List of Suggested Reviewers or Reviewers Not To Include (optional)

		.	
SUGGESTED REVIEWERS: Not Listed			
REVIEWERS NOT TO INCL Not Listed	UDE:		

Pursuant to <u>PAPPG Chapter II.C.1.e.</u>, each PI, co-PI, and other senior project personnel identified on a proposal must provide collaborator and other affiliations information to help NSF identify appropriate reviewers.(v.4/21/2017)

Please complete this template (e.g., Excel, Google Sheets, LibreOffice), save as .xlsx or .xls, and upload directly as a Fastlane Collaborators and Other Affiliations single copy doc.

Do not upload .pdf.

There are five tables:

A: Your Name & Affiliation(s);

B: PhD Advisors/Advisees (all);

C: Collaborators;

D: Co-Editors:

E: Relationships

List names as Last Name, First Name, Middle Initial. Additionally, provide email, organization, and department (optional) to disambiguate common names.

Fixed column widths keep this sheet one page wide; if you cut and paste text, set font size at 10pt or smaller, and abbreviate, where necessary, to make the data fit.

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You may fill-down (crtl-D) to mark a sequence of collaborators, or copy affiliations. Excel has arrows that enable sorting. "Last active" dates are optional, but will help NSF staff easily determine which information remains relevant for reviewer selection.

<u>Table A:</u> List your Last Name, First Name, Middle Initial, and organizational affiliation (including considered affiliation) in the last 12 months.

Α	Your Name:	Your Organizational Affiliation(s), last 12 n	Last Active Date
	Harcourt, Edwin	St. Lawrence University	

<u>Table B:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

G: Your PhD Advisor(s)

T: All your PhD Thesis Advisees

P: Your Graduate Advisors

to disambiguate common names

В	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Mauney, Jon	North Carolina State University	

<u>Table C:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

- A: Co-authors on any book, article, report, abstract or paper (with collaboration in last 48 months; publication date may be later).
- C: Collaborators on projects, such as funded grants, graduate research or others (in last 48 months).

C Name: Organizational Affiliation Optional (email, Department) Last
--

C:	Angstadt, Kevin	University of Michigan	
C:	Carroll, Jim	Clarkson University	
C:	Perconti, Jamie	Northeastern University	
C:			

Table D: List editorial board, editor-in-chief and co-editors with whom you interact. An editor-in-chief should list the entire editorial board.

- B: Editorial board: Name(s) of editor-in-chief and journal (in past 24 months).
- E: Other Co-Editors of journals or collections with whom you directly interacted (in past 24 months).

to disambiguate common names

D	Name:	Organizational Affiliation	Journal/Collection	Last Active

Table E: List persons for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

R: Additional names for whom some relationship would otherwise preclude their service as a reviewer.

D	Name:	Organizational Affiliation	Optional (email, Department)	Last Active

Pursuant to <u>PAPPG Chapter II.C.1.e.</u>, each PI, co-PI, and other senior project personnel identified on a proposal must provide collaborator and other affiliations information to help NSF identify appropriate reviewers.(v.4/21/2017)

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D: Co-Editors:

E: Relationships

List names as Last Name, First Name, Middle Initial. Additionally, provide email, organization, and department (optional) to disambiguate common names.

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<u>Table A:</u> List your Last Name, First Name, Middle Initial, and organizational affiliation (including considered affiliation) in the last 12 months.

Α	Your Name:	Your Organizational Affiliation(s), last 12 n	Last Active Date
	Haney, Robert	St. Lawrence University, University of Massachusetts Lowell	

<u>Table B:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

G: Your PhD Advisor(s)

T: All your PhD Thesis Advisees

P: Your Graduate Advisors

to disambiguate common names

В	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Rand, David	Brown University	

<u>Table C:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

- A: Co-authors on any book, article, report, abstract or paper (with collaboration in last 48 months; publication date may be later).
- C: Collaborators on projects, such as funded grants, graduate research or others (in last 48 months).

C	Name:	Organizational Affiliation	Ontional	(email, Department)	Last Active
•	Ivaille.	Olganizational Anniation	Optional	(email, Department)	Last Active

C:	Ayoub, Nadia	Washington and Lee University	
C:	Bhere, Kanaka	Boehringer Ingelheim Vetmedic, Inc.a	
C:	Clarke, Thomas	Washington and Lee University	
C:	Corbett, Susan	Symbiota, Inc.	
C:	Diaz-Ferguson, Edgardo	Auburn University	
C:	Fitzpatrick, Ryan	University of Massachusetts Lowell	
C:	Gadgil, Rujuta	Ragon Institute	
C:	Garb, Jessica	University of Massachusetts Lowell	
C:	Gendreau, Kerry	Virginia Tech	
C:	Hayashi, Cheryl	University of California Riverside	
C:	Lancaster, Alex	Amber Biology LLC	
C:	Latta, Leigh	Lewis-Clark State College	
C:	Miles, Lindsay	Virginia Commonwealth University	
C:	Richards, Stephen	Baylor College of Medicine	
C:	Schwager, Evelyn	University of Massachusetts Lowell	
C:	Silliman, Brian	Duke University	
C:	Stanke, Mario	Ernst-Moritz-Arndt Universität-Greifswald	
C:	Verrelli, Brian	Virginia Commonwealth University	
C:	Vollmer, Steve	Northeastern University	
C:	Wares, John	University of Georgia	
C:	Wierschin, Torsten	Ernst-Moritz-Arndt Universität-Greifswald	
C:			

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- E: Other Co-Editors of journals or collections with whom you directly interacted (in past 24 months).

to disambiguate common names

D	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:	Samuel Cushman	U.S. Forest Service	Frontiers in Evolutionary and Population Genetics	

Table E: List persons for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

R: Additional names for whom some relationship would otherwise preclude their service as a reviewer.

D	Name:	Organizational Affiliation	Optional (email, Department)	Last Active

Pursuant to <u>PAPPG Chapter II.C.1.e.</u>, each PI, co-PI, and other senior project personnel identified on a proposal must provide collaborator and other affiliations information to help NSF identify appropriate reviewers.(v.4/21/2017)

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<u>Table A:</u> List your Last Name, First Name, Middle Initial, and organizational affiliation (including considered affiliation) in the last 12 months.

Α	Your Name:	Your Organizational Affiliation(s), last 12 n	Last Active Date
	Hill, Adam	St. Lawrence University	

<u>Table B:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

G: Your PhD Advisor(s)

T: All your PhD Thesis Advisees

P: Your Graduate Advisors

to disambiguate common names

В	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Harris, Charles B.	University of California, Berkeley	

<u>Table C:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

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- C: Collaborators on projects, such as funded grants, graduate research or others (in last 48 months).

C	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
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C:	Bowring, Miriam A.	University of Washington	
C:	Frei, Heinz	Lawrence Berkeley National Laboratory	
C:	Glover, Starla D.	Uppsala University	
C:	Henderson, Jane S.	University of California, San Diego	
C:	Katsoukis, Georgios	Lawrence Berkeley National Laboratory	
C:	Krogman, Jeremy P.	Brandeis University	
C:	Kubiak, Clifford P.	University of California, San Diego	
C:	Lomont, Justin P.	University of California, Berkeley	
C:	Nguyen, Son C.	University of California, Berkeley	
C:	Pailloux, Sylvie A.	University of California, Berkeley	
C:	Raymond, Kenneth R.	University of California, Berkeley	
C:	Schlegel, Jacob P.	Merritt College & Chabot College	
C:	Thomas, Christine M.	Brandeis University	
C:	Zoerb, Matthew C.	California Polytechnic State University	
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R: Additional names for whom some relationship would otherwise preclude their service as a reviewer.

D	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
R:	Klemm, Piper K.	Klemm Hill, LLC		

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	Schuckers, Michael	St. Lawrence University	

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P: Your Graduate Advisors

to disambiguate common names

В	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Stern, Hal	Iowa State University	

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C Name: Organizational Affiliation Optional (email, Department) Last
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C:	Coulombe, Grace	Bates College	
C:	O'Neill, Mary	Hamilton College	
C:	Lopez, Michael	Skidmore College	
C:	Mills, Shirley	Carleton University, Ontario, CA	
C:	Schuckers, Stephanie	Clarkson University	
C:	Sharp, Richard	Stanford University	
C:	Argeris, Steve	Carolina Panthers	
C:	Macdonald, Brian	Florida Panthers	
C:	Seppa, Timo	National Hockey League	
C:	Rovito, Mike	Caxton Associates	
C:			
C:			

Table D: List editorial board, editor-in-chief and co-editors with whom you interact. An editor-in-chief should list the entire editorial board.

- B: Editorial board: Name(s) of editor-in-chief and journal (in past 24 months).
- E: Other Co-Editors of journals or collections with whom you directly interacted (in past 24 months).

to disambiguate common names

D	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:	Glickman, Mark	Harvard University	Journal of Quantitative Analysis of Sp	oorts
B:	Ridgon, Steve	St. Louis University	Journal of Quantitative Analysis of Sports	

Table E: List persons for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

R: Additional names for whom some relationship would otherwise preclude their service as a reviewer.

D	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
R:	Schuckers, Stephanie	Clarkson University		

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Chapman, Jessica St. Lawr		St. Lawrence University	

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T: All your PhD Thesis Advisees

P: Your Graduate Advisors

to disambiguate common names

В	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)
G:	Morris, Max D.	Iowa State University	
T:	N/A		
P:			

<u>Table C:</u> List names as Last Name, First Name, Middle Initial, and provide organizational affiliations, if known, for the following.

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C Name: Organizational Affiliation Optional (email, Department) Last
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C:	Anderson-Cook, Christine M Los Alamos National Laboratory		
C:	Lu, Lu University of South Florida		
C:	Rosales, Jon	St. Lawrence University	
C:			

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D	Name:	Organizational Affiliation	Journal/Collection	Last Active
B:				
B:				

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			to alsambiguate common names	
D	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
R:	Ramler, Ivan	St. Lawrence University		

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./DUE DATE			☐ Special E	Exce	eption to Deadline Date Policy FOR NSF USE ONLY			OR NSF USE ONLY		
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FOR CONSIDERATION	BY NSF ORGANIZATION	ON UNIT(S	(Indicate the	most specific unit l	knowi	n, i.e. program, division, etc.)	10	140554	
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PI/PD DEPARTMENT Mathematics &	Computer Science	ee	Corpo		ou	ndation Rels				
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NAMES (TYPED)		High De	•	Yr of Degree	<u> </u>	Telephone Numbe	r	Email Address		
PI/PD NAME										
Edwin Harcourt		PhD		1994		315-229-5444	edharc	edharcourt@stlawu.edu		
CO-PI/PD										
<u> </u>		2008		315-229-5471	jchapn	an@stlawu.edu				
CO-PI/PD			2007		079 024 4722	Dobowt	Homory@ssmal.od			
Robert Haney CO-PI/PD		PhD		2007		978-934-4723	Kobert	_Haney@uml.ed	u	
Adam D Hill		PhD		2013		315-229-5858	ahill@s	stlawu.edu		
CO-PI/PD Michael E Schuo	okore	PhD		1999		315-229-5794	schuelz	ers@stlawu.edu		
Michael E Belluckers 1 IID 1777				1///		313-447-3174	SCHUCK	cise suawu.tuu		

CERTIFICATION PAGE

Certification for Authorized Organizational Representative (or Equivalent) or Individual Applicant

By electronically signing and submitting this proposal, the Authorized Organizational Representative (AOR) or Individual Applicant is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding conflict of interest (when applicable), drug-free workplace, debarment and suspension, lobbying activities (see below), nondiscrimination, flood hazard insurance (when applicable), responsible conduct of research, organizational support, Federal tax obligations, unpaid Federal tax liability, and criminal convictions as set forth in the NSF Proposal & Award Policies & Procedures Guide (PAPPG). Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U.S. Code, Title 18, Section 1001).

Certification Regarding Conflict of Interest

The AOR is required to complete certifications stating that the organization has implemented and is enforcing a written policy on conflicts of interest (COI), consistent with the provisions of PAPPG Chapter IX.A.; that, to the best of his/her knowledge, all financial disclosures required by the conflict of interest policy were made; and that conflicts of interest, if any, were, or prior to the organization's expenditure of any funds under the award, will be, satisfactorily managed, reduced or eliminated in accordance with the organization's conflict of interest policy. Conflicts that cannot be satisfactorily managed, reduced or eliminated and research that proceeds without the imposition of conditions or restrictions when a conflict of interest exists, must be disclosed to NSF via use of the Notifications and Requests Module in FastLane.

Drug Free Work Place Certification

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent), is providing the Drug Free Work Place Certification contained in Exhibit II-3 of the Proposal & Award Policies & Procedures Guide.

Debarment and Suspension Certification

(If answer "yes", please provide explanation.)

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency?

Yes ☐ No 🛛

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) or Individual Applicant is providing the Debarment and Suspension Certification contained in Exhibit II-4 of the Proposal & Award Policies & Procedures Guide.

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding \$100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding \$150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

- (1) No Federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions.
- (3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, Title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

Certification Regarding Nondiscrimination

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is providing the Certification Regarding Nondiscrimination contained in Exhibit II-6 of the Proposal & Award Policies & Procedures Guide.

Certification Regarding Flood Hazard Insurance

Two sections of the National Flood Insurance Act of 1968 (42 USC §4012a and §4106) bar Federal agencies from giving financial assistance for acquisition or construction purposes in any area identified by the Federal Emergency Management Agency (FEMA) as having special flood hazards unless the:

- (1) community in which that area is located participates in the national flood insurance program; and
- (2) building (and any related equipment) is covered by adequate flood insurance.

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) or Individual Applicant located in FEMA-designated special flood hazard areas is certifying that adequate flood insurance has been or will be obtained in the following situations:

- (1) for NSF grants for the construction of a building or facility, regardless of the dollar amount of the grant; and
- 2) for other NSF grants when more than \$25,000 has been budgeted in the proposal for repair, alteration or improvement (construction) of a building or facility.

Certification Regarding Responsible Conduct of Research (RCR) (This certification is not applicable to proposals for conferences, symposia, and workshops.)

By electronically signing the Certification Pages, the Authorized Organizational Representative is certifying that, in accordance with the NSF Proposal & Award Policies & Procedures Guide, Chapter IX.B., the institution has a plan in place to provide appropriate training and oversight in the responsible and ethical conduct of research to undergraduates, graduate students and postdoctoral researchers who will be supported by NSF to conduct research. The AOR shall require that the language of this certification be included in any award documents for all subawards at all tiers.

CERTIFICATION PAGE - CONTINUED

Certification Regarding Organizational Support

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that there is organizational support for the proposal as required by Section 526 of the America COMPETES Reauthorization Act of 2010. This support extends to the portion of the proposal developed to satisfy the Broader Impacts Review Criterion as well as the Intellectual Merit Review Criterion, and any additional review criteria specified in the solicitation. Organizational support will be made available, as described in the proposal, in order to address the broader impacts and intellectual merit activities to be undertaken.

Certification Regarding Federal Tax Obligations

When the proposal exceeds \$5,000,000, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Federal tax obligations. By electronically signing the Certification pages, the Authorized Organizational Representative is certifying that, to the best of their knowledge and belief, the proposing organization:

- (1) has filed all Federal tax returns required during the three years preceding this certification;
- (2) has not been convicted of a criminal offense under the Internal Revenue Code of 1986; and
- (3) has not, more than 90 days prior to this certification, been notified of any unpaid Federal tax assessment for which the liability remains unsatisfied, unless the assessment is the subject of an installment agreement or offer in compromise that has been approved by the Internal Revenue Service and is not in default, or the assessment is the subject of a non-frivolous administrative or judicial proceeding.

Certification Regarding Unpaid Federal Tax Liability

When the proposing organization is a corporation, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Federal Tax Liability:

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that the corporation has no unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

Certification Regarding Criminal Convictions

When the proposing organization is a corporation, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Criminal Convictions:

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that the corporation has not been convicted of a felony criminal violation under any Federal law within the 24 months preceding the date on which the certification is signed.

Certification Dual Use Research of Concern

By electronically signing the certification pages, the Authorized Organizational Representative is certifying that the organization will be or is in compliance with all aspects of the United States Government Policy for Institutional Oversight of Life Sciences Dual Use Research of Concern.

AUTHORIZED ORGANIZATIONAL	REPRESENTATIVE	SIGNATURE		DATE
NAME				
Elizabeth Haney		Electronic Signature		Jan 21 2019 9:26AM
TELEPHONE NUMBER EMAIL ADDRESS			FAX N	UMBER
315-229-1885 ehaney@stlawu.edu			315	5-229-5620
product.	•			

PROJECT SUMMARY

Overview:

St. Lawrence University (SLU) has the goal to give students and faculty access to high performance computing and to significantly expand research and academic activities. This track 1 acquisition project (<\$1M) requests a high-performance computer (HPC), specifically the Warewulf Community Support Cluster, a 18 node cluster with a total of 432 CPUs, 2.6TB RAM, with one node a dedicated GPU node. This HPC's graphics processing unit (GPU), large memory footprint, and processing power will provide essential support for ongoing and new faculty research directions and will also provide outstanding research and educational opportunities for undergraduates at SLU and for faculty and undergraduates at surrounding educational institutions. The 14 SLU faculty participants (five PIs and nine major users) and the three external users involved in this project are active teacher-scholars with records of publishing high quality, impactful papers and mentoring and training STEM students from underrepresented backgrounds. Adding the HPC to SLU's technology base, will strengthen not only faculty research portfolios, but also enhance faculty's capacity to mentor and train dozens and teach hundreds of students over the grant term. Additionally, SLU will make the HPC available to collaborators and other local researchers in northern New York, an economically disadvantaged, rural area.

Intellectual Merit:

The research described in this proposal will address key questions in computer science, statistics, chemistry, biology, physics, and economics that require multiple processors and a large memory footprint for large matrix operations, large-scale simulations, image analysis, large relational databases, and custom software. This research, impossible to execute using desktop computers, will be carried out at 3 times faster speed than with current computing infrastructure and the memory capacity of the requested equipment will allow for larger data sets by 2 times over the current computing infrastructure. A nearby institution (Clarkson University) has an NSF-funded high performance heterogeneous computing platform designed to handle large scale parallelization of processes to improve computation time, and the research projects that are part of this proposal are difficult to parallelize and instead require large amounts of memory. There is an understanding in place with the nearby institution to share computing resources and take advantage of the diversity of computing in the region as projects warrant.

Broader Impacts:

Access to HPC will instill in students a broad perspective on computational thinking, consistent with SLU's liberal arts mission, while simultaneously increasing their preparation for STEM careers by offering early hands-on research and training opportunities and 21st-century workforce skills, such as independent work; modifying thinking/hypotheses in the light of new data/evidence; and collecting, analyzing, evaluating, interpreting, and synthetizing data. The strong mentoring and research components will address workforce needs by providing future employees not only with better research skills, but also with programming skills and practice. SLU's diverse student population (56% female, 17% firstgeneration in college, 21% Pell grant recipients, and 12% underrepresented minorities) ensures that the HPC can impact students from all backgrounds, and collaboration with SLU's successful campus student access programs (e.g., Higher Education Opportunity Program and S-STEM) and with the institutionally funded University Fellows summer research program will assist in attracting underrepresented students. In all, over 80 students will be directly exposed to and trained in the use of high performance computing over the course of this grant via mentored research. Additionally, the research projects carried out using HPC will create research-based educational materials--such as unique datasets--that will enable more sophisticated in-class exercises and homework, as well as more advanced lab exercises for the more than 80 students enrolled in courses such as Advanced Inorganic Chemistry, Programming Languages, Database Systems, as well as in many statistics and data science courses. The proposed projects will also contribute to advancing the professional development of junior faculty participants as scholars and mentors.

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^{*}Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

PROJECT DESCRIPTION

a) Information about the Proposal

Instrument location and type: SLU's Information Technology (IT) Central Server Facility, Canton, NY *Description of the instrument:* High-performance computer

b) Research Activities to be Enabled

St. Lawrence University (SLU) is a predominately undergraduate, liberal arts institution with a long and proud tradition of institutional commitment to STEM excellence. SLU recognizes the importance of computing skills for STEM college graduates, and our faculty research needs continue to grow rapidly. Thus, in this Track 1 instrument acquisition project (<\$1M), we seek to give students and faculty access to state-of-the-art computing that will enable a significant expansion in research and academic activities. We will do so by acquiring a high-performance computer (HPC) that will support ongoing and new faculty research directions as well as support outstanding research and educational opportunities for undergraduates. Specifically, we will acquire the Warewulf Community Support Cluster, a 18-node cluster with a total of 432 CPUs, 2.6 TB RAM, with one dedicated GPU node: a more detailed description of the requested equipment is in section c. The 14 SLU faculty participants (five PIs and nine major users) and the three external users involved in this project are active teacher-scholars with records of publishing high-quality, impactful papers and of mentoring and training STEM students. By adding HPC to SLU's technology base, we will not only strengthen faculty research portfolios, but also enhance faculty's capacity to mentor and train dozens and teach hundreds of students over the grant term. Our diverse student population (17% first-generation in college and 12% underrepresented minorities) ensures that we can reach students from all backgrounds.

The specific research activities that will be enabled, the number of students impacted, and their HPC utilization are listed below.

