master of Science, Advisor: Iman Salehinia

8.3 Other Student Research and Engagement

1. Margo Andrews, B.S. Student, Independent Study, "Automated detection, tracking, and climatology of the elevated mixed layer", Geographic and Atmospheric Science, December 2020, Advisor: V. Gensini
2. Billy Faletti, B.S. Student, Independent Study, "Examining the impacts of the CIN on simulated supercells in CM1", Geographic and Atmospheric Science, December 2020, Advisor: V. Gensini
3. Fall 2018, MEE 697-independent study, 3 credit, 1 student (Jianxiao Hu), Advisor: Jifu Tan
4. Spring 2019, MEE 697 – independent study, 3 credits, 1 student (Michael Roeing-Donna), Advisor: Jifu Tan
5. Spring 2019: MEE 497-independent study, 3 credits, 3 students (Michael Hood, Kyle Alberti, Piotr Mierzwa), Advisor: Jifu Tan
6. Fall 2019, MEE 697-independent study, 3 Credits, 1 student (Michael Hood), Advisor: Jifu Tan
7. Fall 2020, MEE 497-independent study, 3 credits, 1 student (Carson Wallace), Advisor: Jifu Tan

8. Fall 2020, MEE 697, independent study, 3 credits, 1 student, (Dehong Fang), Advisor: Jifu Tan
9. NIU STEM Café, May 8th, 2021, virtual, Machines that learn: understanding robotics, machine learning and artificial intelligence.
10. NIU STEM fest, October 2020 virtual, visualization of flow of circulating tumor cells mixed with blood cell suspensions in microfluidics.
11. NIU STEM fest, October 19, 2019. 8 hours. Interactive real time fluid simulation demonstration, NIU Convocation Center
12. NIU STEM fest, Oct. 27, 2018. 8 hours. Interactive real time fluid simulation demonstration, NIU Convocation Center
13. Michael Zawadzki, Femtosecond Laser Pulse Ablation of Nickel Metal: A Molecular Dynamics Study, independent study (MEE697), Mechanical Engineering, 2019, Advisor: Iman Salehinia

9 CONCLUSION

This report presents an analysis of operations, budget, usage and outcomes of supported research projects for two CRCD computing facilities, Gaea and NICADD, for the period FY2019-FY2021. The results show GAEA and NICADD clusters were operated efficiently and at low cost while assisting faculty in there research and attracting external funds.