Research Area/Activity	SLU Faculty and External Users	# research students	HPC Ir	nstrument Ca Utilization	pability
		impacted in grant term	Minimum GPU Needs	Minimum CPU Needs	Minimum Memory Needs
Computer Science: Reinforcement Learning	E. Harcourt (PI) and L. Torrey (major internal user)	10	Both Tesla GPU cards	24	128 GB
Chemistry: Quantum Chemical Calculations; the Warner-Juaregg Reaction; Chemotherapeutic Drugs	hemistry: Quantum Chemical A. Hill (co-PI); S. Tartakoff (major internal user); S. Glazier (major		-	24–72	Up to 512 GB
Biology: Bioinformatics of Spiders; Citizen Science Participation; Gene Regulation in Yeast; Metagenomics of Microbial Communities	R. Haney (co-PI); E. Barthelmess (major internal user) and J. Malcomb (major external user); E. Dixon (major internal user); L. Olendzenski (major internal user)	18 (3, 9, 3, and 3 respectively)	-	64–128	Up to 512 GB
Statistics: Multivariate Longitudinal Clustering and Adjusted Plus-Minus Models; Clustering Time Series and Simulation-based Methods; Spatial Statistics on 2D matrices M. Schuckers (co-PI); J. Chapman (co-PI); I. Ramler (major internal user) and R. Sharp (major external user)		23 (10, 3, and 10 respectively)	-	4–36	Up to 512 GB
Economics, Physics and Physics	Yang (major internal user); Armendanz-Picon (major internal user); Helenbrook (major external user);	9 (3, 3, and 3 respectively)	-	4–36	Up to 512 GB

Table 1. Research activities that will benefit from the requested instrument, their computing needs, and their impact on students.

We describe below representative research projects for which the HPC is critical for success and which will involve over 80 undergraduate student research trainees over the three-year grant term. The students are full research partners; these experiences often culminate in co-authored peer-reviewed papers and presentations at professional meetings and conferences. The projects will leverage the HPC's graphics processing unit (GPU), large memory footprint, and processing power (described below in section c) for *large matrix operations, large-scale simulations, image analysis, large relational databases, bioinformatics and genomics research, and custom software* to meet the growing research needs of faculty and students. The first three projects heavily utilize the GPU, memory, and processing capabilities, respectively, and show how these capabilities will be used for research in computer science, chemistry, and biology by PIs Harcourt, Hill, and Haney. Additional projects by PIs and major users in statistics, mathematics, chemistry, biology, physics, economics, and engineering that leverage the computing power of the HPC are described in less detail subsequently. Projects are currently supported by SLU internal funds and external grants, and the results can be leveraged to secure additional funding, including funding from NSF.

Project #1. Deep Learning-Based Object Perception for Reinforcement Learning, Ed Harcourt, PI, Charles A. Dana Professor of Computer Science, St. Lawrence University, Dr. Lisa Torrey, Major Internal User, Associate Professor of Computer Science, St. Lawrence University.

Intellectual Merit and Research Plan. Work in reinforcement learning (RL), in which agents learn autonomously to complete tasks based on environmental feedback, focuses on helping RL agents learn more efficiently by applying knowledge from previous tasks¹ or advice from other agents². In the current project, an RL agent acquires knowledge to facilitate learning by watching a human demonstrate a task. Like humans, agents think about their environments in terms of the objects they contain. Unlike humans, they do not perceive objects naturally and effortlessly. In the first stage of this project, we circumvented the object perception problem and engineered a custom object detector for each experimental environment. In the next stage, to be carried out with the proposed HPC, the goal is to return to this problem and train agents to perceive objects autonomously. Additional work will involve learning involve image processing with a convolutional neural network (CNN)³-5 using TensorFlow (a deeplearning neural network software library developed by Google) and Keras (a Python neural network library that sits on top of TensorFlow and allows for a rapid prototyping of deep-learning models).

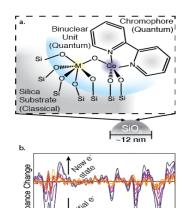
Project #2. Quantum Chemical Calculations of Bimetallic Catalyst Structures for Renewable Energy, Adam Hill, Co-PI, Assistant Professor of Chemistry, St. Lawrence University.

Intellectual Merit and Research Plan. Artificial photosynthesis (AP), the process of capturing sunlight and using its energy to transform atmospheric carbon dioxide and water into chemical fuels, is a promising source of clean, renewable energy. The challenging nature of the chemistry involved means that a new generation of catalysts (molecular machines) is necessary to make the conversion economically feasible. Heterobimetallic chemistry uses two commonly available metal atoms to form a potent, scalable, affordable catalytic center for artificial photosynthesis. In earlier studies, heterobimetallic units have been shown to perform AP, but the relationship (geometry and bonding) of the metal atoms to their silicon dioxide support remains ambiguous (Fig. 1a). Building from our earlier expertise modeling metal systems, 11-13 and recent publication on binuclear units, 14 we will create computational models of

this interaction to reveal the geometry relationship and allow for the rational design of high-efficiency devices.

This bonding relationship can be determined by simulating experimental observations of the units' spectroscopic properties when paired with a "chromophore" reporter molecule like bipyridine: color, vibrations (infrared absorption), fluorescence, and photochemical reactivity. The theoretical models that most accurately match the AP unit will be those that most closely match experimental spectra (**Fig. 1b**). ^{15,16}

Modeling spectroscopic properties requires quantum mechanics to describe the behaviors of electron wavefunctions; all of which can be correlated with one another; changes in one part of the structure impact wavefunctions in the remainder of the structure, resulting in $O(N_{electrons}^{8})$ scaling for most techniques.¹⁷ Density functional theory (DFT) has proven itself to be a flexible tool to efficiently determine electron behaviors, but it still struggles with very large systems due to these scaling issues. ^{17,18} So-called "embedding" approaches place the quantum core inside a classical (non-quantum) structure (Fig. 1a) that allow a large system to simulate more quickly, making calculations of a whole silica nanoparticle feasible. 19,20 Nonetheless, the resources of an HPC are necessary to complete calculations within a reasonable (sub-month) timescale. Because the computations involve searching multiple possible configurations, multiple instances of the computation described above will be occurring at the same time. The reasonable usage of the proposed machine will permit computation of approximately 3–4



IR Frequency (cm-1)

Figure 1. (a) Structure of heterobimetallic unit on silica nanoparticle and indicated component theory levels; (b) time-resolved infrared spectrum of a similar system that will be matched to theoretical simulations to confirm structure and properties.

structures/week, keeping up with the rate of data taking for new chromophore molecules by undergraduate researchers in the laboratory. These calculations will be performed primarily by undergraduate researchers, including McNair and S-STEM students; this research training will help to prepare them for graduate programs in theoretical chemistry or careers in data science that use these or similar techniques to model complex systems.²¹

<u>Project #3.</u> Evolution of the Toughest Spider Silk and the Population Genomics of Spider Urbanization, *Robert Haney, Co-PI, Instructor in the First Year Program and Adjunct Faculty of Statistics, St. Lawrence University.*

<u>Intellectual Merit and Research Plan.</u> Spiders are key predators in terrestrial ecosystems—this status is enabled by their production of silk and venom, which are used in prey capture. Two ongoing projects focus on achieving evolutionary insights into these key spider systems in distinct species.

The striking architecture of spider webs is enabled by spider silks, which include some of the toughest-known material: the combined strength and elasticity of spider silks exceeds that of nearly all other biological and engineered materials. The recently described Darwin's bark spider of Madagascar (*Caerostris darwini*) is heralded as the pinnacle of dragline silk toughness, with large webs that cross rivers up to 25 meters wide. Connecting the phenotype of this spider's unique dragline silk to its underlying genetic basis is necessary to potentially replicate this toughness in biomimetic materials. Recent work identified an unexpected diversity of spidroin (spider fibroin) genes expressed in the major ampullate silk gland of the Darwin's bark spider, with repetitive motifs that differ from those previously identified, which together with an unusual gland morphology, likely contributes to the toughness of this spider's dragline silk. Ongoing and future work includes assaying the protein composition of silk with high-throughput tandem mass-spectrometry and testing patterns of gene expression among differentiated silk glands in multiple species of *Caerostris*, to determine how expression changes have led to evolved differences in silk composition among species.

The western black widow is an important urban pest of the desert southwest and serves as a model of an "urban adapter", with increased population densities and phenotypic modifications in urban compared to their natural habitats. The goal of this work is to determine the genetic and epigenetic basis for urban phenotypes in this species, using genomic sequence and data from multi-tissue transcriptomes. This research will reveal up- and down-regulated genes in multiple disjunct urban populations relative to non-urban groups, to specify gland specific expression phenotypes underpinning adaptation to a novel environment, and test whether the functional systems involved in urban adaptation are convergent, as well as testing for outlier loci in the genome-wide distribution of population structure, to find putative target genes for positive selection and urban adaptation.

This proposed research requires the proposed HPC, as the analyses utilize hundreds of GBs of memory and consist of highly parallelizable tasks can be accelerated greatly by multi-threading. Some jobs may consume 48 or more CPUs (75% of the current HPC's capacity) and in excess of 100 GB of RAM.

<u>Project #4.</u> Multivariate Longitudinal Clustering and Adjusted Plus-Minus Models, *Michael Schuckers*, Co-PI, Charles A. Dana Professor of Statistics, St. Lawrence University.

<u>Intellectual Merit.</u> Prof Schuckers' work develops statistical methods using sports data, recognizing that these methods can also apply to other data and that sports is useful for harnessing student interest in statistics research.²⁴ Projects include multivariate longitudinal clustering, which have applications in metabolonomics or electroencephalography data, and adjusted plus-minus models.²⁵⁻³¹ As these datasets grow, the necessity for fast matrix processing grows in parallel. Parallel matrix libraries will leverage the capabilities of the proposed HPC.

<u>Project #5.</u> Clustering and Simulation-based Methods with Application to Dendrochronology, Jessica Chapman, Co-PI, Associate Professor of Statistics and Grace J. Fippinger '48 Professor of Sciences, St. Lawrence University.

<u>Intellectual Merit.</u> Dendrochronology of driftwood requires comparison of driftwood samples to known sites (e.g., the International Tree Ring Data Bank).³² This work develops a simulation-based approach to evaluate different methods for this comparison using parallel computing. As these datasets grow, the necessity for fast matrix processing grows in parallel. Parallel matrix libraries will leverage the capabilities of the proposed HPC.

Project #6. Using Big Data to Map the Diversity of Citizen Scientist Participation, Erika Barthelmess, Major Internal User, Professor of Biology, St. Lawrence University; Jacob Malcomb, Major External User, Ph.D. student, Environmental Sciences, University of Virginia.

Intellectual Merit. National-scale citizen science (Cit Sci) projects aim to make scientific knowledge more robust and democratic, 33 engage communities that have traditionally remained uninvolved in science, 44 and connect people to science; 55 yet, reports from single projects indicate that Cit Sci participants are not diverse and representative of the public at large but tend to be highly educated and more affluent. 66 Given that one of the goals of Cit Sci is to encourage interest in scientific careers, lack of diversity among participants may contribute to reduced diversity in the current and future scientific workforce. 75 This project examines factors affecting engagement by a diverse audience of participants in national-scale Cit Sci projects to broaden their reach and impact. The methodology of logistic regression with more than 20 predictor variables requires more computational power with datasets of this size than can easily be accomplished with the current HPC

Project #7. Using Metagenomics to Understand Complex Microbial Communities in Meromictic Lake Sediments, Ed Harcourt, Co-PI, Professor of Computer Science and the Peterson Professor of Mathematics, St. Lawrence University; Robert Haney, Co-PI, Instructor in the First Year Program and Adjunct Faculty of Statistics, St. Lawrence University; Lorraine Olendzenski, Major Internal User, Associate Professor of Biology, St. Lawrence University.

<u>Intellectual Merit.</u> This work uses metagenomics to characterize microbial community composition and metabolic capabilities present in the sediments of Fayetteville Green Lake³⁷, and to understand how

sediment depth affects microbial community dynamics and metabolism by characterizing the diversity of sediment sulfate reducing bacteria, the metabolic capabilities of the lineages present, and their potential interactions with other members of the sediment bacterial community. This proposed research requires the proposed HPC, as the analyses utilize hundreds of GBs of memory and consist of highly parallelizable tasks can be accelerated greatly by multi-threading. Some jobs may consume 48 or more CPUs (75% of the current HPC's capacity) and in excess of 100 GB of RAM.

<u>Project #8.</u> DNA Binding Strengths of Chemotherapeutic Drugs, Samantha Glazier, Major Internal User, Associate Professor of Chemistry, St. Lawrence University.

Intellectual Merit. Creating targeted chemotherapeutics that biological targets requires estimating the equilibrium constant (K_{eq}) for binding and the free energy changes (ΔG) for each "molecular step" along a binding pathway. This work correlates experimental K_{eq} and ΔG results measured via fluorescence spectroscopy with computed binding energies for a class of chemotherapeutics called acridines. Calculations of chemical structures requires for this research scale in difficulty with the cube of the number of particles being simulated; drug molecules are large enough that a single-structure calculation would take days to weeks on the current HPC. Furthermore, these calculations parallelize with decreasing efficiency so the high individual processor speeds of the proposed HPC are critical.

<u>Project #9.</u> Forest Edge Degradation of Global Carbon Forest Stocks, *Ivan Ramler, Major Internal User, Associate Professor of Statistics, St. Lawrence University; Richard Sharp, Major External User, Natural Capital Project, Stanford University.*

<u>Intellectual Merit.</u> Carbon stock estimates based on land-cover type are critical for informing climate change assessment and landscape management. Preliminary work^{45,46} used a combination of R, Python, and C to calculate distance transforms and spatial statistics on 2D matrices but was limited to an analysis on a grid of 500-km cells across the planet due to computational limitations of the statistical analysis code. With the new HPC, a parallel implementation of this model will be developed, and results will be released as part of InVEST⁴⁷, a free and open-source environmental software analysis package. Currently, many analyses incur a computational cost of approximately 100 computing days on a single core. Even with a desktop quad-core parallelization, these analyses face a month of computing time. With the proposed HPC, those processes can be performed in a single day to allow iteration on models and derivative works.

<u>Project #10.</u> The Wagner-Jauregg reaction, Samuel Tartakoff, Major Internal User, Assistant Professor of Chemistry, St. Lawrence University.

Intellectual Merit. The proposed work focuses on elucidation of the mechanism for the Wagner-Jauregg reaction, ⁴⁸ as well as developing catalytic methods for this process. Specifically, the reaction can be applied to morphine analogues, such as commercially available isovanillin, 2,4-dihydroxy-5-methoxybenzaldehyde, or 3,4,5-trihydroxybenzaldehyde, to make a variety of novel molecules that can then be tested for potency in pain relief. This work will not only provide information about what novel types of molecular structures are effective in treatment of pain, but also validate the Wagner-Jauregg reaction as a method. Calculations of chemical structures requires for this research scale in difficulty with the cube of the number of particles being simulated; drug molecules are large enough that a single-structure calculation would take days to weeks on the current HPC. Furthermore, these calculations parallelize with decreasing efficiency so the high individual processor speeds of the proposed HPC are critical.

<u>Project #11.</u> Regulation of Gene Expression in Yeast, *Emily Dixon, Major Internal User, Associate Professor of Biology, St. Lawrence University.*

<u>Intellectual Merit.</u> The proposed work studies the molecular mechanisms that lead to altered gene regulation following nutrient limitation and focuses on the roles of histone-modifying enzymes, such as the histone deacetylase RPD3, and chromatin remodeling enzymes, such as SNF2, in *Saccharomyces*

cerevisiae. This proposed research requires the proposed HPC, as the analyses utilize hundreds of GBs of memory and consist of highly parallelizable tasks can be accelerated greatly by multi-threading. Some jobs may consume 48 or more CPUs (75% of the current HPC's capacity) and in excess of 100 GB of RAM.

<u>Project #12.</u> Endogenous Skills and Labor Income Inequality, *Guanyi Yang, Major Internal User, Assistant Professor of Economics, St. Lawrence University.*

<u>Intellectual Merit.</u> The proposed work develops a model of the role of education on lifetime earnings inequality. The model introduces education decisions through life cycle to an overlapping generations model of human capital and can be used to evaluate policies designed to mitigate the impact of early-life conditions on life outcomes. As datasets grow, the necessity for fast matrix processing will leverage the capabilities of the proposed HPC.

<u>Project #13.</u> Estimating the Strength of the Gravitational Waves Produced at the Beginning of the Big-Bang, Cristian Armendariz-Picon, Major Internal User, Associate Professor of Physics, St. Lawrence University.

<u>Intellectual Merit.</u> According to the inflationary paradigm, the early universe underwent an epoch of accelerated expansion that ended with the production of matter and radiation particles, observable as gravitational waves. By analyzing temperature fluctuations in the cosmic microwave background, this work will estimate the strength of the gravitational waves produced at the beginning of the Big-Bang via the calculation of three-dimensional integrals of a set of functions that lack analytical forms. As datasets grow, the necessity for fast matrix processing will leverage the capabilities of the proposed HPC.

Project #14. Horizontal Ribbon Growth of Single-Crystal Silicon for Use in Solar Cells, Brian Helenbrook, Major External User, Professor of Mechanical and Aeronautical Engineering and Paynter-Krigman Endowed Chair in Engineering Science Simulation, Clarkson University.

Intellectual Merit. The manufacture of high-efficiency solar cells to convert solar energy to electrical energy requires a manufacturing approach for creating high-quality single-crystal silicon wafers. One approach, called horizontal ribbon growth (HRG), has been developed and has the potential for up to 75% cost savings. Commercialization of the HRG process has been difficult, however, due to a lack of information about the underlying physics of the process. The goal of this work is to develop a model of HRG and use the model to optimize the process for commercialization. The model will use an in-house high-order finite element method for moving meshes and typically have more than a million unknowns and require parallel computing techniques. The proposed HPC is the ideal machine for computing jobs of this size and will vastly increase the ability to parametrically explore the HRG process. Because of the potential for cost savings noted above, this work has potential to bring down the cost of solar energy to be competitive with other sources, or even to make it the cheapest energy source of all.

Results from Prior NSF Support

PI Harcourt was co-PI on an MRI titled, "Acquisition of High Performance Computer and Microarray Scanner for Interdisciplinary Research in Computer Science and Biology at St. Lawrence University," Award #0959713, \$179,336; 5/10/10–4/30/13. Intellectual Merit: This project advanced image synthesis, comparative genome analysis in yeast, phylogenetic analysis of microbial communities, and comparative analysis of bacterial genomes, microarray analysis of gene expression, and bird foraging studies. Both of these instruments were the first of their kind on the SLU campus; the microarray scanner was the first in New York State north of Syracuse; and the HPC was the first among neighboring universities. Broader Impacts: Eight SLU faculty from six majors utilized the instrument for research, resulting in over 50 projects, including individual faculty research projects, as well as mentored research projects with over 30 students. Collaborations were established with Clarkson University and Los Alamos National Labs. One of the projects developed using this instrument, THOR (Total Hockey Ranking), spawned interest in a predictive data analytics center to be housed in Massena, NY. Publications: Fifteen

publications in the fields of statistics, biology, computer science, and economics utilized this equipment.⁴⁹⁻⁶³ **Operations and Maintenance, Downtime, and Usage History:** The equipment has been successfully operated and maintained with minimal downtime—fewer than three days over its life.

PI Chapman and co-PI Hill are PI and co-PI, respectively, on an S-STEM titled, "Liberal Arts Science Scholars Program," Award #1458712, \$618,524; 4/1/15–8/31/20. Intellectual Merit: This program is increasing the number and diversity of students in the STEM pipeline and improving their retention and success by helping them build knowledge in core subject areas and supporting them through mentoring, support services, and research and career-building opportunities. Broader Impacts: SLU has seen an influx of strong students with improved confidence in their research and scientific communication skills and students have begun research projects with faculty members. The PI team will share how their model may prepare the next generation of STEM researchers and educators. Publications: Two conference presentations.

Co-PI Haney is co-PI on a grant from NSF's Division of Integrative Organismal Systems titled "Collaborative Research: Comparative analyses of structural designs underlying functional performance of the toughest spider silk," Award #1656458, \$335,168; 9/1/17–8/31/21. Intellectual Merit: This project investigates silk production, structure and biomechanics among Caerostris darwini and its close relatives in a comparative framework to determine the key design features underlying super-tough spider silk and how they evolved with web ecology. Broader Impacts: The super-silk protein sequences obtained in this work can be exploited to develop new bio-inspired materials; the work will train diverse undergraduates, graduate students, and post-docs; and outreach activities will be developed for K-12 students at the Tsongas Industrial History Center in Lowell, MA and for the public at large at the UVM Natural History Museum. Publications: None to date.

Co-PI Schuckers was PI on a workshop grant titled, "Quantitative and Mathematics Support Center Workshop to Develop Handbook of Best Practices, Professional Organization and STEM Infrastructure," Award #1255945, \$49,652; 1/1/13–6/30/15. Intellectual Merit: Quantitative and Mathematical Support Centers (QMaSCs) exist in many institutions of higher learning across the country and those centers for a backbone of support for STEM disciplines. This workshop began a national conversation about the role of QMaSCs and increased the visibility of directors of these centers. Broader Impacts: The publication of a handbook for directors of these centers creates a vital resource for center directors nationally and internationally. This reference gives QMaSC directors a set of best practices and a set of case studies that enables them to better lead and manage their centers. Over 1,700 chapters from the handbook have been downloaded since its publication in 2016. Publications: Coulombe, GC, O'Neill, MB, Schuckers, ME,(eds), A Handbook for Directors of Quantitative and Mathematical Support Centers, University of South Florida Scholar Commons (2016), which is freely available for download by chapter at the University of South Florida Scholar Commons website.

Conference (HRUMC) 2018," Award # 1807502, \$13,886; 2/15/18–7/31/18. Intellectual Merit: This grant supported the 2018 HRUMC and incorporated four novel innovations to strengthen and broaden the impact of HRUMC: 1) presentations on opportunities in mathematical sciences (REUs and internships, graduate school, and career options); 2) three lunch panels: one featuring recent student experiences in graduate school, one composed of recent graduates who have gone into industry to inspire undergraduate students to consider careers in mathematical sciences, and one for faculty on the mentoring of student research projects; 3) practical evaluation tools for undergraduate mathematics conferences to assess their impact; and 4) outreach to increase attendance by students from underrepresented groups. Broader Impacts: HRUMC provides presentation and networking opportunities for approximately 300 undergraduate students per year; raises awareness about research, conference, graduate school, and career opportunities in the mathematical sciences; offers faculty development in mentoring of undergraduate research; and encourages underrepresented minorities and women to participate in the mathematics, computer science, and statistics communities. Publications: None to date.

PI Chapman is co-PI on "EAGER: Reducing Scientific Uncertainty of Storm Trends in Savoonga and Shaktoolik, Alaska with Traditional Knowledge," Award #1640960, \$90,366; 6/15/16–5/31/18.

Intellectual Merit: This research represents a novel merging of traditional ecological knowledge (TEK) and dendrochronology science and contributes to the enhancement of climate science by approaching the topic of storm intensity from a TEK perspective. The untested elements of this project are: 1) whether enough babies have been named after storms in these two villages to date past weather events; and 2) whether an independent untested method of dating past driftwood lines will corroborate this "stored information" to determine the direction of storm intensity change. If successful, this project will help reduce uncertainty related to storm intensity in the scientific literature on climate change in the Arctic and/or uncover a potentially rich store of TEK, while also advancing knowledge in the growing field of driftwood studies. Broader Impacts: If successful, this project will verify a widely-held claim by traditional and local knowledge holders in Savoonga and Shaktoolik that storm intensity is increasing and generate data for government authorities working on climate change adaptation plans. Publications: None to date.

Research Training to be Strengthened

SLU's research training is already strong, and acquiring state-of-the-art equipment is essential to maintain this strength. National rankings rate SLU as #58 in the US News & World Report "Best Colleges" guidebook and give it high recognition by the Princeton Review for Best Science Lab Facilities (#17) and one of the "25 Great Schools for Mathematics Majors." Over the past several years, we have also been noted by Forbes as one of the top 20 institutions of higher education for excellence in educating women in the sciences. Currently, almost half of SLU graduates attend graduate school within four years, and over 20% attain a graduate degree within five years. Each summer, 35 to 50 students participate in our \$250,000 annual institutionally-funded "University Fellowship" program, which involves an 8-10-week experience of participating in intensive faculty-mentored research. The majority of these projects are consistently in STEM fields—63% of the most recent summer projects represented STEM disciplines. This approach has led to student success; for graduates with majors in chemistry and biochemistry since 2008, over 30% are in graduate programs at schools including Columbia, Dartmouth, University of Indiana, University of Michigan, and Yale. Moreover, over the past six years, the Department of Computer Science, Mathematics, and Statistics has graduated 49 computer science majors (an average eight per year), 19 of whom have gone on to graduate school (39%), Recent graduate schools include Johns Hopkins, The University of Florida, Boston University, Harvard, The University of Maryland, New York University, The University of Virginia, and the University of Michigan. Job placement is also excellent, with recent graduates being employed by EMC, BAE Systems, General Electric, Stanford University, New York State, DirecTV, and the U.S. Army.

SLU trains a diverse student population with great success. In the incoming class in Fall 2017 (most recent year with data), 17% of students were first-generation in college and 12% were underrepresented minorities. The University data for the past five years show that 97% of alumni are placed in graduate school or employment within nine months of graduation. This indicates the strength of the curriculum, as well as the power of the SLU alumni network, which is ranked by The Princeton Review as third in the nation. In the overall mobility index—a measure that represents the likelihood that a student moves up two or more income quintiles—SLU was ranked 18th out of 71 highly-selective private colleges by *The New York Times* in 2017. Furthermore, the PIs involved have strong histories of working with students from all backgrounds across a variety of disciplines including computer science, chemistry, biology, and statistics (**Table 2**, *below*).

Having the HPC on campus will impact three major mechanisms for training students. First, students involved in the research projects described above will be trained in the usage of the HPC. Depending upon the project, these students will learn to program the HPC to varying degrees in order to complete aspects of the highlighted projects. Second, SLU will offer specific course modules on parallel computing based on the popular Open Message Passing Interface (MPI) library. These modules will range from a guest lecture in lower-level courses to projects in our Programming Languages course to an entire senior-level elective on High Performance Programming taught twice over the period of this grant by PI Harcourt. Third and most importantly, many students complete a senior year experience (SYE) that

involves original research. As students gain valuable skills, the SYE also provides opportunities to improve their communication skills; in addition to writing a final paper, students give two departmental talks on their research and present posters at our Festival of Science at the end of the year. Students who leverage their SYE into completing honors projects deliver an oral defense of their thesis.

SLU Faculty	Discipline	Total Students Mentored (# female, # underrepresented
Member		minority)
Chapman (co-PI)	Statistics	15 (8, 4)
Haney (co-PI)	Biology	8 (2,0)
Harcourt (PI)	Computer	40 (10,3)
	Science	
Hill (co-PI)	Chemistry	19 (13,2)
Schuckers (co-PI)	Statistics	43(21,5)

Table 2. PIs have long and successful experience with mentoring of students from diverse backgrounds.

Exposure to the proposed, state-of-the-art HPC will build on and expand these strengths. Access to the HPC will instill in students a broad perspective on computational thinking, consistent with the University's liberal arts mission, while simultaneously increasing their marketability to prospective employers. This is a critical factor in our students' post-baccalaureate success, as specific high-value skills, such as computing ability, are particularly scarce relative to demand and, thus, particularly valuable to employers. HPC experience and training will also contribute to our students' successful transition to graduate school, which is another key pathway to future professional work in STEM fields. Between the student involvement in the proposed faculty-driven research projects and enrollment in high-performance computing courses and course components, we estimate that over 80 students will be directly exposed to and trained in the use of high-performance computing over the course of this grant via mentored research (Table 1) and that hundreds of students will be directly exposed to high-performance computing via their interaction with the HPC through their coursework.

The proposed projects will also contribute to advancing the professional development of junior faculty participants as scholars and mentors; senior faculty (PIs Schuckers, Harcourt, Chapman) will take an active role in mentoring junior faculty (PIs Haney and Hill). Additionally, the close-knit community of scientists at a small liberal-arts college encourages interdisciplinary collaboration. For example, as a computer scientist, Harcourt will lend technical assistance in computing to the other research scientists in their projects, including in a proposed collaborative project with co-PIs Haney and Harcourt and major internal user Olendzenski (Project #7). Similarly, the statistician Schuckers (co-PI) frequently assists colleagues such as Barthelmess (major internal user) in data analysis. Additionally, the PI and co-PIs will host a series of talks and seminars at SLU and other local institutions to encourage additional faculty utilization of the HPC, including workshops as part of the local R (the statistical software) Users Group which is co-organized by Schuckers and Barthelmess.

c) Description of the Research Instrumentation and Needs

Limited Existing Resources

We have seen growth of both student interest and faculty need for computing, based upon rising departmental enrollments (e.g., the combined enrollment in mathematics, computer science, and statistics has risen by 19% in the last two years); recent hiring of new faculty members, such as co-PIs Haney and Hill, who will conduct research that uses the HPC (e.g., since 2013, SLU has hired eight new tenure-track faculty members in STEM fields); and a current proposal to offer a new data science major—a combined major in computer science and statistics—that will likely attract additional students to conduct research in these fields. The HPC will allow for a significant upgrade in the computing facilities available to faculty and students. Simply stated, we will be unable to maximize the potential for faculty and student research and training in the projects we propose without new HPC infrastructure.

The only research computing resources currently available at St. Lawrence, other than individual desktops and laptops, is a Linux-based multicore computer purchased with NSF grant #0959713 in 2010.

The main feature of this existing HPC is a 1-TB main memory with only 64 older-model processors (CPUs). The large main memory (RAM) helps with research problems that are memory intensive but does little to assist with problems that are compute bound (**Fig. 2**). Furthermore, with limited-compute resources, the current HPC is often overloaded and less responsive; given our computing needs, we are faced with the challenge of growing faculty and student demand for greater computing capacity, performance, and infrastructure.

We note that nearby Clarkson University also has an NSF-funded high performance heterogeneous computing platform, which is designed to handle large-scale parallelization of processes to improve computation time. The research projects that are part of this proposal are difficult to parallelize and instead require large amounts of RAM for their computation; they require different computing infrastructure than what can be provided by Clarkson's instrument

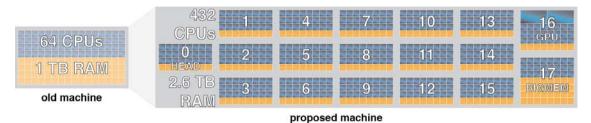


Figure 2. Visual comparison of improvement between the current HPC and new the proposed HPC (1 gray block = 1 processor; 1 gold block = 16 GB RAM): more, faster processors split across multiple nodes, as well as specialized GPU and BIGMEM nodes for particular applications.

The requested HPC configuration consists of 18 compute nodes, each with 24 cores (48 threads) and 128 Gigabytes (GB) of main memory. Each CPU core is an Intel Xeon Gold processor capable of running two threads at 3.2 Gigahertz (GHz). Each compute node contains a one-Terabyte (TB) hard drive. To assist with memory-bound projects, one of the compute nodes will have 512 GB of main memory. For the GPU-based projects, an additional compute node will contain two NVIDIA Tesla v100 GPUs; each with 5,120 CUDA cores and 640 Tensor cores. The HPC also has one additional head node that is used for logging on to the HPC and controls the submission of jobs and monitoring of the compute nodes. The head node also contains a one-Terabyte (TB) disk for scratch space, a 32-TB RAID disk for user data, and a separate 480-GB disk for the Linux installation. The head node will be connected to the compute nodes with a 100-Gigabyte per second (Gbps) Infiniband (EDR) interconnect allowing parallel job across multiple compute nodes. The system design is shown below (Fig. 3)

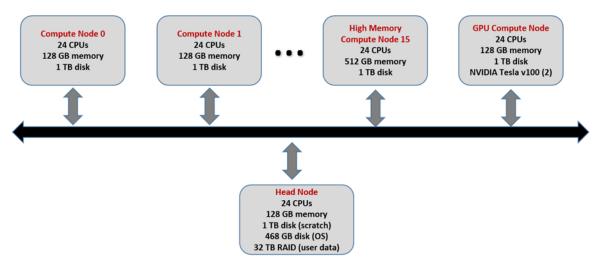


Figure 3. Proposed HPC system design and parameters

The proposed research projects are either compute bound and/or memory bound and require the increased capabilities of the proposed HPC as compared to SLU's current configuration (**Fig. 2**). Furthermore, some of the compute-bound projects are amenable to GPU implementations, such as the deep-learning neural-network-based projects are most suitable for GPU computing (Project 1). Specific ways in which the capabilities of the proposed HPC will enable the research projects described above are elaborated on below by disciplinary area.

Research Capabilities Enabled by this MRI Proposal

The proposed machine will greatly improve computing infrastructure. More CPUs allow for faster run times—three times as many jobs—or for individual jobs to run three times faster. More RAM allows for larger datasets by two times over the current computing infrastructure. Finally, the processors in the proposed HPC are 2–3 generations newer than the processors in the computer purchased with NSF grant #0959713 in 2010, which means faster computation time

Needs for HPC in Chemistry

Calculations of chemical structures like those proposed by co-PI Hill and major users Glazier and Tartakoff are effectively high-dimensionality optimization problems, seeking to determine the optimal positions of atoms and electrons. As a result, these calculations generally scale in difficulty with the cube of the number of particles being simulated; real-world-applicable molecules like catalysts and drug molecules are large enough that a single-structure calculation would take weeks to months on a typical desktop. More processors reduce this time somewhat, but the correlated nature of the structures (behavior of an electron in one part of a molecule influences the behavior of an electron in a different part) means that substituent calculations need to frequently check the status of other substituents. Read/write times mean the density functional theory calculations parallelize with decreasing efficiency, so high individual processor speeds are critical. Though the final output from a density functional theory calculation is small, the intermediate steps generate large amounts of data on electron densities; large amounts of RAM result in fewer read/writes to scratch and substantial improvements in speed—the high memory compute node with its 512 GB of RAM will be invaluable for all chemical calculations, but it is expected that the memory and processors of other nodes in the proposed HPC will also be recruited. This will allow calculations to keep pace with laboratory results.

Needs for HPC in Biology

Co-PI Haney's proposed work requires computationally-intensive assembly and annotation of transcriptomes from multiple spider tissues, including venom glands, silk glands, and ovaries, as well as the assembly of the large genomes of Theridiid spiders. Transcript reconstruction in genome-enabled species involves the spliced alignment to genomes of Illumina libraries consisting of hundreds of millions of reads. Assessment of venom composition requires the characterization of spider venom proteomes through matching of tandem mass spectra against protein databases generated from transcriptomes. Large datasets from next-generation sequencing require significant computational resources to analyze them and require demanding tasks such as genome assembly, the characterization and annotation of genomes via sequence comparison using the Basic Local Alignment Search Tool (BLAST) with locally hosted databases, as well as phylogenomic analysis—all of which require the proposed HPC. Depending on installed software and dataset size, hundreds of GBs of memory may be required to run analyses, or highly parallelizable tasks can be accelerated greatly by multi-threading. While memory and CPU requirements vary depending on existing software, large jobs may consume 48 or more CPUs (75% of the current HPC's capacity) and in excess of 100 GB of RAM.

Dixon's and Olendzenski's work has similar computing requirements. For Barthelmess and Malcomb's work, the data files from national-scale Cit Sci projects contain from hundreds of thousands to millions of records. Logistic regression with more than 20 predictor variables requires more computational power with datasets of this size than can easily be accomplished with the current HPC.

Furthermore, manipulating these files in statistical packages like R requires a large amount of memory that can not met by the existing HPC.

Needs for HPC in Statistics, Economics, Physics, and Engineering

Many of the statistical models being utilized in the research proposed by Chapman, Schuckers, Ramler, Sharp, Yang, Armendanz-Picon, and Helenbrook require large matrix computations that can be accelerated by the use of sparse matrices; however, as these datasets grow, the necessity for fast matrix processing grows in parallel. Parallel matrix libraries will leverage the capabilities of the proposed HPC. Currently, many analyses incur a computational cost of approximately 100 computing days on a single core. Even with a desktop quad-core parallelization, these analyses face a month of computing time. With the proposed HPC, those processes can be performed in a single day to allow iteration on models and derivative works.

d) Broader Impacts (Including Impact on Research and Training Infrastructure) Attract Researchers and Improve Capacity to Conduct Leading-Edge Research

Acquiring state-of-the-art equipment is essential to maintaining SLU's strong research and training infrastructure. Major infrastructure investments completed during the last decade include: (1) the \$37 million Johnson Hall of Science, a 115,000-square-foot, Gold LEED-certified science facility housing the Biology, Neuroscience, Chemistry, and Biochemistry programs (2007); (2) major renovation of space within the former Biology building to establish the 2,500-square-foot Peterson Quantitative Resource Center (2012) to provide walk-in peer tutoring in all areas of quantitative reasoning within the Department of Mathematics, Statistics and Computer Science; and (3) \$229,000 to renovate and equip three new computer labs dedicated for Computer Science.

The research infrastructure will be further strengthened by the addition of the proposed HPC. Its multiple processors and large memory footprint will enable new research directions that involve large matrix operations, massive simulations, image analysis, large relational databases, and custom software to meet the growing research needs of faculty (as show by the eight new tenure-track faculty members in STEM fields) and students (as shown by the increase in the combined enrollment in mathematics, computer science and statistics by 19% in the last two years). The HPC will also support the new Data Science major, which will likely attract additional students to conduct research, as well as be supported by one new tenure-track faculty hire in Data Science and one new tenure-track faculty hire in Bioinformatics, both of whom will begin in fall of 2019. The new HPC will also enable collaborative projects across disciplines, such as Project #7.

Quality of Research Training

The research training infrastructure will be further strengthened by the addition of the HPC, which will add to the overall training capacity at SLU. First, it will support training of student researchers via mentoring. Recognizing that faculty have an active role in influencing students' engagement through their interactions with students both inside and outside of classrooms and that such interactions are closely related to students' collegiate experiences, development, and success^{67,68}, SLU faculty are committed to a mentoring model that maximizes relationships and interactions between PIs and students during research. Such intense interaction results in positive outcomes, including students' self-assessed leadership abilities and social self-confidence⁶⁹ and is especially effective for students of color⁷⁰ and female students.⁷¹ Through active, hands-on participation with the use of the HPC, students will develop not only practical computing skills, but also essential skills for researchers, including creativity, judgment, communication, organization, and persistence.⁷² Furthermore, mentoring relationships will also provide students with information about possible careers and industries that are possible with a STEM degree and with HPC skills. Mentored research at SLU occurs during SYEs and in the annual "University Fellows" undergraduate summer research program. Over the most recent summer, STEM projects accounted for 63% of these summer fellowships, and projects in Mathematics, Computer Science, or Statistics accounted for 14% of STEM projects. Given these participation data, it is important for SLU to continue

to offer state-of-the-art computing resources to engage and train students. Second, via its implementation by PIs and other faculty in courses—such as Chemistry 403 Advanced Inorganic Chemistry, Computer Science 364 Programming Languages, and Computer Science 345 Database Systems, as well as in many statistics courses and in to-be-determined courses as designed and offered by the new tenure-track faculty member in data science—the HPC will enable more sophisticated in-class exercises and homework, as well as more advanced lab exercises for the more than 80 students enrolled in these classes annually. Third, the HPC will enable the creation of entirely new training opportunities for undergraduate students via new courses. For example, PI Harcourt will teach an MPI-based software development course using HPC as an upper-level elective for computer science students. Through our consortial relationship with other neighboring institutions (SUNY Potsdam and SUNY Canton), we plan to expand the reach of the HPC well beyond our campus by holding a series of "open houses" for faculty colleagues with research and teaching interests involving HPC. There is significant potential to increase collaboration between our institutions. SUNY Potsdam, for example, has a Computer Science program with four faculty members serving 90 majors, and these students will be able to cross-register in St. Lawrence's new HPC programming courses via existing agreements as part of the Associated Colleges of the St. Lawrence Valley.

Broaden Participation of Women, Underrepresented Minorities, and Students with Disabilities

SLU serves a diverse population of 2,414 undergraduates (44% men and 56% women). Our students represent 43 states and 53 foreign countries: 33.8% New York State; 57.6% U.S., non-New York State; and 8.6% from outside the U.S. Currently, 100% of undergraduates receive financial aid (need or merit based); 21% of our students are Pell grant recipients (a rate higher than at most select, small private colleges in the U.S.); and the average total aid package is \$40,737. Over the past 20 years, we have made significant progress in diversifying our campus, doubling the percentages of students of color (now 14%) and first-generation students (now 17%). This is especially significant, as our surroundings in rural, upstate New York are 92% white, with only 22% of adults having bachelor's degrees or higher. This diverse student body will benefit from the implementation by PIs and other faculty in courses of the proposed HPC by gaining an understanding of scientific concepts and processes; how different hardware and software can be used to achieve specific goals; and the use of computational and programming tools. Participation in the proposed research projects will further help students' skills by honing independent work; modifying their thinking/hypotheses in the light of new data/evidence; and providing practice in collecting, analyzing, evaluating, and interpreting data. All of these are essential skills for the 21st century workforce.

Guided by the inclusive excellence principle 72,73, course and research opportunities described above using HPC will be targeted to all traditionally underrepresented student populations, as identified by the Admissions Office. There is a substantial target population; in the incoming class in Fall 2017 (most recent year with data), 16% of students were first-generation in college and 12% were underrepresented minorities. In addition, SLU has an active NSF S-STEM grant that offers scholarships to 20 underrepresented students in STEM fields. The project team will use processes similar to those in the S-STEM project to identify underrepresented science students to target for recruitment to research projects (Co-PI Hill is a Co-PI on the S-STEM). Furthermore, SLU has several existing programs that can also be useful for promoting projects using the HPC to students from underrepresented groups. The New York State (NYS) Higher Education Opportunity Program (HEOP) supports 70 low-income students each year who are capable of college success but do not meet regular admissions standards; they graduate and go on for post-baccalaureate education at the same rates as the overall SLU student body. The Ronald E. McNair Post-baccalaureate Achievement Program (McNair) is a highly competitive program supporting 27 students annually who are first-generation, come from economically disadvantaged families, or are from groups underrepresented in doctoral programs. It prepares eligible students to become competitive for Ph.D. programs. McNair Scholars currently enroll in graduate school immediately following their graduation at a rate of 67.3% annually, and, to date, 23% have earned advanced degrees. The NYS Collegiate Science and Technology Entry Program (CSTEP) works to increase the number of students

from underrepresented groups pursuing professional licensure and careers in mathematics, science, technology, law and health-related fields and serves 36 students annually. Other promotion activities will include featuring students' HPC research projects in *The Hill News* (SLU's student-run newspaper), on SLUWire (an online platform in which University offices, campus organizations, associations, and fellow Laurentians find and share information about campus happenings), and through emails, bulletin board posters, presentations at campus family weekends (fall and spring); personal communication of faculty in their classes; and personal interactions by faculty with students.

Projects using the HPC will help SLU improve the preparation of students for STEM careers by offering hands-on research and training opportunities and 21st-century workforce skills. This will address workforce needs by providing future employees with not only better computing and research skills, but also with interpersonal, teaming, and communication skills and practice. The strong mentoring by the faculty on each research project will foster positive outcomes in students, especially underrepresented students (women, minority, low-income, first-generation), ⁶⁷⁻⁷⁴ helping them to persist in STEM majors and go on to graduate school and/or careers in STEM.

e) Management Plan

SLU has a track record of successfully managing an HPC from a prior NSF grant. In the prior grant, PI Harcourt and the other PIs constituted a management committee that worked closely with SLU's IT server support staff to oversee: (a) access to the HPC; (b) the software installed; (c) maintenance; and (d) equitable use among the users. Building on this past experience, we are seeking assistance from a consultancy group, Sly Media Networks, LLC, who specializes in HPC installations and support. The previous HPC was one large, shared memory computer, which eased the administration of the system. This new proposal has many nodes, so continual support by the consulting group is needed to handle all aspects of the system administration; this will allow the PIs to concentrate on their research projects. Sly Media Networks will work with SLU IT for hardware and facilities issues. They will also work with users, install specialized software and system updates, and perform any other system administration tasks.

For the proposed instrument, PI Harcourt will again chair a multidisciplinary Project Steering Committee to oversee the use and management of the requested equipment. Steering Committee members will be: PIs Harcourt, Chapman, and Hill; a representative of Sly Media Networks; and the SLU IT server manager. Specifically, the committee will: (a) evaluate how the equipment is being used; (b) plan how to optimize its future use; (c) monitor purchases and use of equipment supplies; (d) facilitate cooperation among users; and (e) identify potential other opportunities in which the equipment will enhance faculty and faculty-student research, mentoring, and collaborative partnerships. The Steering Committee will meet on a regular basis to ensure the advancement of the research programs described in this proposal and the submission of the required reports.

The HPC is a fundamental component of the research programs described in this proposal, but, like most modern computer technology, the HPC will have a limited research shelf life (approximately five years). Consequently, another primary role of the Steering Committee will be to coordinate with the senior administrative staff in the Academic Affairs and Finance divisions, as well as the grants office, to plan for the eventual replacement of the HPC when needed.

Installation and Training/Facility Where Instrument Will Be Housed

Sly Media Networks, LLC will install the equipment, configure it for the institution's infrastructure and train the PI, co-PIs, and other senior personnel on its use. The HPC will be housed in the SLU IT Central Server Facility, a stand-alone building of approximately 2,000 sq. ft. It currently houses 60 IBM Intel servers, one IBM z800 mainframe, and two EMC storage systems. The facility includes the following features: 1) secure physical access; 2) fire suppression system; 3) redundant environment control and air-conditioning units; 4) 40-KVA UPS backup power for all systems; 5) natural gas generator backup power for the entire building; and 6) environment and access control, monitored by security and IT staff.

Housing, Maintenance, and Long-Term Operation

SLU is committed to the long-term operation and maintenance of HPC sought through this proposal and has permanent, dedicated space, as well as experienced faculty and a consultant who will manage day-to-day use, ongoing operation, and long-term maintenance of the HPC. PI Harcourt and the co-PIs will coordinate with Sly Media Networks, SLU's IT department, and the equipment manufacturers/suppliers, to develop a protocol and schedule for maintenance to ensure proper long-term operation of the equipment. On an ongoing basis, Sly Media Networks will teach new users how to operate the equipment.

The new HPC will be maintained by Sly Media Networks, LLC, which will work with the SLU IT server manager. Management tasks conducted by Sly Media Networks will include software and server installation, monitoring of server status, and system security policies. User accounts will be maintained, and training will be conducted by Sly Media Networks with assistance from PI Harcourt and co-PIs as needed. Any physical maintenance will be conducted by Sly Media Networks and SLU IT. NSF support will cover the costs for hardware and software support for the HPC during the 36-month project period, and thereafter SLU will assume all costs for the day-to-day operation and long-term maintenance of the equipment. The HPC comes with a three-year warranty, and Sly Media Networks will provide service via an annual consulting contract; after the grant term these costs are incorporated into the operating budget. Because the shelf life of an HPC is approximately five years, the Steering Committee will work closely with key administrators to pursue funding opportunities that will enable project personnel to acquire updated technology. The PI and colleagues will use improved data and strong project results to plan strategically for future funding.

We anticipate near-continuous use of the proposed HPC for research projects and training during courses (**Table 3**).

Purpose	Average Weekly Use (hours)
Faculty Research Projects during Summer	120
Faculty Research Projects during Academic Year	70
Student Research Projects during Summer	45
Student Research Projects during Academic Year	35

Table 3. Expected usage by faculty and students of HPC.

Procedures for Allocating Instrument Time

Priority will be managed by the scheduling software provided and installed by Sly Media Networks, defined by the policies of the Steering Committee, and assigned to SLU faculty and students and to external users by the software when batch jobs are submitted. A software-based queue system will ensure fairness in the utilization of resources as defined by the scheduling policy. Unless otherwise necessary, short computation jobs will be given priority over long ones, to maximize throughput on the HPC. Conflicts will be resolved by PI Harcourt, and, if necessary, the Steering Committee.

Plans for Attracting and Supporting New Users

The PI and co-PIs will communicate with science department chairs at SLU and at several universities and colleges in Northern New York and will use existing networks, including the Associated Colleges of the St. Lawrence Valley, to inform the science community of the new HPC. Training/scheduling of new users will be managed through existing training and calendar systems. SLU will not charge fees to outside collaborators/users of the HPC. Each co-PI attends small regional meetings in their disciplines, where they will present their research. At each venue, they will provide equipment usage and contact information and also explore collaboration with other faculty. The Department websites will contain contact information for usage, and each year the PI and co-PIs will directly contact potential user institutions (Clarkson, SUNY Potsdam, and SUNY Canton) with instrument/user updates.

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(PI, co-PI, and major internal and external users in **bold**) (*undergraduate co-author)

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- 14. **Hill, A. D.**; Katsoukis, G.; Frei, H. "Photoinduced Electron Transfer from ZrOCo Binuclear Light Absorber to Pyridine Elucidated by Transient Optical and Infrared Spectroscopy." *The Journal of Physical Chemistry C* **2018**, *122*, 20176. http://dx.doi.org/10.1021/acs.jpcc.8b06435
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- 50. **Schuckers, M.E.** "An Alternative to the NFL Draft Pick Value Chart Based upon Player Performance", *Journal of Quantitative Analysis in Sports* (2011).
- 51. **Schuckers, M.E.**, "Statistical Evaluation of Hockey Goaltending" in <u>Handbook of Statistical Methods for Design and Analysis in Sports</u> Chapman & Hall/CRC Handbooks of Modern Statistical Methods (2016).
- 52. **Schuckers, M.E.**, "Draft by Numbers: Using Data and Analytics to Improve National Hockey League (NHL) Player Selection", in *Proceedings of the 2016 MIT Sloan Sports Analytics Conference*, March 2016.
- 53. **Schuckers, M.E.** and *Brozowski, L.C. "Referee Analytics: An Analysis of Penalty Rates by National Hockey League Officials, in *Proceedings of the 2012 MIT Sloan Sports Analytics Conference*, March 2012.

- 54. **Schuckers, M.E.** "DIGR: A Defense Independent Rating of NHL Goaltenders using Spatially Smoothed Save Percentage Maps" in *Proceedings of the 2011 MIT Sloan Sports Analytics Conference*, March 2011.
- 55. Sylvain, J. and **Schuckers M.E.,** "Can We Predict Injuries? The Probability and Severity of Man Games Lost Due to Injury in an NHL Season" in *Rob Vollman's Hockey Abstract 2017* (2017)
- 56. Humphrey-Dixon, E.L., **Sharp, R., Schuckers, M**., Lock R. "Comparative genome analysis suggests characteristics of yeast inverted repeats that are important for transcriptional activity", *Genome* (2011). 54(11):934-42.
- 57. **Chapman, J.L.**, Morris, M.D., and Anderson-Cook, C.M. "Computationally Efficient Comparison of Experimental Designs for System Reliability Studies with Binomial Data." *Technometrics* (2012). 54 (4): 410-424
- 58. **Harcourt, E.** and Perconti, J. "A SystemC library for specifying pipeline abstractions." *Microprocessors and Microsystems* (2014). 38(1):76-81.
- 59. L. Lu, **J.L. Chapman**, C.M. Anderson-Cook. "A Case Study on Selecting a Best Allocation of New Data for Improving the Estimation Precision of System and Subsystem Reliability Using Pareto Fronts." *Technometrics* (2013). 55 (4): 473-487.
- 60. Lopez, M.L. and **Schuckers M.E.** "Predicting Coin Flips: Using Resampling And Hierarchical Models To Help Untangle The NHL's Shootout." *Journal of Sports Science* (2016). 35(9): 888-897.
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- 73. Williams, D. A. (2007). Achieving inclusive excellence: Strategies for creating real and sustained change in quality and diversity. *About Campus*, 12, 8–14.
- 74. Packard, B. W.-L. (2016). <u>Successful STEM mentoring initiatives for underrepresented students:</u> A research–based guide for faculty and administrators. Sterling, VA: Stylus Publishing, 141 p.

Edwin A. Harcourt

St. Lawrence University 23 Romoda Drive Canton, NY 13617 (315) 299-5858 edharcourt@stlawu.edu

Professional Preparation

State University of New York, Plattsburgh, NY	Computer Science	B.S.	1986
North Carolina State University, Raleigh, NC	Computer Engineering	M.S.	1989
North Carolina State University, Raleigh, NC	Computer Science	Ph.D.	1994
Chalmers University of Technology,	Computer Science	Postdoctoral	1994-6
Gothenburg, Sweden			

Appointments

2016 – present	Professor, Computer Science, Martha E.'62 and Gregg E. Peterson Professor of
	Mathematics, Department of Mathematics, Computer Science, and Statistics, St.
	Lawrence University, Canton, NY
2010 - 2014	Chair, Department of Mathematics, Computer Science, and Statistics, St.
	Lawrence University, Canton, NY
2009 - 2016	Associate Professor, Computer Science, St. Lawrence University, Canton, NY
2003 - 2009	Assistant Professor, Computer Science, St. Lawrence University, Canton, NY
1996-2003	Software Architect, Cadence Design Systems, Chelmsford, MA

Most Closely Related Products

- 1. Kevin Angstadt and Ed Harcourt. *A Virtual Machine Model for Accelerating Relational Database Joins using a General Purpose GPU*. In Proceedings of the High Performance Computing Symposium (HPC'15). Society for Computer Simulation International, 2015.
- 2. Ed Harcourt and Jamie Perconti. *A SystemC library for specifying pipeline abstractions*. Microprocessors and Microsystems, 38(1):76-81, February 2014.
- 3. Ed Harcourt. *Policies of system level pipeline modeling*. Electronic Notes in Theoretical Computer Science 238: 13-23. 2009.
- 4. Paolo Giusto, Grant Martin, and Ed Harcourt. *Reliable estimation of the execution time of embedded software*. In Proceedings of the Design Automation and Test Europe, pages 580-588. IEEE Press, March 2001.
- 5. Jwahar Bammi, Ed Harcourt, Wido Kruitzer, Luciano Lavagno, and Mihai Lazarescu. *Software performance estimation strategies in a system level design tool*. In Proceedings of the Eighth International Workshop on Hardware/Software Codesign (CODES). IEEE Press, March 2000.

Other Related Products

- 1. Ed Harcourt. *Teaching computer organization and architecture using SystemC*. The Journal of Computing Science in Colleges, 21(2), December 2005.
- 2. Performance Level Modeling and Simulation of Electronic Systems Having Both Hardware and Software, U.S. Patent 7,069,204. June 27, 2006. Also published under the Patent Cooperation Treaty, International Publication Number WO 02/027565 A1.
- 3. *Method and System for Simulation of Mixed-Language Circuit Designs*, U.S. Patent 7,424,703. September 9, 2008.
- 4. Ed Harcourt, Richard Sharp, Kevin Angstadt and Yuxi Zhan, *StatKey*, A web based statistics package http://www.lock5stat.com/statkey/index.html (also available as a Google Chrome app at the Chrome Web Store).

5. Richard Sharp and Ed Harcourt. Design and construction of general purpose computing resources for Linux based computer science education. *Journal of Computing Science in Colleges*, 26(1):150-156, October 2010.

Synergistic Activities

1. Prior Grants

New York State Education Department grant for "Summer Institutes for Teachers in Mathematics and Science. Level 2 Lego/Vex Curriculum Development Workshop;" 05/01/2008-10/31/2008; \$98,319; co-PIs: **Edwin Harcourt** (St. Lawrence), Jim Carroll (Clarkson University), Donna Kennedy (St. Lawrence, SUNY Potsdam), Glenn Simonelli (SUNY Potsdam); supported 20 research and teaching activities in partnership with 8 regional institutions and resulted in 3 publications.

- 2. *Software:* Consultant, NexID Biometrics; developed StatKey software (with Kevin Angstadt, Rich Sharp and the authors of the book *Statistics: Unlocking the Power of Data* by Robin Lock, Patti Lock, Kari Lock Morgan, Eric Lock, Dennis Lock. Wiley, 2013).
- 3. Professional Service: Program Chair, Consortium for Computing Science in Colleges Northeast Region, 2017-2018; Steering Committee, Hudson River Undergraduate Math Conference, 2008; Reviewer for numerous technical conferences, journals, and publishers including McGraw-Hill, Wiley, IEEE Design Automation Conference (DAC), ACM Computing Reviews (reviews.com), SIGCSE, ITiCSE, CCSC, ACM Computing Surveys, ACM Programming Language Design and Implementation, and CONCUR; Member of the Association for Computing Machinery and of Sigma Xi, the Scientific Research Society.
- St. Lawrence Service: Quantitative Resource Center Advisory Board (2007 present); Director, Engineering Combined Program (2008 - present); Coordinator, New Zealand study abroad program (2010 - present); Institutional Strategy and Assessment Committee (Spring 2011); Academic Advising Committee (2015 - present)
- 5. *Outreach:* Led workshops for K-12 teachers

Summer 2015. Android Mobile Development for Middle School Teachers. Carthage Central School District.

Summer 2008. Advanced Robotics Workshop on Sensors, Data Acquisition, and Analysis and Developing Rigorous and Relevant Lesson Plans. Clarkson University. Funded by the New York State Education Department.

Summer 2008 and Summer 2009. First Tech Challenge Robotics Workshop for High School Teachers. Clarkson University. Funded by the New York State Education Department.

Jessica L. Chapman

127 Bewkes Hall St. Lawrence University Canton, NY 13617 (315) 229-5471 jchapman@stlawu.edu

Professional Preparation

- Truman State University; Kirksville, MO; Mathematics B.S., Statistics and Computer Science minors, 2003
- Iowa State University; Ames, IA; Statistics M.S., 2006
- Iowa State University; Ames, IA; Statistics, Ph.D., 2003 2008

Appointments

- 2014 present Associate Professor of Statistics (with Tenure), St. Lawrence University
- 2009 2014 Assistant Professor of Statistics, St. Lawrence University

Related Products

- Chapman, J.L., Lu, L., and Anderson-Cook, C.M. (2018). "Using Multiple Criteria Optimization and Two-Stage Genetic Algorithms to Select a Population Management Strategy with Optimized Reliability." Complexity, Vol. 2018, Article ID 7242105. https://doi.org/10.1155/2018/7242105.
- Lu, L., Chapman, J.L., and Anderson-Cook, C.M. (2017). "Multiple Response Optimization for Higher Dimensions in Factors and Responses." Quality and Reliability Engineering International, 33, 727-744; DOI: 10.1002/qre.2051.
- Rosales, J. and **Chapman, J.L.** (2015). "Identifying the Exposure of Two Subsistence Villages in Alaska to Climate Change Using Traditional Ecological Knowledge." *Climate* (Climate Risk Assessment and Management Special Issue), 3, 812-832; doi:10.3390/cli3040812.
- Chapman, J.L., Lu, L., and Anderson-Cook, C.M. (2015). "Impact of Response Variability on Pareto Front Optimization." *Statistical Analysis and Data Mining* (CODA Special Issue), 8, 314-328.
- **Chapman, J.L.**, Lu, L., and Anderson-Cook, C.M. (2014). "Incorporating Response Variability and Estimation Uncertainty into Pareto Front Optimization." *Computers and Industrial Engineering* 76: 253-267.

Other Significant Products

- Chapman, J.L., Lu, L., and Anderson-Cook, C.M. (2014). "Process Optimization for Multiple Responses Utilizing the Pareto Front Approach." *Quality Engineering*, 26(3), 253-268.
- Lu, L., Chapman, J.L., and Anderson-Cook, C.M. (2013). "A Case Study on Selecting a Best Allocation of New Data for Improving the Estimation Precision of System and Subsystem Reliability Using Pareto Fronts." *Technometrics* (CODA Special Issue), 55(4), 473-487.
- **Chapman, J.L.** (2013). "A Matrix Representation of System Structure with Application to Computational Reliability Assessments." *Quality Engineering*, 25(4), 418-436.

- Chapman, J.L., Morris, M.D., and Anderson-Cook, C.M. (2012). "Computationally Efficient Comparison of Experimental Designs for System Reliability Studies with Binomial Data." *Technometrics*, 54(4), 410 424.
- Ramler, I.P. and **Chapman, J.L.** (2011) "Introducing Statistical Research to Undergraduate Mathematical Statistics Students using the Guitar Hero Video Game Series." *Journal of Statistics Education*, 19(3).

Synergistic Activities

- *Honors:* Named to Grace J. Fippinger '48 Professorship in the Sciences, established in 1998 to honor St. Lawrence alumna Grace J. Fippinger '48 by encouraging the success of women in the sciences.
- <u>Mentoring</u>: Mentoring of fifteen undergraduates (eight women) in statistics, including collaborative efforts with the Los Alamos National Laboratory.
- <u>Pedagogy:</u> Offered pedagogical presentations at international and domestic statistics teaching conferences, including: Chapman, J.L. (2017). "Developing a Research and Writing Intensive Introductory Statistics Course for Science Majors." US Conference on Teaching Statistics (USCOTS); Ramler, I.P. and Chapman, J.L. (2014). "Advice for Using Faculty Connections to Create Research Opportunities for Undergraduates." International Conference on Teaching Statistics (ICOTS); and Ramler, I.P. and Chapman, J.L. (2011). "Using Video Games to Introduce Statistical Research in Undergraduate Statistics Courses." US Conference on Teaching Statistics (USCOTS).
- <u>Teaching:</u> Iowa State University Teaching Excellence Award
- <u>Professional Service</u>: Member, American Statistical Association (ASA), ASA Section on Statistical Education; Member-at-large, Executive Committee of the ASA Section on Statistical Education; Reviewer for *Quality Engineering, Journal of Statistics Education, The American Statistician, and Applied Stochastic Models in Business and Industry*; Associate Editor for Reviews, *Journal of the American Statistical Association and The American Statistician, 2011-2015*; Session Chair, Joint Statistical Meetings, 2010, 2014, and 2015.

Robert A. Haney

121-2 Bewkes Hall St. Lawrence University Canton, NY 13617 (315) 229-5220 rhaney@stlawu.edu

Professional Preparation

<u>Undergraduate Institution</u> SUNY Buffalo 2001	Amherst, NY,	USA Biology	B.S.,
Graduate Institution Brown University	Providence, RI, USA	Evolutionary Biology	Ph.D., 2007
Postdoctoral Institutions			
University of Chicago	Chicago, IL, USA	Organismal Biology	2007-2010
Harvard University	Cambridge, MA, USA	Molecular Biology	2010-2012
Northeastern University	Nahant, MA, USA	Marine Sciences	2012-2013
University of Massachusetts	Lowell, MA, USA	Biological Sciences	2013-present

Appointments

Instructor in the First Year Program and Adjunct Faculty of Statistics, St. Lawrence
Instructor in Biology, Middlebury College
Postdoctoral Researcher, University of Massachusetts Lowell
Postdoctoral Researcher and Instructor, Northeastern University
Postdoctoral Researcher, Harvard University
Postdoctoral Researcher, University of Chicago

Publications

(i) 5 significant publications most closely related to proposed project

- (1) Clarke, T.H., Garb, J.E., Haney, R.A., Chaw, R.C., Hayashi, C.Y., Ayoub, N.A. 2017. Evolutionary shifts in gene expression decoupled from gene duplication across functionally distinct spider silk glands. *Scientific Reports*. 7: 8393.
- (2) Haney, R.A., Clarke, T.H., Gadgil, R., Fitzpatrick, R., Hayashi, C.Y., Ayoub, N.A. and J.E Garb. 2016. Effects of gene duplication, positive selection and shifts in gene expression on the evolution of the venom gland transcriptome in widow spiders. *Genome Biology and Evolution*. 8: 228-242.

- (3) Bhere, K.V., Haney, R.A., Ayoub, N.A. and J.E. Garb. 2014. Gene structure, regulatory control, and evolution of black widow venom latrotoxins. *FEBS Letters*. 588: 3891-3897.
- (4) Clarke, T.H., Garb, J.E., Hayashi, C.Y., Haney, R.A., Lancaster, A.K., Corbett, S. and N.A. Ayoub. 2014. Multi-tissue transcriptomics of the black widow spider reveals expansions, co-options, and functional processes of the silk gland gene toolkit. *BMC Genomics*. 15: 365.
- (5) Haney, R.A., Ayoub, N.A., Clarke, T.H., Hayashi, C.Y. and J.E. Garb. 2014. Dramatic expansion of the black widow toxin arsenal uncovered by multi-tissue transcriptomics and venom proteomics. *BMC Genomics*. 15: 366.

(ii) 5 other significant publications

- (1) Gendreau K.L., Haney, R.A., Schwager, E.E., Wierschin, T., Stanke, M., Richards, S., Garb, J.E. 2017. House spider genome uncovers evolutionary shifts in the diversity and expression of black widow venom proteins associated with extreme toxicity. *BMC Genomics*. 18:178.
- (2) Haney, R. A., Silliman, B.R. and D.M. Rand. 2010. Effects of selection and mutation on mitochondrial variation and inferences of historical population expansion in a Caribbean reef fish. *Molecular Phylogenetics and Evolution*. 57: 821-828.
- (3) Haney, R.A. and M.E. Feder. 2009. Contrasting patterns of transposable element insertions in *Drosophila* heat-shock promoters. *PLoS One.* 4: e8486.
- (4) Haney, R.A., Silliman, B.R., Fry, A.J., Layman, C.A. and D.M. Rand. 2007. The Pleistocene history of the sheepshead minnow (*Cyprinodon variegatus*): non-equilibrium evolutionary dynamics within a diversifying species complex. *Molecular Phylogenetics and Evolution*. 43: 743-754.
- (5) Rand, D.M., Haney, R.A. and A.J. Fry. 2004. Cytonuclear coevolution: the genomics of cooperation. *Trends in Ecology and Evolution*. 19: 645-653.

Synergistic Activities

- [1] Review Editor: Frontiers in Evolutionary and Population Genetics
- [2] <u>Professional Service:</u> I have served as an invited reviewer of submitted manuscripts for the following journals: Molecular Biology and Evolution, Science, Genetica, Genome Research, International Journal of Molecular Sciences, Diversity, Molecular Ecology, Functional Ecology, Environmental Biology of Fishes, Molecular Ecology Resources.
- [3] <u>Undergraduate mentoring</u>: I have mentored eight undergraduate students, including two Asian-Americans and two women, at five different universities, and the research involved has contributed to three publications on which undergraduates have served as co-authors.

Adam D. Hill

St. Lawrence University 23 Romoda Drive Canton, NY 13617 (315) 299-5858 ahill@stlawu.edu

Professional Preparation

Trinity College, Hartford, CT. B.S. Chemistry, 2008. University of California, Berkeley, CA. Ph.D. Chemistry 2013.

Appointments

Assistant Professor of Chemistry, St. Lawrence University (August 2013 – present)
Lab Affiliate, Lawrence Berkeley National Laboratory (December 2016 – present)
Lecturer, University of California, Berkeley (October 2012 – December 2012)
Graduate Student Researcher, University of California, Berkeley (October 2008 – May 2013)
Graduate Student Instructor, University of California, Berkeley (August 2008 – May 2011)

Most Closely Related Products

- 1. **Hill, A. D.**; Katsoukis, G.; Frei, H. "Photoinduced Electron Transfer from ZrOCo Binuclear Light Absorber to Pyridine Elucidated by Transient Optical and Infrared Spectroscopy." *The Journal of Physical Chemistry C* **2018**, *122*, 20176. http://dx.doi.org/10.1021/acs.jpcc.8b06435
- Zoerb, M. C.; Henderson, J. S.; Glover, S. D.; Lomont, J. P.; Nguyen, S. C.; Hill, A. D.; Kubiak, C. P.; Harris, C. B. "Electron Dynamics and IR Peak Coalescence in Bridged Mixed Valence Dimers Studied by Ultrafast 2D-IR Spectroscopy." *The Journal of Physical Chemistry B* 2015, 119, 10738. http://dx.doi.org/10.1021/acs.jpcb.5b06734
- 3. **Hill, A. D.**; Zoerb, M. C.; Nguyen, S. C.; Lomont, J. P.; Bowring, M. A.; Harris, C. B. "Determining equilibrium fluctuations using temperature-dependent 2D-IR." *Journal of Physical Chemistry B* **2013**, *117*, 15346. http://dx.doi.org/10.1021/jp403791k
- 4. Lomont, J. P.; Nguyen, S. C.; Schlegel, J. P.; Zoerb, M. C.; Hill, A. D.; Harris, C. B. "Ultrafast Observation of a Solvent Dependent Spin State Equilibrium in CpCo(CO)." *Journal of the American Chemical Society* **2012**, *134*, 3120. http://dx.doi.org/10.1021/ja2098468
- 5. Nguyen, S. C.; Lomont, J. P.; Zoerb, M. C.; **Hill, A. D.**; Schlegel, J. P.; Harris, C. B. "Chemistry of the Triplet 14-Electron Complex Fe(CO)3 in Solution Studied by Ultrafast Time-Resolved IR Spectroscopy." *Organometallics* **2012**, *31*, 3980. http://dx.doi.org/10.1021/om3002075

Other Related Products

- Lomont, J. P.; Nguyen, S. C.; Zoerb, M. C.; Hill, A. D.; Schlegel, J. P.; Harris, C. B. "Observation of a Short-Lived Triplet Precursor in CpCo(CO)-Catalyzed Alkyne Cyclotrimerization." *Organometallics* 2012, *31*, 3582. http://dx.doi.org/10.1021/om300058y
- 2. **Hill, A.D.;** Lehman, A.H.; Parr, M.L. "Using Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy To Analyze Archaeological Materials." *Journal of Chemical Education* **2007**, *84*, 810. http://dx.doi.org/10.1021/ed084p810

Synergistic Activities

- 1. Mentor to student research projects, including SYE (senior year experiences) in which students design and pursue independent research projects (10 students), and summer research students, including McNair scholars (3), St. Lawrence University fellows (5), and Clark L. Gage fellows (3)
- 2. Academic mentor to chemistry majors (30 students, 70% female) and first-year students (16 students, 10% URM).
- 3. Development of interdisciplinary course (CHEM-347 "Independent Study: Python for Chemists") integrating computer science into the chemistry curriculum.
- 4. Laboratory Affiliate at Lawrence Berkeley National Laboratory, working with Heinz Frei Group in Molecular Biosciences on the development of new artificial photosynthesis devices (December 2016 present).

Michael Schuckers

Department of Mathematics, Computer Science, and Statistics 23 Romoda Drive St. Lawrence University Canton, NY 13617 (315) 229-5028 schuckers@stlawu.edu

Professional Preparation

The Pennsylvania State University, State College, PA, Mathematics B.A., 1992 The University of Michigan, Ann Arbor, MI, Statistics A.M., 1994 Iowa State University, Ames, IA, Statistics Ph.D., 1999

Appointments

2015-present	Professor of Mathematics, St. Lawrence University, Canton, NY
2007-present	Director, Martha E. '62 and Gregg E. Peterson Quantitative Resource Center,
	Canton, NY
2007-2015	Associate Professor of Mathematics, St. Lawrence University, Canton, NY
2002-2007	Assistant Professor of Mathematics, St. Lawrence University, Canton, NY
1999-2002	Assistant Professor of Statistics, West Virginia University, Morgantown, WV
1999	Visiting Assistant Professor of Statistics, West Virginia University, Morgantown,
	WV

Products

Related Products

- 1. Coulombe, GC, O'Neill, MB, Schuckers, ME,(eds), *A Handbook for Directors of Quantitative and Mathematical Support Centers*, University of South Florida Scholar Commons (2016).
- 2. Schuckers, ME, Curro, JM "Total Hockey Rating (THoR): A comprehensive statistical rating of National Hockey League forwards and defensemen based upon all on-ice events", in Proceedings of the 2013 MIT Sloan Sports Analytics Conference, March 2013 (2nd Place in Research Paper Competition).
- 3. Schuckers, ME, Computational Methods in Biometrics: Statistics for Performance Evaluation Springer (2010).
- 4. Schuckers, ME, "Test Sample and Size" in Encyclopedia of Biometrics, Li, SZ and Elliot SJ (eds), (2009).
- 5. Schuckers, ME "DIGR: A Defense Independent Rating of NHL Goaltenders using Spatially Smoothed Save Percentage Maps" Proceedings of the MIT Sloan Sports Analytics Conference, March 2011.

Other Significant Products

- 1. Humphrey-Dixon, EL, Sharp, R, Schuckers, M, Lock R "Comparative genome analysis suggests characteristics of yeast inverted repeats that are important for transcriptional activity," Genome (2011).
- 2. Schuckers, ME "An Alternative to the NFL Draft Pick Value Chart Based upon Player Performance," Journal of Quantitative Analysis in Sports (2011).
- 3. Lewicke, A, Corwin, W, Schuckers, M., Xueyan, X, Neuman, M, Schuckers, S "Analysis of Heart Rate Variability for Predicting Cardiorespiratory Events in Infants," Biomedical Signal Processing and Control (2011).

4. Schuckers, ME "A parametric correlation framework for the statistical evaluation and estimation of biometric-based classification performance in a single environment," IEEE Transactions on Information Forensics and Security 4 (2009), 231-241.

Synergistic Activities

- Overseen 30 + undergraduate senior theses at St. Lawrence University since 2002.
- Established Quantitative Resource Center for St. Lawrence University.
- Host Math Support Center listsery (mathcenters-1@listsery.stlawu.edu)
- Host Quantitative Literacy listsery (qr-list@listserv.trinity.edu)
- J. Calvin Keene award from St. Lawrence University in 2018in recognition of high standards of personal scholarship, effective teaching and moral concerns

SUMMARY YEAR 1
PROPOSAL BUDGET FOR NSF USE ONLY

ORGANIZATION	DPOSAL	NO. DURATIO		ON (months)		
Saint Lawrence University					Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		A۱	WARD N	O.		
Edwin Harcourt						
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates		NSF Fund Person-mo	led nths		unds	Funds
(List each separately with title, A.7. show number in brackets)	CAL	ACAD	SUMR	Requ pr	lested By oposer	granted by NSF (if different)
1.	0.00		0.00			
2.	0.00	0.00	0.00			
3.						
4.						
5.						
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00		0	
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)	0.00		0.00		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)	0.00	0.00	0.00		U	
,	0.00	0.00	0.00			
1. () POST DOCTORAL SCHOLARS	0.00				0	
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0	
3. (0) GRADUATE STUDENTS					0	
4. (0) UNDERGRADUATE STUDENTS					0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. (0) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEED	NG \$5,0	000.)				
High Performance Computer		\$ 2	200,078			
TOTAL EQUIPMENT					200,078	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
2. INTERNATIONAL					0	
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS \$						
2. TRAVEL						
3. SUBSISTENCE						
4. OTHER						
TOTAL NUMBER OF PARTICIPANTS (()) TOTAL PAR	TICIPAN	IT COST	<u> </u>		0	
G. OTHER DIRECT COSTS	I ICIF AIN	11 0001	<u> </u>		U	
1. MATERIALS AND SUPPLIES					0	
NATERIALS AND SUPPLIES PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					0	
3. CONSULTANT SERVICES						
4. COMPUTER SERVICES					12,928	
					0	
5. SUBAWARDS					<u>0</u>	
6. OTHER					5,615	
TOTAL OTHER DIRECT COSTS					18,543	
H. TOTAL DIRECT COSTS (A THROUGH G)					218,621	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)						
(Rate: , Base:)						
(Rate: , Base:) TOTAL INDIRECT COSTS (F&A)					0	
					0 218,621	
TOTAL INDIRECT COSTS (F&A)					218,621 0	
TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					218,621	
TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE	VEL I <u>F</u> [DIFFERE	NT\$		218,621 0	
TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)	VEL IF [DIFFERE			218,621 0	
TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LE	VEL IF [FOR N	ISF US	218,621 0 218,621	CATION
TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 0 0 0 0 0 0 0 0 0 0 0 0			FOR N	ISF US	218,621 0 218,621 SE ONLY	CATION Initials - ORG

SUMMARY YEAR 2
PROPOSAL BUDGET FOR NSF USE ONLY

PROPOSAL BUDGET			FOR		R NSF USE ONLY	
ORGANIZATION		PRO	POSAL	NO.	DURATIO	ON (months
Saint Lawrence University					Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		ΑV	WARD N	<u> </u>		
		'`'	, , , , , , , , , , , , , , , , , , ,	O .		
Edwin Harcourt		NSE Fund	ed			Funda
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates		NSF Fund Person-mo		Regu	Funds Jested By	Funds granted by N
(List each separately with title, A.7. show number in brackets)	CAL	ACAD	SUMR	pr	oposer	(if different
1.	0.00	0.00	0.00			
2.						
3.						
4.						
5.						
	0.00	0.00	0.00			
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00		0.00		0	
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	0.00		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (0) POST DOCTORAL SCHOLARS	0.00	0.00	0.00		0	
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0	
3. (0) GRADUATE STUDENTS					0	
4. (0) UNDERGRADUATE STUDENTS					0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. (0) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEED	ING \$5.0	000.)				
TOTAL EQUIPMENT E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL					0 0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 0 0					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL 0 0 0					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 1. DOMESTIC (INCL. U.S. POSSESSIONS) 0 0 0 0 0 0 0 0 0 0 0 0 0					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANTS	TICIPAN	IT COSTS	6		0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 1. DOMESTIC (INCL. U.S. POSSESSIONS) 0 0 0 0 0 0 0 0 0 0 0 0 0	TICIPAN	IT COSTS	6		0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 0 2. TRAVEL 0 3. SUBSISTENCE 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR	TICIPAN	IT COSTS	6		0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS	TICIPAN	IT COSTS	6		0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES	TICIPAN	IT COSTS	6		0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION	TICIPAN	IT COSTS	6		0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES	TICIPAN	IT COSTS	S		0 0 0 0 0 8,928 0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS	TICIPAN	IT COSTS	S		0 0 0 0 0 8,928 0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER	TICIPAN	IT COSTS	S		0 0 0 0 0 8,928 0 0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS	TICIPAN	IT COSTS	5		0 0 0 0 8,928 0 0 0 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G)	TICIPAN	T COSTS	5		0 0 0 0 0 8,928 0 0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPA	TICIPAN	T COSTS	5		0 0 0 0 8,928 0 0 0 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPA	TICIPAN	IT COSTS	5		0 0 0 0 8,928 0 0 0 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPA	TICIPAN	IT COSTS	5		0 0 0 0 8,928 0 0 0 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPA	TICIPAN	T COSTS	5		0 0 0 0 8,928 0 0 0 8,928 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I)	TICIPAN	T COSTS	5		0 0 0 0 8,928 0 0 8,928 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE	TICIPAN	T COSTS	5		0 0 0 0 8,928 0 0 8,928 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:) TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					0 0 0 0 8,928 0 0 8,928 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$			NT \$		0 0 0 0 8,928 0 0 8,928 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LE		DIFFERE	NT \$ FOR N		0 0 0 8,928 0 0 8,928 8,928 0 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LE PI/PD NAME Edwin Harcourt	VEL IF [DIFFERE	NT \$ FOR N	T RAT	0 0 0 8,928 0 0 8,928 8,928 0 8,928	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) II. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LE	VEL IF [DIFFERE	NT \$ FOR N		0 0 0 8,928 0 0 8,928 8,928 0 8,928	CATION Initials - OF

SUMMARY YEAR 3
PROPOSAL BUDGET FOR NSF USE ONLY

ORGANIZATION	OPOSAL	SAL NO. DURATIO		ON (months)		
Saint Lawrence University					Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		Α	WARD N	Ο.		
Edwin Harcourt						
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associate	es	NSF Fund Person-mo	ded onths		unds ested By	Funds granted by NSF
(List each separately with title, A.7. show number in brackets)	CA		SUMR	pro	poser	(if different)
1.	0.0	0.00	0.00			
2.						
3.						
4.						
5.						
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PA	GE) 0.0	_			0	
7. (1) TOTAL SENIOR PERSONNEL (1 - 6)	0.0	0.00	0.00		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (0) POST DOCTORAL SCHOLARS	0.0				0	
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.) 0.0	0.00	0.00		0	
3. (0) GRADUATE STUDENTS					0	
4. (0) UNDERGRADUATE STUDENTS					0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. (0) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXC	EEDING \$	5,000.)				
TOTAL EQUIPMENT					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
2. INTERNATIONAL					0	
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS \$						
2. TRAVEL 0						
3. SUBSISTENCE 0						
4. OTHER						
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL I	PARTICIPA	ANT COST	S		0	
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES					0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					0	
3. CONSULTANT SERVICES					8,928	
4. COMPUTER SERVICES					0	
5. SUBAWARDS					0	
6. OTHER					0	
TOTAL OTHER DIRECT COSTS					8,928	
H. TOTAL DIRECT COSTS (A THROUGH G)					8,928	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)						
(Rate: , Base:)						
TOTAL INDIRECT COSTS (F&A)					0	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					8,928	
K. SMALL BUSINESS FEE					0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					8,928	
	D LEVEL II	DIFFERE	NT \$			
PI/PD NAME				NSF US	E ONLY	
Edwin Harcourt		INDIR			E VERIFIC	CATION
ORG. REP. NAME*		Date Checke		e Of Rate		Initials - ORG
Elizabeth Haney						

SUMMARY Cumulative
PROPOSAL BUDGET FOR NSF USE ONLY

PROPOSAL BUDGET			FOR	R NSF USE ONLY		
ORGANIZATION		PRO	POSAL	NO.	DURATIO	ON (months
Saint Lawrence University					Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		Δ١	WARD N	<u></u>	1, 1130	
Edwin Harcourt		'''	, , , , , , , , , , , , , , , , , , ,	O .		
		NSE Fund	ed		- unds	Funda
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates		NSF Fund Person-mor		Regi	uested By	Funds granted by NS
(List each separately with title, A.7. show number in brackets)	CAL	ACAD	SUMR	pr	oposer	(if different)
1.	0.00	0.00	0.00			
2.						
3.						
4.						
5.	0.00	0.00	0.00			
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00		0	
7. (0) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	0.00		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (0) POST DOCTORAL SCHOLARS	0.00	0.00	0.00		0	
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00		0.00		0	
3. (0) GRADUATE STUDENTS	0.00	0.00	0.00		0	
/						
4. (0) UNDERGRADUATE STUDENTS					0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. (0) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEED	ING \$5 C	100.)				
		\$2	00,078			
TOTAL FOURNIENT					000 070	
TOTAL EQUIPMENT					200,078	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS					0	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 0 0					0	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION	TICIPAN	T COSTS	5		0 0 0 0 0 30,784	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER	TICIPAN	T COSTS	5		0 0 0 0 0 30,784 0 0 5,615	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G)	TICIPAN	T COSTS	6		0 0 0 0 0 30,784 0 0 5,615	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)	TICIPAN	T COSTS	5		0 0 0 0 30,784 0 0 5,615 36,399 236,477	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A) (SPECIFY RATE AND BASE) TOTAL INDIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE	TICIPAN	T COSTS	5		0 0 0 0 30,784 0 0 5,615 36,399 236,477	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					0 0 0 0 30,784 0 0 5,615 36,399 236,477	
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPA		DIFFERE	NT \$ FOR N		0 0 0 30,784 0 0 5,615 36,399 236,477 0 236,477	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LE PI/PD NAME Edwin Harcourt	EVEL IF [DIFFERE	NT \$ FOR N	ST RAT	0 0 0 30,784 0 0 5,615 36,399 236,477 0 236,477	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS) 2. INTERNATIONAL F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (0) TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PAR G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. SMALL BUSINESS FEE L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K) M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LE	EVEL IF [DIFFERE	NT \$ FOR N		0 0 0 30,784 0 0 5,615 36,399 236,477 0 236,477	CATION Initials - OR

Budget Justification

Equipment (\$200,078)

The PIs worked with St. Lawrence University's IT department to design the requested high-performance computing (HPC) equipment. In pricing high performance computing equipment, we compared quotes from Red Barn and Dell. Both the Red Barn and the Dell contain a number of compute nodes, a head node, and a GP node. Both use the latest version of Red Hat Enterprise Linux (RHEL), and both provide 24/7 support. The table below shows a high-level summary of the two machine quotes.

Vendor	Nodes	Total CPUs	Total Mem	GPUs	Hardware Cost
Red Barn	18	432	2.6TB	2	\$200,078
Dell	19	708	4.1TB	1	\$432,878

The total number of CPUs and the total memory reflect the total in the compute nodes, plus the head node, and the GPU node. In both quotes the processors are Intel Xeon Gold processors with the GPU node containing NVidia Tesla v100 GPU card(s). As outlined in the project description, the Red Barn configuration is adequate for our compute needs and is less than half the price of the Dell quote. As such we are proposing that we purchase the Red Barn configuration.

This quoted price (\$200,078) includes 432 Intel Xeon Gold 5118 processors (12 core) running at 2.3-3.2 GHz (each core is hyperthreaded allowing for 768 concurrent processes); 2.6 TB of main memory (RAM); and the CentOS operating system across eighteen (18) compute nodes. In addition, there is a GPU compute node with (2) Nvidia V100 32Gb Graphics processors, 2 - Intel Xeon Gold 5118 (12 core) CPU, 128Gb Memory, 480 Gb Disk and a head node (server) with (2) Intel Xeon Gold 5118 (12 core), 128 Gb Memory, (2) 480 Gb Mirrored operating system disks, 4TB scratch/temporary disk space, and 32TB for data storage. This equipment represents sufficient computing capability to meet our needs and final computing specifications listed above. The quoted price also includes a 3-year hardware warranty.

Service of the instrument during the 3-year project period will be covered by the warranty and the consultant, Sly Media Networks, as described in the management plan. After that time, ongoing costs of service will be included in the University's budget.

Software (\$5,615)

The Q-Chem quantum chemistry program is requested to support research projects in chemistry using the proposed HPC. This software includes the ability to perform density functional theory methods and algorithms, nuclear magnetic resonance (NMR) property evaluation, coupled cluster and perturbation theories, methods for electronically excited and open-shell species, tools for treating extended environments, algorithms for walking on potential surfaces, analysis tools, energy and electron transfer modelling, parallel computing capabilities, and graphical user interfaces.

Consulting Services (\$30,784)

One of the challenges for a small liberal arts college like St. Lawrence, when acquiring this type of equipment, is the lack of professional expertise within the organization to be able to administer the technically specific needs that a HPC compute cluster requires. To address this, we are including a support contract with Sly Media Networks, LLC to manage the cluster and allow the PIs to concentrate on research instead of system administration. The quoted price of \$30,784 for HPC installation and support will provide HPC System Administrator services for the equipment by Sly Media Networks, LLC as follows

Installation (\$4,000)

Although the Red Barn quote includes the Warewulf Community Support Cluster Suite Full Installation, this one-size-fits-all approach is not sufficient. Sly Media Networks has developed an HPC cluster Infrastructure that will integrate into our enterprise academic infrastructures and our institution's IT department. This additional installation cost includes:

- CentOS 7.x (Community ENTerprise Operating System) Free version of Red Hat Enterprise Linux (RHEL)
- FreeIPA (Identity Policy and Audit) authentication system with the ability to set security policies, integrate with Active Directory, provide local DNS, Automount service for NFS mounts, LDAP (users/groups/hosts), Kerberos, Certificate Authority (SSL certs).
- SLURM Queue/Scheduling software scheduling and running of jobs on the compute node resources.
- Ganglia Performance Monitoring software web based tool for visualizing resource utilization
- Nagios Alert Monitoring software Alert administrators of problems with the resources.
- Git based documentation website (using MkDoc) with basic user guides for using the HPC customized for the institution's policies.
- Network File System (NFS) used to store all the data on the large raid disk (32 TB), to house all the software and data and mounted across all the compute resources.

Sly Media Networks will work with St. Lawrence IT to determine the best possible configuration for the equipment in order to integrate it into the institution's infrastructure. Once all the configuration details are discovered, Sly Media Networks will setup these details on St. Lawrence's cloud servers in a private git repository. Installation is done on the head server by running a script that will pull the installation instructions from the internet and consistently install the operating system and all the needed software to build the rest of the cluster. The technology used to install the cluster nodes is called kickstart. This system, initially configured on and served by the head node, will allow for all the compute nodes to be booted over the network (netboot) and automatically installed. No user data is ever stored on a compute node which eliminates the need for a data backup system for any of the nodes (excluding the head node where all the data resides). Storing the initial server installation in the cloud also serves as a disaster recovery solution in the event of a failure. All data from accounts, software and compute node operating system installation instructions are stored in the large raid array (32TB) connected to the head node. As long as this raid disk is available from the head node, any other equipment can be rebuilt as needed in the event of a hardware failure. No data is stored on the compute nodes and it is all mounted (via automount) over the network file system (NFS) from the head node server.

Monthly Support (\$8,928 per year - \$26,784 over 3 years)

Monthly support cost includes:

- Maintain cluster uptime and respond to outages.
- Software installation, support and updates for the operating systems and research applications.
- Queue maintenance and customization (adjust queue scheduling rules as needed).
- Work with HPC users to execute jobs on the cluster to perform their research.
- Work with St. Lawrence IT on issues that arise with the equipment

Facilities and Administrative Costs (\$0)

N/A. Facilities and Administrative costs are calculated at St. Lawrence University's negotiated rate of 49.9% of salaries and benefits, and none are included in this proposal.

Summary

The total amount requested in this proposal is \$236,477. Of the total budget request, 85% reflects the cost of the instrumentation purchase, including hardware, software, and shipping. The remainder of the costs are for the QChem software and for the consultant, Sly Media Networks, who will install all hardware and software needed for St. Lawrence to utilize the cluster for faculty research, as well as assist in software installation requests, cluster maintenance, and working with users to utilize the cluster for their research throughout the term of the award.

ITEM	YEAR 1		YEAR 2		YEAR 3		TOTA	AL
	NSF Request	Cost Share	NSF Request	Cost Share	NSF Request	Cost Share	NSF Request	Cost Share
High performance computing equipment	\$200,078	\$0	\$0	\$0	\$0	\$0	\$200,078	\$0
QChem software	\$5,615	\$0	\$0	\$0	\$0	\$0	\$5,615	\$0
Consulting services	\$12,928	\$0	\$8,928	\$0	\$8,928	\$0	\$30,784	\$0
TOTAL Direct Costs	\$218,621	\$0	\$8,928	\$0	\$8,928	\$0	\$236,477	\$0
TOTAL F&A (49.9% rate, salaries and benefits base)	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
GRAND TOTAL	\$218,621	\$0	\$8,928	\$0	\$8,928	\$0	\$236,477	\$0

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal
Other agencies (including NSF) to which this proposal has been/will be submitted. Investigator: Edwin Harcourt
Support: □ Current ☑ Pending □ Submission Planned in Near Future □ *Transfer of Support Project/Proposal Title: MRI: Acquisition of a high-performance computer (HPC)
Source of Support: NSF Total Award Amount: \$ 236,477 Total Award Period Covered: 09/01/19 - 08/31/22 Location of Project: St. Lawrence University Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.00
Support: □ Current □ Pending □ Submission Planned in Near Future □ *Transfer of Support Project/Proposal Title:
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:
Support: Current Pending Submission Planned in Near Future *Transfer of Support Project/Proposal Title:
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:
Support: Current Pending Submission Planned in Near Future *Transfer of Support
Project/Proposal Title:
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:
Support: □ Current □ Pending □ Submission Planned in Near Future □ *Transfer of Support Project/Proposal Title:
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.
Other agencies (including NSF) to which this proposal has been/will be submitted. Investigator: Jessica Chapman
Support: ☑ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support Project/Proposal Title: Liberal Arts Science Scholars Program
Source of Support: NSF Total Award Amount: \$ 618,524 Total Award Period Covered: 04/01/15 - 03/31/20 Location of Project: St. Lawrence University Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.30
Support: ☑ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support Project/Proposal Title: EAGER: Reducing Scientific Uncertainty of Storm Trends in Savoonga and Shaktoolik, Alaska with Traditional Knowledge
Source of Support: NSF Total Award Amount: \$ 90,366 Total Award Period Covered: 06/01/16 - 05/31/19 Location of Project: St. Lawrence University Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.10
Support: ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support Project/Proposal Title: MRI: Acquisition of a high-performance computer (HPC)
Source of Support: NSF Total Award Amount: \$ 236,477 Total Award Period Covered: 09/01/19 - 08/31/22 Location of Project: St. Lawrence University
Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.00
Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support Project/Proposal Title:
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:
Support: Current Pending Submission Planned in Near Future *Transfer of Support Project/Proposal Title:
Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project:
1 =====================================

The following information should be provided for each	investigator and other senior pers	onnel. Failure to provide this information	on may delay consideration of this proposal.
Investigator: Robert Haney	Other agencies (inc	cluding NSF) to which this proposa	I has been/will be submitted.
, structur	rative Research: C	Planned in Near Future Comparative analyses ing functional perform	of
	,168 Total Award Pe ity of Massachuse itted to the Project.		/17 - 08/31/21 00 Sumr: 0.00
Support: □ Current ☑ Pendi Project/Proposal Title: MRI: Ad	· ·	Planned in Near Future -performance compute	□*Transfer of Support er (HPC)
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Person-Months Per Year Comm	itted to the Project.	Cal: Acad:	Summ:

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposa								
Other agencies (including NSF) to which this proposal has been/will be submitted. Investigator: Adam Hill								
Support: ☑ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support Project/Proposal Title: Liberal Arts Science Scholars Program								
Source of Support: NSF Total Award Amount: \$ 618,524 Total Award Period Covered: 04/01/15 - 03/31/20 Location of Project: St. Lawrence University Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.15								
Support: □ Current ☑ Pending □ Submission Planned in Near Future □ *Transfer of Support Project/Proposal Title: MRI: Acquisition of a high-performance computer (HPC)								
Source of Support: NSF Total Award Amount: \$ 236,477 Total Award Period Covered: 09/01/19 - 08/31/22 Location of Project: St. Lawrence University Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.00								
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Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project: Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:								
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Source of Support: Total Award Amount: \$ Total Award Period Covered: Location of Project:								
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:								

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this propose							
Other agencies (including NSF) to which this proposal has been/will be submitted. Investigator: Michael Schuckers							
Support: □ Current ☑ Pending □ Submission Planned in Near Future □ *Transfer of Support Project/Proposal Title: MRI: Acquisition of a high-performance computer (HPC)							
Source of Support: NSF Total Award Amount: \$ 236,477 Total Award Period Covered: 09/01/19 - 08/31/22 Location of Project: St. Lawrence University Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 0.00							
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Person-Months Per Year Committed to the Project. Cal: Acad: Summ:							

Facilities, Equipment, and Other Resources

St. Lawrence University Facilities and Equipment

Johnson Hall of Science

Constructed in 2007, the Johnson Hall of Science is designed to lead the way in science education for the 21st century. Johnson Hall features two interconnected buildings for biology, chemistry, neuroscience, biochemistry, and psychology, with the most innovative sustainable design features possible. The 115,000-square-foot Gold-LEED certified building includes teaching labs, research labs, conference rooms, departmental and individual faculty offices, and informal student spaces.

Mathematics, Computer Science, and Statistics

Valentine Hall and Bewkes Hall are adjoining office and classroom buildings connected by an indoor walkway. These two buildings house the Mathematics, Computer Science and Statistics Department and its three computer science labs and two statistics computer labs. In these spaces, each student station has a 24-inch monitor, eight square feet of work space, and access to high performance computing and public printing. A 400 square foot room contains file servers and networking equipment to support the labs.

Drs. Ed Harcourt and Michael Schuckers each have a roughly 160 square foot office, with ample space for meeting with students, and an additional 500 square foot meeting space available nearby.

Chemistry

Faculty and student research is conducted primarily in two, large, dedicated shared spaces, a 2250 square foot synthesis lab, and a 1250 square foot analytical and environmental lab. These lab spaces are located in the 130,000 square foot, Gold-LEED certified Johnson Hall of Science and are utilized cooperatively departmental faculty. A smaller spectroscopy lab houses Raman and fluorescence instrumentation, and a smaller laser lab is also under the supervision of Glazier. The synthesis lab is equipped with a Biotage Horizon Flash Chromatograph (2003), Innovative Technology drybox (2007) and PureSolve solvent purification unit (2007) along with everything required to support synthetic projects. The two large research labs can accommodate 18-20 simultaneous users. Student researchers each have desks with PCs within these large community-style, open floor-plan laboratories.

The majority of shared instrumentation used in teaching and research is housed in the Stradling Instrument Facility in Johnson Hall. This instrumentation includes:

- JEOL Eclipse+ 300 MHz Full Broadband Probe NMR Spectrometer (2000) with additional upgrades (subsequent).
- Jobin Yvon Fluoromax 3 Fluorescence Spectrometer (2005) with Hi-Tech Scientific SFA-20
- Rapid Kinetics Stopped-Flow Accessory (2007) and DeltaTime nanosecond pulsed light source (2014)
- Centaurus FT-IR Microscope with MCT-A detector, Transmission / Reflection modes, Si ATR slide (August 2007)
- Nicolet 4700 FT-Infrared Spectrometer (2005)
- Jasco V-570 UV/VIS/NIR Spectrophotometer (2004)
- Agilent 6890/5973 Capillary Gas Chromatograph-Mass Spectrometer (2002)
- ThermoSep HPLC with dual channel UV/VIS absorption detectors (2001)
- Rigaku Supermini200 benchtop wavelength-dispersive (WD) x-ray fluorescence spectrometer (2014)

Dr. Adam Hill has a roughly 160 square foot office, with ample space for meeting with students, and an additional 500 square foot meeting space available nearby.

Biology

The Department of Biology is housed on the first two floors of the Johnson Hall of Science and contains ample working room and lab space for students. Research and teaching labs typically run from 900 to 1,200 square feet. Other major instrumentation and research spaces include:

- Leica laser scanning confocal microscope TCS SP2 acquired in 2001 via an NSF MRI grant (#0116408) awarded to Dr. T. Budd, Professor of Biology
- Scanning electron microscope FEI Quanta 450 Scanning Electron Microscope with Oxford EDS and Gatan cathodoluminescence acquired in 2009 via the NSF-MRI grant (#0923398) to Dr. Jeff Chiarenzelli, Professor of Geology
- Olympus B-MAX 50 fluorescence microscope
- Four Sorvall ultra-microtomes (2 motorized, 2 manual drive)
- EMS Sputter Coater
- Cell culture lab (1,200 sq. ft.) containing laminar flow hoods, incubators, inverted scope for viewing cultures, work benches and two PC work stations
- Animal colony room, a 2,300 sq. ft., environmentally controlled (temperature, humidity and light) facility used to maintain our own colonies of rats and mice. The facility has separate rooms for surgery, recovery, cage cleaning, bedding/food storage, and animal euthanasia.
- Lab for molecular studies of developmental biology which include: PCR clean room of 100 square feet, a teaching laboratory of 1,200 square feet, and an equipment room of 200 square feet. This facility is equipped with two chemical hoods, one tissue culture hood, three 30 cu ft 5-600C temperature incubators, two Bio-Rad thermocyclers, a Tissue Tek Embedding Center, paraffin microtome, two hybridization ovens, agarose gel units, acrylamide gel units, semidry blotters, a refrigerated centrifuge, microcentrifuges, a BTX electroporator, Olympus photomicroscope for phase and DIC, compound and dissecting student microscopes, waterbaths, a pH meter, a two door chromatography refrigerator, refrigerator/freezers, and -800C and -200C freezers.
- Research laboratory is 600 square feet and is equipped with: inverted epifluorescence microscope outfitted with cooled charge-coupled device (CCD) camera, imaging software and electrophysiology set-up; three dissection microscopes one of which has fluorescence capabilities; pipette puller; air table; analytical balance; pH meter; laminar flow hood; three low temperature incubators for worm culture; high temperature incubator for bacterial culture; clinical centrifuge; water bath; hot plate; microcentrifuge; -20 °C freezer, vapor pressure osmometer; chemical store; student work areas.

Dr. Erika Barthelmess' main laboratory is 900 sq. ft. with an additional 100 sq. ft. prep lab space. The main laboratory includes: a PCR machine, hybridization oven, bench top centrifuge, water bath, spectrophotometer, dissecting microscope with CCD (charge-coupled device) camera, analytical balance, pH meter, sample freezer, refrigerator, and electrophoresis set-ups. There is also chemical storage, a chemical/fume hood, and student work areas including one GIS workstation, a video-editing workstation, and two Macintosh Pro workstations. The prep lab space houses optics for wildlife viewing (binoculars, spotting scopes) and miscellaneous field equipment (game cameras, boots, bait supplies, animal handling supplies etc.). Dr. Barthelmess also has a second shared lab for teaching/research purposes (1,200 square feet) that adjoins the prep lab and includes three student PC workstations; she has access to these labs except when one or two other classes are in session there. Dr. Barthelmess has access to a field equipment storage room (900 sq. ft.) that stores a wide variety of ecological research equipment, including nets, waders, traps, buckets, etc. Dr. Barthelmess has an office (300 sq. ft.) with a GIS workstation and desktop computer. Both labs and office are equipped with phone and wireless and wired high speed internet.

Dr. Robert Haney has a roughly 160 square foot office, with ample space for meeting with students, and an additional 500 square foot meeting space available nearby. He has shared access to all major instrumentation and research spaces in the Biology Department.

Physics

The Physics Department, located in Bewkes Hall on the St. Lawrence campus, consists of 5 full-time faculty members, an Astronomer/Lab Coordinator, and a science shop technician. Equipment includes

- Single photon detectors and various optics for Quantum Optics experiments
- Raman Spectroscopy System with 532 nm and 405 nm lasers
- Ellipsometer
- Near-field scanning optical microscope
- Thermal evaporator
- 17 kG electromagnet
- Liquid Nitrogen cooled cryostat
- Automated Hall and resistivity measurement system
- Portable telescopes: Celestron Nexstar GPS (11"); Celestron C-8 (8"); Meade LX6 (8")

Economics

The Laboratory for Experimental Economics in the Economics Department provides St. Lawrence University faculty and students with a facility for studying how people make choices. The laboratory supports classroom experiments, as well as faculty and student research on principles of economics, making key concepts like competitive markets and public goods clear and meaningful.

St. Lawrence University Other Resources

SLU Student Research Funds – Student Research Funds support various scholarly activities of full-time St. Lawrence University students including materials, laboratory supplies, and travel related to research. These funds, administered by the Academic Dean's office, are awarded on a case-by-case basis with awards as high as \$600 per student per academic year.

SLU Student Travel Funds – Full-time St. Lawrence University students may access funds up to \$600 per academic year to present at a conference. These funds are awarded on a case-by-case basis and are administered by the Academic Dean's office.

Peterson Quantitative Resource Center (PQRC) – The PQRC is a focal point for quantitative resources for students and faculty in the St. Lawrence University community. It facilitates research that involves quantitative reasoning. Students use it to analyze data, and use quantitative software to calculate and interpret statistics.

SLU Libraries and Information Technology Division – Guided by the university mission and strategic map, the Libraries (main and science) and Information Technology division provides scholarly and technology services, resources, and infrastructure which are critical for student learning at a residential liberal arts University.

Personnel to Support Broader Impacts – The project will receive support for recruiting students researchers from underrepresented groups from Marsha Sawyer, Director, CSTEP & McNair Scholars Programs, who brings over 20 years of experience serving student populations who are underrepresented in the professions and in graduate programs at the doctoral level; from Associate Dean for Academic Advising Programs Elun Gabriel and his staff; from Director of Admissions Jeremy Freeman; and from Director of Financial Aid Patricia Farmer.

Other Resources in the Region

Clarkson University, which is 12 miles from St. Lawrence University, was awarded an NSF MRI for a high-performance Heterogeneous Computing Platform for Biometrics Research in 2016, CNS-1626360. Clarkson's machine is designed to handle large scale parallelization of processes to improve computation time. The research projects that are part of this current St. Lawrence University proposal are difficult to parallelize and instead require large amounts of RAM, compute nodes, and GPU nodes. Consequently, the

instrument that we are requesting in this grant is chosen to address our specific computational needs, which are different from those addressed by Clarkson's nearby instrument. Indeed, the capabilities of our requested instrument are so different from the existing instrument at Clarkson that one of the major users is a Clarkson researcher who requires the unique capabilities of our proposed system for his NSF-funded research on methods to fabricate silicon wafers for solar cells.

We have an understanding in place with Clarkson to share our computing resources such that St. Lawrence researchers can use the Clarkson instrument for projects that require large scale parallelization of processes and Clarkson researchers can use St. Lawrence's proposed instrument for projects that require large amounts of RAM, compute nodes, and GPU nodes. This agreement allows faculty researchers and students at each institution to take advantage of the diversity of computing in our region as projects warrant, as well as expose students to a diversity of high-performance computing platforms.

Additionally, we will make the HPC available to collaborators and other local researchers in northern New York, an economically disadvantaged, rural area that is also home to two public colleges within the State University of New York (SUNY) system with limited resources and significant populations of students from underrepresented backgrounds.

Data Management Plan

1. The types of data, samples, physical collections, software, curriculum materials, and other materials to be produced in the course of the project

The PIs and the St. Lawrence University (SLU) will have overall responsibility for data management over the course of the project and will monitor compliance with the plan. The types of data to be produced from the project include research data from projects in in computer science (testing hardware configurations for machine learning algorithms), statistics (methods for longitudinal clustering of multivariate data), chemistry (understanding bimetallic catalysts for artificial photosynthesis and DNA binding pathways for acridines), and biology (evolutionary genomics, gene regulation, microbial community ecology, and forest ecology). Custom software to meet research needs may also be produced.

2. The standards to be used for data and metadata format and content

Scientific data generated through the project will be stored both as raw data (RAW, DXF, KML and ASCII files) and in standard formats such as HTML, DOCX, XLSX, TIFF, fasta, fastq, .sf3, and PDF formats.

3. Policies for access and sharing including provisions for appropriate protection of privacy, confidentiality, security, intellectual property, or other rights or requirements

Data sharing from this project will be consistent with NSF's policy for accessing and sharing research data. Research data and custom software will be made available for sharing upon request to the PIs by qualified parties, given that the request does not occur prior to data curation in accepted databases, in any way interfere with the process of publication, or compromise intellectual property interests.

4. Policies and provisions for re-use, re-distribution, and the production of derivatives

Scientific data and custom software will be made available for use in research and education, either by visiting SLU or on loan (free of charge). Journal publications will be available according to the individual journal's copyright policies. Data available in online databases is subject to the terms and conditions of use as set forth in the database documentation.

5. Plans for archiving data, samples, and other research products, and for preservation of access to them

The raw research project data (for students and faculty) will be maintained in SAKAI, which is the online environment designed to facilitate teaching, learning, and assessment at SLU. The raw and analytical data will be stored in SAKAI and available upon publication. All data will be submitted to accepted online databases as required. All other materials related to the projects, such as laboratory notebooks and physical samples, will be stored in the laboratory of the PIs.

List of Supplementary Documents

Statement classifying the organization as non-Ph.D.-granting, p2

Letter documenting the performing institution's commitment to ensuring successful operations and maintenance over the expected lifetime of the instrument, p3-4

Vendor quotes, p5-27

Red Barn quote for requested instrument, p5-10

Sly Media Networks quote for installation and management of requested instrument, p11

Q Chem quote for software for use on requested instrument, p12

Dell quote (representative), p13-27

Statements from individuals confirming substantive collaboration efforts, p28-40

To: NSF MRI Coordinator

By signing below I certify that St. Lawrence is classified as *non-Ph.D.-granting* as defined in Section IV of the MRI solicitation.

Signed: Elizabeth B. Henry?

Print Name: Elizabeth B. Haney_

Title of Signatory: _Senior Officer for Strategic Initiatives, Corporate and Foundation Relations/Sponsored Research_

Date: _January 9, 2019_



January 15, 2019

Dr. Randy Phelps
Office of International and Integrative Activities
Major Research Instrumentation Program
National Science Foundation, Room 935
4201 Wilson Boulevard
Arlington, VA 22230

Dear Dr. Phelps:

On behalf of PI Ed Harcourt and co-PIs Jessica Chapman, Robert Haney, Adam Hill, and Michael Schuckers, please accept this letter as verification that St. Lawrence University is committed to providing the long-term operation and maintenance of the Warewulf Community Support Cluster requested through the proposed project *MRI: Acquisition of a high-performance computer (HPC)*. This will be true during the grant period and beyond the life of the NSF award.

As detailed in our proposal, the St. Lawrence project team (consisting of 14 SLU faculty participants (five PIs and nine major users) along with three external users) will use the requested instrument to conduct research in a wide array of STEM disciplines, including: computer science, statistics, chemistry, biology, physics, and economics. The proposed HPC has the specialized capabilities needed to pursue these lines of research, as well as the potential to expand research, training, and teaching activities for faculty and students. We anticipate that the proposed acquisition of the HPC will have an impact on almost 80 students via mentored research during the grant period and over 220 undergraduate students annually via courses during the grant period.

As a non-Ph.D. granting undergraduate institution, St. Lawrence University is not required to provide institutional cost-sharing for the NSF-MRI program. However, it is important to note that the University not only has an excellent track record in maintaining our scientific equipment, but also makes our instrumentation available for use by other scientists, faculty, and students from throughout our northern New York region at no cost.

MRI awards to St. Lawrence University with an end date in the last five years:

Joseph Erlichman, PI, NSF Award # 1626166; \$282,390 (9/01/16-8/31/19)

Project Title: MRI: Acquisition of Confocal Laser Scanning Microscope for Research and Training in the Biological Sciences

This most recent MRI award supported the purchase of a Nikon C2+ spectral imaging confocal microscope with wide field camera and environmental chamber systems during the fall semester of 2016. The new instrument augments the research, teaching, and training activities of eleven faculty and science professionals in cell and developmental biology and ecology and evolution.

Edwin Harcourt, PI, NSF Award #0959713; \$179,336 (5/1/2010-4/30/2013)

Project Title: MRI-R2: Acquisition of High Performance Computer (HPC) and Microarray Scanner for Interdisciplinary Research in Computer Science and Biology at St. Lawrence University.

Eight SLU faculty from six majors utilized the instrument for research, resulting in over 50 projects, including individual faculty research projects as well as mentored research projects with over 30 students, in fields such as advanced image synthesis, comparative genome analysis in yeast, phylogenetic analysis of microbial communities and comparative analysis of bacterial genomes, microarray analysis of gene expression, and bird foraging studies. One of the projects developed using this instrument, THOR (Total Hockey Ranking), spawned interest in a predictive data analytics center to be housed in Massena, NY. Collaborations were established with Clarkson University and Los Alamos National Labs. Fifteen publications in the fields of statistics, biology, computer science, and economics utilized this equipment. The equipment has been successfully operated and maintained with fewer than three days of downtime over its life.

All instruments are in excellent condition and are in continuous use for research and teaching purposes.

On behalf of St. Lawrence University, I confirm that our institution will provide all necessary resources for the ongoing care and maintenance of the requested equipment. The new HPC will be maintained by PI Harcourt, IT server manager R. Thacher, and consultant Steve Young. The HPC comes with a warranty for the life of the grant. We have also included costs for consultant Steve Young to provide monthly support for the life of the grant to assist in software installation requests, cluster maintenance, and working with users to utilize the cluster for their research. SLU maintains service contracts for all major science equipment (as available), and these costs are incorporated into the relevant departments' annual operating budgets. Costs for maintenance and support of the HPC will be handled in the same manner.

Thank you for the opportunity to submit this proposal.

Sincerely,

Karl K. Schonberg

Vice President and Dean for Academic Affairs



Red Barn Technology Group, Inc. 37 Pine St., Binghamton, NY 13901

phone: 607-772-1888 fax: 607-584-9217

Sales Quotation

SQ - 1078957

Dec-03-2018



Bill To Contact Ship To

St. Lawrence University 23 Romoda Dr BUCKS BRIDGE NY 13617 UNITED STATES Phone # (1315)229-5011 St. Lawrence University 23 Romoda Dr BUCKS BRIDGE NY 13617 UNITED STATES

Account	Terms	Due Date	Rep	Ship Date
127395	1% 10 Days-Net 30 Days	Jan-02-2019	Jonathan Layish	Dec-03-2018
SQ	PO	Reference	Ship Via	Page 1 of 6
1078957				Printed : Dec-03-2018 13:56:00

L	Item Code	Description	Ordered	Shipped	Price	UOM	Discount %	Amount
1	TURNKEY-CLSTR	Warewulf Community Support Cluster Suite Full Installation	1	0	\$131,575.00	EA	5.00	\$124,996.25
2		At no charge RBTG, Inc will install & configure open source Clustering OS, provisioning, monitoring, message passing, scheduling solution. All packages are supplied and supported free of charge by the open source community.						
3	2U-SC-TY-TN70E	Red Barn HPC 2U Rack Svr DP Intel Scalable w/NVME Tyan	1	0	\$0.00	EA	0.00	\$0.00
4	635872044229	Tyan 2U B7106T70EV8E4HR Scalable Svr Bare	1	0	\$0.00	EA	0.00	\$0.00



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SQ - 1078957 Page 2 of 6

L	Item Code	Description	Ordered	Shipped	Price	UOM	Discount %	Amount
5		Socket Type / Q'ty LGA3647/ (2) Supported CPU Series Intel Xeon Scalable Processor Thermal Design Power (TDP) wattage to 165W Chipeset Intel C621 Supported DIMM Qty (8)+(8) DIMM slots DIMM Type / Speed DDR4 RDIMM/RDIMM 3DS/LRDIMM/LRDIMM 3DS 2666 Capacity Up to 512GB RDIMM 1,024GB LRDIMM/ 2,048GB LRDIMM 3DS *Follow latest Intel DDR4 Memory POR PCI-E: (2) sets of the following expansion combination: / (2) PCI-E Gen3 x8 slots / (1) PCI-E Gen3 x16 slots (w/ x8/16 link) Pre-install TYAN Riser Card M7106-L24-3F / M7106-R24-3F Others: (1) PCI-E Gen3 x16 OCP 2.0 slots (conn.A+conn.B) Pre-install TYAN Mezz Card M7106-4E w/ (2) OCulink 8x connectors for (4) NVMe ports Port Q'ty (2) GbE ports / (1) PHY Controller Intel I210-AT PHY Realtek RTL8211E Connector: (2) Mini-SAS HD (8-ports), Controller Intel C621, Speed 6.0 Gb/s RAID RAID 0/1/10/5 (Intel RSTe), M.2 connector, (1) M.2 connector (2242/2260/2280) by PCI-E interface, NVMe(4) NVMe ports default from 1x M7106-4E cards, SATA Connector (2) SATA-III / (1) Mini-SAS HD (4-ports), Controller Intel C621, Speed 6.0 Gb/s, RAID RAID 0/1/10/5 (Intel RSTe) Graphic Connector type D-Sub 15-pin Resolution Up to 1920x1200 Chipset Aspeed AST2500 I/O Ports USB(2) USB2.0 ports (at front) / (2) USB3.0 ports (at rear) COM (1) DB-9 COM port VGA (1) D-Sub 15-pin port RJ-45 (2) GbE ports, (1) GbE dedicated for IPMI Output Watts 770 Watts Efficiency 80 plus Platinum Redundancy 1+1						
6	CD8067303536100	Intel Xeon Gold 5118 12C 2.3-3.2GHz	2	0	\$0.00	EA	0.00	\$0.00
7		12 MB - 16.50 MB Cache - 64-bit Processing - 3.20 GHz Overclocking Speed - 14 nm - 105 W - 177.8°F (81°C)						
8	128GBDDR4-SVR	128GB DDR4 2400/2666 ECC/REG (8x16GB)	1	0	\$0.00	EA	0.00	\$0.00
9		192Gb +\$800/Node	6					



Description

Intel 480Gb DC S4500 Ent. SSD

Dedicated IPMI 2.0 LAN
5. 3 Hot-swap 3.5" SATA3 drive bays
6. Up to 2200W Redundant Power Supplies

Mellanox 2Pt EDR 100Gb/s Adapter

TMC 2M QSFP28 to QSFP28 100GbE

Intel Xeon Gold 5118 12C 2.3-3.2GHz

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SQ - 1078957

Dec-03-2018

Page 3 of 6

Amount

\$0.00



Discount %

0.00

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Item Code

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C9797-2M-100G

CD8067303536100

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St. Lawrence University 23 Romoda Dr BUCKS BRIDGE NY 13617 UNITED STATES Phone # (1315)229-5011 Contact

Ship To

Price

\$0.00

UOM

EΑ

St. Lawrence University 23 Romoda Dr BUCKS BRIDGE NY 13617 UNITED STATES

	11	RAID-5	Raid 5-Redundancy Over 3+ Drives	1	0	\$0.00	EA	0.00	\$0.00	
	12	735858321037	Intel 1TB DC P4500 2.5In U.2	4	0	\$0.00	EA	0.00	\$0.00	
-	13	ST4000NM0125	Seagate 4TB SAS Enterprise HDD	8	0	\$0.00	EA	0.00	\$0.00	
	14	MCX556A-ECAT	Mellanox 2Pt EDR 100Gb/s Adapter (upg from 10G)	1	0	\$754.00	EA	0.00	\$754.00	
	15	C9797-2M-100G	TMC 2M QSFP28 to QSFP28 100GbE	1	0	\$129.00	EA	0.00	\$129.00	
	16	RAID-6	Raid 6 Redundancy w/HW RAID ONLY	1	0	\$0.00	EA	0.00	\$0.00	
	17	830343003068	LSI MegaRaid 9361-8i 4+ HD's	1	0	\$0.00	EA	0.00	\$0.00	
	18	830343003082	LSI CVM02 Cache Vault Module	1	0	\$0.00	EA	0.00	\$0.00	
	19	Linux	Courtesy Linux installation-Detail info TBD	1	0	\$0.00	EA	0.00	\$0.00	
2	20		per customer specification-TBD Open source distribution of choice.							
2	21	WAR-HI-ED-SVR	Warranty 3 Year FULL Warranty SVR/HPC	1	0	\$0.00	EA	0.00	\$0.00	
2	22		Includes 24 Hour Cross ship including 2 way shipping coverage.							
2	23									
2	24	2U-SC-SM-TWIN	Red Barn HPC 2U Twin Rack Server 4 Node Xeon Scalable	4	0	\$0.00	EA	0.00	\$0.00	
2	25	B7108T200X4- 220PE6HR	Tyan 2U 4 Node B7108 3.5HD	4	0	\$0.00	EA	0.00	\$0.00	
2	26		Four hot-pluggable systems (nodes) in a 2U form factor. Each node supports the following: 1. Dual socket P (LGA 3647) supports Intel® Xeon® Scalable Processors, Dual UPI up to 10.4GT/s 2. Up to 2TB ECC 3DS LRDIMM, up to DDR4-2666MHz; 16 DIMM slots 3. (1) PCI-E Gen3 x16 slot (Half-height, Half-length) / (1) PCI-E Gen3 x8 slot (Half-height, Half-length) / (1) PCI-E Gen3 x16 OCP 2.0 slot (conn.A+conn.B+conn.C) 4. Flexible Networking support via OCP;							

Ordered Shipped

16

169

32

\$754.00

\$129.00

\$0.00

EΑ

EΑ

EΑ

0.00

0.00

0.00

\$12,064.00

\$21,801.00 \$0.00



Red Barn Technology Group, Inc. 37 Pine St., Binghamton, NY 13901

phone: 607-772-1888 fax: 607-584-9217

Sales Quotation

SQ - 1078957

Dec-03-2018



Bill To Contact Ship To

St. Lawrence University 23 Romoda Dr **BUCKS BRIDGE NY 13617 UNITED STATES** Phone # (1315)229-5011

SQ - 1078957

St. Lawrence University 23 Romoda Dr **BUCKS BRIDGE NY 13617 UNITED STATES**

Page 4 of 6 Ordered Shipped L Item Code Description Price UOM Discount % Amount

12 MB - 16.50 MB Cache - 64-bit Processing - 3.20 GHz Overclocking Speed - 14 nm - 105 W - 177.8°F (81°C)	\$0.00 \$4,499.20
192Gb +\$800/Node \$3200 Total	·
33 512GBDDR4-SVR1 (16x32GB) 512GB DDR4 2133/2400MHz ECC/REG (16x32GB) 1 0 \$4,736.00 EA 5.00 34 MZ-V7P1T0E Samsung 1Tb 970 Pro NVMe M.2 16 0 \$0.00 EA 0.00 35 Linux Courtesy Linux installation-Detail info TBD 16 0 \$0.00 EA 0.00 36 WAR-HI-ED-SVR Warranty 3 Year FULL Warranty SVR/HPC 16 0 \$0.00 EA 0.00 38 Includes 24 Hour Cross ship including 2 way shipping coverage. 1 0 \$0.00 EA 0.00 40 40 <	\$4,499.20
33 ST2GBDDR4-SVR1 (16x32GB) 1	\$4,499.20
Linux Courtesy Linux installation-Detail info TBD 16 0 \$0.00 EA 0.00 per customer specification-TBD Open source distribution of choice. Warranty 3 Year FULL Warranty SVR/HPC 16 0 \$0.00 EA 0.00 Includes 24 Hour Cross ship including 2 way shipping coverage. Netgear 28 Port GS728TX-100NES 1 0 \$0.00 EA 0.00 EA	
per customer specification-TBD Open source distribution of choice. WAR-HI-ED-SVR Warranty 3 Year FULL Warranty SVR/HPC 16 0 \$0.00 EA 0.00 Includes 24 Hour Cross ship including 2 way shipping coverage. Netgear 28 Port GS728TX-100NES 1 0 \$0.00 EA 0.00 EA 0.00 24 Ports - Manageable - Stack Port - 2 x Expansion Slots - 10GBase-T, 10GBase-X,	\$0.00
distribution of choice.	\$0.00
Includes 24 Hour Cross ship including 2 way shipping coverage.	
shipping coverage. shipping coverage. shipping coverage. 100 \$0.00 EA 0.00 24 Ports - Manageable - Stack Port - 2 x Expansion Slots - 10GBase-X,	\$0.00
40	
41 606449103007 Netgear 28 Port GS728TX-100NES 1 0 \$0.00 EA 0.00 24 Ports - Manageable - Stack Port - 2 x Expansion Slots - 10GBase-X,	
24 Ports - Manageable - Stack Port - 2 x Expansion Slots - 10GBase-X,	
Expansion Slots - 10GBase-T, 10GBase-X,	\$0.00
Supported - Rack-mountable	
43 MSB7800-ES2F Mellanox 36Pt EDR Managed IB Switch-Upgrade from 10G Switch 1 0 \$11,515.00 EA 0.00	311,515.00
Switch-IB -2 based EDR InfiniBand 1U Switch, 36 QSFP28 ports, 2 Power Supplies (AC), x86 dual core, standard depth, P2C airflow, Rail Kit, RoHS6	
45 065030820752 Startech - 22U Enclosed Rack 1 0 \$0.00 EA 0.00	\$0.00
46 731304197287 APC Smart-UPS SMT1500RM2U 1500VA 1 0 \$0.00 EA 0.00	\$0.00
47 373321166732 Tripp Lite PDU1220 20A/120V 13Dev 1U/0U 4 0 \$0.00 EA 0.00	\$0.00
48	
49 2U-SC-TY-B7102N Red Barn HPC 2U Tesla GPU Rack Server DP Intel Xeon Scalable 1 0 \$6,895.00 EA 5.00	\$6,550.25
50 B7102T76V12HRN Tyan Thunder SX TN76B7102 2U Passive GPU	\$0.00
8	



Red Barn Technology Group, Inc. 37 Pine St., Binghamton, NY 13901

phone: 607-772-1888 fax: 607-584-9217

Sales Quotation

SQ - 1078957

Dec-03-2018



Bill To Contact Ship To

St. Lawrence University 23 Romoda Dr BUCKS BRIDGE NY 13617 UNITED STATES Phone # (1315)229-5011 St. Lawrence University 23 Romoda Dr BUCKS BRIDGE NY 13617 UNITED STATES

SQ - 1078957 Page 5 of 6

L	Item Code	Description	Ordered	Shipped	Price	UOM	Discount %	Amount
51		2U-2 Socket server platform with maximum memory support for 2 x GPGPU, technical computing and virtualization -(12) 3.5"/2.5" Hot-Swap SSD/HDDs devices -Dual LGA3647 socket supports (2) Intel® Xeon® Scalable Processor Family -(12+12) DIMM slots DDR4 RDIMM/RDIMM 3DS/LRDIMM/LRDIMM 3DS 2666 -Supporting up to 768GB RDIMM/ 1,536GB LRDIMM/ 3,072GB RDIMM 3DS/LRDIMM 3DS *Follow latest Intel DDR4 Memory POR* - Max up to (4) PCI-E Gen3 x8 slots (w/ x8/x0 link) -(2) 10GbE posrts + (1) PHY port (via Intel® X550-AT2 + via Realtek® RTL8211E) -Onboard BMC w/ IPMI and iKVM support -(1+1) 1,200W RPSU, 80 PLUS Platinum						
52	CD8067303536100	Intel Xeon Gold 5118 12C 2.3-3.2GHz	2	0	\$0.00	EA	0.00	\$0.00
53		12 MB - 16.50 MB Cache - 64-bit Processing - 3.20 GHz Overclocking Speed - 14 nm - 105 W - 177.8°F (81°C)						
54	128GBDDR4-SVR	128GB DDR4 2400/2666 ECC/REG (8x16GB)	1	0	\$0.00	EA	0.00	\$0.00
55	735858347907	Intel 480GB DC S4500 2.5IN	1	0	\$0.00	EA	0.00	\$0.00
56	MCX556A-ECAT	Mellanox 2Pt EDR 100Gb/s Adapter	1	0	\$759.00	EA	0.00	\$759.00
57	C9797-2M-100G	TMC 2M QSFP28 to QSFP28 100GbE	1	0	\$12.00	EA	0.00	\$12.00
58	GPU-NVTV100-32	NVIDIA Tesla V100 32Gb PCle	2	0	\$9,999.00	EA	15.00	\$16,998.00
59		5120 CUDA cores, 640 New Tensor Cores, 7.5 TeraFLOPS double-precision performance with NVIDIA GPU Boost, 15 TeraFLOPS single-precision performance with NVIDIA GPU Boost, 120 TeraFLOPS mixed-precision deep learning performance with NVIDIA GPU Boost, 300 GB/s bi-directional interconnect bandwidth with NVIDIA NVLink 900 GB/s memory bandwidth with CoWoS HBM2 Stacked Memory, 32 GB of CoWoS HBM2 Stacked Memory, 300 Watt						
60	RAID_CONFIG	Choose Your Raid Configuration	1	0	\$0.00	EA	0.00	\$0.00
61	Linux	Courtesy Linux installation-Detail info TBD	1	0	\$0.00	EA	0.00	\$0.00
62		per customer specification-TBD Open source distribution of choice.						
63	WAR-HI-ED-SVR	Warranty 3 Year FULL Warranty SVR/HPC	1	0	\$0.00	EA	0.00	\$0.00
64		Includes 24 Hour Cross ship including 2 way shipping coverage.	9					



SQ - 1078957

Red Barn Technology Group, Inc. 37 Pine St., Binghamton, NY 13901

phone: 607-772-1888 fax: 607-584-9217

Sales Quotation

SQ - 1078957

Dec-03-2018

Page 6 of 6



Bill To		Contact	Ship To	
23 Romoo BUCKS B UNITED S	RIDGE NY 13617		23 Romoda	RIDGE NY 13617

<u> </u>	- 1070937							1 agc 0 01 0
L	Item Code	Description	Ordered	Shipped			Discount %	Amount
65	SHIP-95	Choose a Shipping Method	1	0	\$0.00	EA	0.00	\$0.00
Pric	ces quoted here are v	alid for 30 days.	Payment D	Details			Taxable	\$0.00
							Tax	\$0.00
rie:	ase contact us at 60 <i>7</i> es@thinkredbarn.com	-772-1888 or email to our sales team at with any questions.					Non Taxable	\$200,077.70
		,,					Total	\$200,077.70
							Paid	\$0.00
							Pay Discount	
							Balance	\$200,077.70



63 Bridge St. Pulaski, NY 13142 (315) 298-8294

Quote #	Subject	Date Created	Valid Until
69	St. Lawrence HPC Cluster installation and management	11/02/2018	12/31/2019

Recipient

St. Lawrence University ATTN: Rene Thatcher 23 Romoda Drive Canton, New York, 13617 United States

This quote is for the installation and monthly support of a new HPC Cluster at St. Lawrence University . Sly Media Networks, LLC will install the Cluster at the customers location. This will include the installation of all hardware and software needed for St. Lawrence to utilize the cluster for faculty research.

Once the cluster is in production, Sly Media Networks, LLC will provide monthly support (based on 5 hours a month) for 36 months to assist in software installation requests, cluster maintenance, and working with users to utilize the cluster for their research.

Qty	Description	Unit Price	Discount %	Total
1	High Performance Computing - Compute Cluster Installation	4000.00	0.00	\$4000.00 USD
36	High Performance Computing Support - Monthly Managed Support 5HPC	744.00	0.00	\$26784.00 USD
			Sub Total	\$30784.00 USD
Sales Tax @ 8.00%			\$0.00 USD	
			Total	\$30784.00 USD



Quote

181203-ST3 14-Dec-18

Invoice:Ship To:Adam HillAdam HillSt. Lawrence Universityvia download toCanton, NYahill@stlawu.edu

(Prices are quoted in US Dollars)

Quantity	Description	Unit Price	Amount
1	Q-Chem 5.1 unlimited-core license upgrade, single academic research group.	\$2,339.40	\$2,339.40
3	QMP for above license, to expire 8/31/22, including upgrade to Q-Chem 5.4	\$1,091.72	\$3,275.16
	End Users: Research group of Adam Hill, St. Lawrence University		
	PLEASE NOTE: All licenses are for the express use of the specified		
	End User. No other person or group is authorized to use this license.		
	Order # 6806		
	Total USD Due		\$5,614.56

Payments payable to: Q-Chem, Inc.

Remittance Address: 1228 Vine Street, McKees Rocks, PA 15135

MarySue Flick, (412) 687-0695 ex. 801

Payment terms: Net 30 days

All Duties, Customs, Tariffs, Taxes-Local, State, National and bank fees paid by the receiver

Accepted payment methods: Check, Money Order, Credit Card, and Wire Transfer

Wire transfer information:

Note: WHEN PAYING BY WIRE TRANSFER, PLEASE ADD \$30 FOR SERVICE FEES.

Bank Name: PNCBANK PITTSBURGH

Swift Code: PNCCUS33 Routing / ABA Number: 043 000 096

Account: 11 3324 0176 IBAN: 1133240176

Bank address: 249 5th Ave., Ste 30, Pittsburgh PA 15222 USA

EIN: 25-1771588 DUNS: 837635556 hs. Code 991699

1226 Vine Street, McKees Rocks, PA 15136
Telephone: (412) 687-0695, Fax: (412) 687-0698, Email: office@q-chem.com



A quote for your consideration!

Total: \$ 432,878.41

Based on your business needs, we put the following quote together to help with your purchase decision. Please review your quote details below, then contact your sales rep when you're ready to place your order.

Quote number:	Quote date:	Quote expiration:	Solution ID: 10340788
3000030961383.1	Nov. 16, 2018	Dec. 16, 2018	
Company name:	Customer number:	Phone:	
ST LAWRENCE UNIV	83639750	(315) 229-5413	
Sales rep information: Dylan Baylosis Dylan_Baylosis@Dell.com (800) 456-3355 Ext: +15130178	Billing Information: ST LAWRENCE UNIV BUSINESS OFFICE/ VILAS HALL 23 ROMODA DR CANTON NY 13617-1423 US (315) 229-5413		

Pricing Summary

Qty	Unit Price	Subtotal
4	\$9,136.02	\$36,544.08
57	\$156.75	\$8,934.75
20	\$7.67	\$153.40
2	\$72.38	\$144.76
16	\$18,552.24	\$296,835.84
1	\$26,016.46	\$26,016.46
1	\$29,671.54	\$29,671.54
1	\$7,339.62	\$7,339.62
1	\$6,952.76	\$6,952.76
1	\$20,285.20	\$20,285.20
	4 57 20 2 16 1	4 \$9,136.02 57 \$156.75 20 \$7.67 2 \$72.38 16 \$18,552.24 1 \$26,016.46 1 \$29,671.54 1 \$7,339.62 1 \$6,952.76

Subtotal: \$432,878.41 Shipping: \$0.00

Environmental Fees: \$0.00
Non-Taxable Amount: \$432,878.41
Taxable Amount: \$0.00
Estimated Tax: \$0.00

Total: \$432,878.41

Special lease pricing may be available for qualified customers. Please contact your DFS Sales Representative for details.

Shipping Address: 23 ROMODA DR

Dear Customer,

Your Quote is detailed below; please review the quote for product and information accuracy. If you find errors or desire certain changes please contact me as soon as possible.

Shipping via:

Standard Delivery

Regards,

Dylan Baylosis

Order this quote easily online through your Premier page, or if you do not have Premier, using Quote to Order

Shipping phone:

(315) 229-5908

Group 1 - Group 1

Shipping Contact:

JAMIE RICHARDSON

o, will receive	(STS) 227 S700 Standard Detriv	Ciy	BUSINESS OFFI HALL CANTON NY 13617 US	CE/ VILAS
SKU	Description	Qty	Unit Price	Subtotal
	PowerEdge C6400 Enclosure - [amer_c6400_12252]	4	\$9,136.02	\$36,544.08
	Estimated delivery date: Jan. 4, 2019 Contract No: 70137 Customer Agreement No: Dell Std Terms			
210-ALBU	PowerEdge C6400 Enclosure	4	-	-
321-BCOM	PowerEdge C6400 Chassis	4	-	-
321-BCOO	PowerEdge C6400 Enclosure, 2.5" NVME	4	-	-
340-BLEV	PowerEdge C6400 Shipping	4	-	-
340-BSLZ	PowerEdge C6420/C6400 User Doc Shipping Material	4	-	-
818-BBGS	PowerEdge C6400 Shipping Material	4	-	-
450-AFMQ	Dual, Hot-plug, Redundant Power Supply (1+1), 1600W, 250 Volt Power Cord Required for Use	4	-	-
770-BCFZ	PEC Static Rails	4	-	-
631-AACK	No Systems Documentation, No OpenManage DVD Kit	4	-	-
611-BBBH	No Factory Installed Operating System	4	-	-
332-1286	US Order	4	-	-
813-7219	Dell Hardware Limited Warranty Plus On Site Service	4	-	-

A7228203 SKU A0100686 SKU	Contract No: 70137 Customer Agreement No: Dell Std Terms Acad Bright Cluster Manager Advanced Sub 16-31 1YR Description C2G 10ft Cat6 Snagless Unshiel ded (UTP) Ethernet Network Pat ch Cable - Red - patch cable - 10 ft - red Estimated delivery date: Nov. 28, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms C2G 10ft Cat6 Snagless Unshielded (UTP) Ethernet Network Patch Cable - Red - patch cable - 10 ft - red Description	57 Qty 20 Qty	Unit Price \$7.67	\$153.40
SKU	Contract No: 70137 Customer Agreement No: Dell Std Terms Acad Bright Cluster Manager Advanced Sub 16-31 1YR Description C2G 10ft Cat6 Snagless Unshiel ded (UTP) Ethernet Network Pat ch Cable - Red - patch cable - 10 ft - red Estimated delivery date: Nov. 28, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms C2G 10ft Cat6 Snagless Unshielded (UTP) Ethernet Network	Qty 20	Unit Price	Subtotal
SKU	Contract No: 70137 Customer Agreement No: Dell Std Terms Acad Bright Cluster Manager Advanced Sub 16-31 1YR Description C2G 10ft Cat6 Snagless Unshiel ded (UTP) Ethernet Network Pat ch Cable - Red - patch cable - 10 ft - red Estimated delivery date: Nov. 28, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms	Qty 20	Unit Price	Subtotal
	Contract No: 70137 Customer Agreement No: Dell Std Terms Acad Bright Cluster Manager Advanced Sub 16-31 1YR Description C2G 10ft Cat6 Snagless Unshiel ded (UTP) Ethernet Network	Qty	Unit Price	Subtotal
	Contract No: 70137 Customer Agreement No: Dell Std Terms Acad Bright Cluster Manager Advanced Sub 16-31 1YR		· -	-
A7228203	Contract No: 70137 Customer Agreement No: Dell Std Terms	57	-	ψ 0 ,73 4 .73
	Contract No: 70137		,	ψ0,734.73
			,	ψ0,734.73
	Acad Bright Cluster Manager Ad vanced Sub 16-31 1YR	57	\$156.75	\$8,934.75
SKU	Description	Qty	Unit Price	Subtotal
818-0961	ProDeploy for HPC Base SKU (Pr imary SKU; no HW Instl)	4	-	-
463-7922	High Performance Computing Cluster Information SKU	4	-	-
492-BBDH	C13 to C14, PDU Style, 12 AMP, 2 Feet (.6m) Power Cord, North America	8	-	-
421-5736	No Media Required	4	-	-
900-9997	On-Site Installation Declined	4	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)	4	-	-
989-3439	Thank you choosing Dell ProSupport. For tech support, visit //www.dell.com/support or call 1-800- 945-3355	4	-	-
955-9041	Dell Hardware Limited Warranty Plus On Site Service Extended Year	4	-	-
813-7231	ProSupport: 7x24 HW / SW Tech Support and Assistance, 3 Year	4	-	-
813-7225	Mission Critical Package: 4-Hour 7x24 On-Site Service with Emergency Dispatch, Ext to 2 Year	4	-	-

	Estimated delivery date: Nov. 30, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms			
770-BBIN	Ready Rails 2U Sliding Rails, CusKit	2	-	-
SKU	Description	Qty	Unit Price	Subtotal
	PowerEdge C6420 - Compute Nodes	16	\$18,552.24	\$296,835.84
	Estimated delivery date: Dec. 10, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms			
210-ALBP	PowerEdge C6420	16	-	-
461-AADZ	No Trusted Platform Module	16	-	-
321-BCPD	PE C6420 Motherboard	16	-	-
340-BLEY	PowerEdge C6420/C6400 Shipping	16	-	-
331-7591	PowerEdge C6420/C6400 Complex Tied Order Ship	16	-	-
338-BLMH	Intel Xeon Gold 6138 2.0G, 20C/40T, 10.4GT/s , 27M Cache, Turbo, HT (125W) DDR4-2666	16	-	-
374-BBOC	Intel Xeon Gold 6138 2.0G, 20C/40T, 10.4GT/s , 27M Cache, Turbo, HT (125W) DDR4-2666	16	-	-
370-ADPN	Memory, Filler, Blank DIMM, Qty 8	16	-	-
412-AAIX	C6420 Heatsink for CPU1	16	-	-
412-AAIZ	C6420 Heatsink for CPU2	16	-	-
750-AAUR	NonFabric CPU Clip for C6420	16	-	-
750-AAUR	NonFabric CPU Clip for C6420	16	-	-
370-ADNU	2666MT/s RDIMMs	16	-	-
370-AAIP	Performance Optimized	16	-	-
405-AANF	PERC H330 Controller Card	16	-	-
540-BBWM	PERC Bridge Card for C6420	16	-	-
575-BBNY	MiniPerc Bracket for C6420	16	-	-
780-BCEG	C10A, PERC H330 Controller, C6420 1U NVMe, NO RAID, Supports up to 6x2.5in Hard Drives	16	-	-
470-ACJM	NVMe MiniPerc Cable for C6420	16	-	-
370-ADRU	M.2 Blank Riser for C6420	16	-	-

619-ABVR	No Operating System	16	-	-
421-5736	No Media Required	16	-	-
385-BBKX	iDRAC9,Enterprise	16	-	-
528-BBWT	OME Server Configuration Management	16	-	-
379-BCQV	iDRAC Group Manager, Enabled	16	-	-
540-BBWN	PCIe Riser for C6420	16	-	-
750-AABF	Power Saving Dell Active Power Controller	16	-	-
384-BBBI	HPC BIOS Settings	16	-	-
631-AACK	No Systems Documentation, No OpenManage DVD Kit	16	-	-
332-1286	US Order	16	-	-
813-8553	Dell Hardware Limited Warranty Plus On Site Service	16	-	-
813-8562	ProSupport: Next Business Day Onsite Service After Problem Diagnosis, 3 Year	16	-	-
813-8575	ProSupport: 7x24 HW / SW Tech Support and Assistance, 3 Year	16	-	-
989-3439	Thank you choosing Dell ProSupport. For tech support, visit //www.dell.com/support or call 1-800- 945-3355	16	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)	16	-	-
900-9997	On-Site Installation Declined	16	-	-
370-ADND	16GB RDIMM, 2666MT/s, Dual Rank	192	-	-
400-AXTV	480GB SSD SATA Read Intensive 6Gbps 512 2.5in Hot-plug AG Drive, 1 DWPD, 876 TBW	16	-	-
400-ASDP	2.5in HDD Blank, C6400	64	-	-
400-AUMP	Dell 1.6TB, NVMe, Mixed Use Express Flash, 2.5 SFF Drive, U.2, PM1725a with Carrier	16	-	-
540-BCDL	Mellanox ConnectX-5 Single Port EDR VPI QSFP28 100Gb PCIe Adapter, Low Profile	16	-	-
463-7922	High Performance Computing Cluster Information SKU	16	-	-
SKU	Description	Qty	Unit Price	Subtotal
	PowerEdge R740 - Accelerator Node	1	\$26,016.46	\$26,016.46
	Estimated delivery date: Dec. 7, 2018 Contract No: 70137			

	Customer Agreement No: Dell Std Terms			
210-AKXJ	PowerEdge R740 Server	1	-	-
329-BDKH	PowerEdge R740/R740XD Motherboard	1	-	-
461-AADZ	No Trusted Platform Module	1	-	-
321-BCSM	Chassis with up to 8 x 2.5" SAS/SATA Hard Drives for 2CPU Configuration	1	-	-
340-BLKS	PowerEdge R740 Shipping	1	-	-
343-BBFU	PowerEdge R740 Shipping Material	1	-	-
338-BLMH	Intel Xeon Gold 6138 2.0G, 20C/40T, 10.4GT/s , 27M Cache, Turbo, HT (125W) DDR4-2666	1	-	-
374-BBOC	Intel Xeon Gold 6138 2.0G, 20C/40T, 10.4GT/s , 27M Cache, Turbo, HT (125W) DDR4-2666	1	-	-
750-AAXX	HS Install Kit, GPU Config, EPS12V Cable	1	-	-
370-ADNU	2666MT/s RDIMMs	1	-	-
370-AAIP	Performance Optimized	1	-	-
780-BCDI	No RAID	1	-	-
405-AANP	PERC H330 RAID Controller, Adapter, Low Profile	1	-	-
619-ABVR	No Operating System	1	-	-
421-5736	No Media Required	1	-	-
379-BCQV	iDRAC Group Manager, Enabled	1	-	-
379-BCSG	iDRAC,Legacy Password	1	-	-
330-BBHH	Riser Config 4, 3x8, 4 x16 slots	1	-	-
540-BBBW	Broadcom 5720 QP 1Gb Network Daughter Card	1	-	-
429-ABBU	DVD ROM, SATA, Internal	1	-	-
384-BBPZ	6 Performance Fans forR740/740XD	1	-	-
450-ADWM	Dual, Hot-plug, Redundant Power Supply (1+1), 1100W	1	-	-
325-BCHU	PowerEdge 2U Standard Bezel	1	-	-
350-BBKG	Dell EMC Luggage Tag	1	-	-
350-BBJV	No Quick Sync	1	-	-
384-BBBL	Performance BIOS Settings	1	-	-
384-BBBI	HPC BIOS Settings	1	-	-

210-AKZR	PowerEdge R740XD Server	1	-	-
	Estimated delivery date: Dec. 7, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms			
	PowerEdge R740XD - Large Memory Node	1	\$29,671.54	\$29,671.54
SKU	Description	Qty	Unit Price	Subtotal
463-7922	High Performance Computing Cluster Information SKU	1	-	-
492-BBDI	C13 to C14, PDU Style, 12 AMP, 6.5 Feet (2m) Power Cord, North America	2	-	-
490-BENY	NVIDIA Tesla V100 32G Passive GPU	1	-	-
403-BBQL	Dell 1.6TB, NVMe, Mixed Use Express Flash, HHHL AIC, PM1725a, DIB	1	-	-
540-BCDK	Mellanox ConnectX-5 Single Port EDR VPI QSFP28 100Gb PCIe Adapter, Full Height	1	-	-
528-BBWT	OME Server Configuration Management	1	-	-
385-BBKT	iDRAC9,Enterprise	1	-	-
400-ASEO	480GB SSD SAS Mix Use 12Gbps 512n 2.5in Hot-plug Drive, PX05SV,3 DWPD,2628 TBW	1	-	-
370-ADND	16GB RDIMM, 2666MT/s, Dual Rank	12	-	-
973-2426	Declined Remote Consulting Service	1	-	-
818-0965	ProDeploy for HPC Add-on for Nodes: Rack and Stack (Requires PD for HPC Base)	1	-	-
989-3439	Thank you choosing Dell ProSupport. For tech support, visit //www.dell.com/support or call 1-800- 945-3355	1	-	-
813-9129	ProSupport Mission Critical: 7x24 HW / SW Technical Support and Assistance, 3 Years	1	-	-
813-9123	ProSupport Mission Critical: 4-Hour 7x24 On-Site Service with Emergency Dispatch, 3 Years	1	-	-
813-9119	Dell Hardware Limited Warranty Plus On-Site Service	1	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)	1	-	-
332-1286	US Order	1	-	-
631-AACK	No Systems Documentation, No OpenManage DVD Kit	1	-	-
770-BBBS	No Rack Rails	1	-	-

329-BDKH	PowerEdge R740/R740XD Motherboard	1	-	-
461-AADZ	No Trusted Platform Module	1	-	-
321-BCPY	Chassis with Up to 24 x 2.5" Hard Drives for 2CPU	1	-	-
340-BLBE	PowerEdge R740XD Shipping	1	-	-
343-BBFU	PowerEdge R740 Shipping Material	1	-	-
338-BLMH	Intel Xeon Gold 6138 2.0G, 20C/40T, 10.4GT/s , 27M Cache, Turbo, HT (125W) DDR4-2666	1	-	-
374-BBOC	Intel Xeon Gold 6138 2.0G, 20C/40T, 10.4GT/s , 27M Cache, Turbo, HT (125W) DDR4-2666	1	-	-
412-AAIQ	Standard 1U Heatsink	1	-	-
412-AAIQ	Standard 1U Heatsink	1	-	-
370-ADNT	2666MT/s LRDIMMs	1	-	-
370-AAIP	Performance Optimized	1	-	-
780-BCDI	No RAID	1	-	-
405-AAMR	PERC H730P RAID Controller, 2GB NV Cache, Adapter, Full Height	1	-	-
619-ABVR	No Operating System	1	-	-
421-5736	No Media Required	1	-	-
385-BBKT	iDRAC9,Enterprise	1	-	-
528-BBWT	OME Server Configuration Management	1	-	-
379-BCQV	iDRAC Group Manager, Enabled	1	-	-
379-BCSF	iDRAC,Factory Generated Password	1	-	-
330-BBHC	Riser Config 5, 6 x8, 2 x16 slots	1	-	-
540-BBBW	Broadcom 5720 QP 1Gb Network Daughter Card	1	-	-
384-BBPZ	6 Performance Fans forR740/740XD	1	-	-
450-ADWS	Dual, Hot-plug, Redundant Power Supply (1+1), 750W	1	-	-
325-BCHU	PowerEdge 2U Standard Bezel	1	-	-
389-BTTO	PE R740XD Luggage Tag	1	-	-
350-BBJV	No Quick Sync	1	-	-
750-AABF	Power Saving Dell Active Power Controller	1	-	-

384-BBBI	HPC BIOS Settings	1	-	-
770-BBBS	No Rack Rails	1	-	-
631-AACK	No Systems Documentation, No OpenManage DVD Kit	1	-	-
332-1286	US Order	1	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)		-	-
813-6068	Dell Hardware Limited Warranty Plus On-Site Service	1	-	-
813-6072	ProSupport Mission Critical: 4-Hour 7x24 On-Site Service with Emergency Dispatch, 3 Years	1	-	-
813-6078	ProSupport Mission Critical: 7x24 HW / SW Technical Support and Assistance, 3 Years	1	-	-
989-3439	Thank you choosing Dell ProSupport. For tech support, visit //www.dell.com/support or call 1-800- 945-3355	1	-	-
818-0965	ProDeploy for HPC Add-on for Nodes: Rack and Stack (Requires PD for HPC Base)	1	-	-
973-2426	Declined Remote Consulting Service	1	-	-
370-ADNH	64GB LRDIMM, 2666MT/s, Quad Rank	12	-	-
400-ASEO	480GB SSD SAS Mix Use 12Gbps 512n 2.5in Hot-plug Drive, PX05SV,3 DWPD,2628 TBW	1	-	-
540-BCDK	Mellanox ConnectX-5 Single Port EDR VPI QSFP28 100Gb PCIe Adapter, Full Height	1	-	-
403-BBQL	Dell 1.6TB, NVMe, Mixed Use Express Flash, HHHL AIC, PM1725a, DIB	1	-	-
492-BBDI	C13 to C14, PDU Style, 12 AMP, 6.5 Feet (2m) Power Cord, North America	2	-	-
463-7922	High Performance Computing Cluster Information SKU	1	-	-
SKU	Description	Qty	Unit Price	Subtotal
	PowerEdge R440 - Head Node	1	\$7,339.62	\$7,339.62
	Estimated delivery date: Dec. 7, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms			
210-ALZE	PowerEdge R440 Server	1	-	-
384-BBQW	Motherboard	1	-	-
461-AADZ	No Trusted Platform Module	1	-	-

321-BCUU	3.5" Chassis with up to 4 Hot Plug Hard Drives	1	-	-
405-AAOM	Internal PERC	1	-	-
340-BSFX	PowerEdge R440 Shipping	1	-	-
343-BBIC	PowerEdge R440 x4 Drive Shipping Material	1	-	-
338-BLUO	Intel Xeon Silver 4108 1.8G, 8C/16T, 9.6GT/s , 11M Cache, Turbo, HT (85W) DDR4-2400	1	-	-
374-BBPL	Intel Xeon Silver 4108 1.8G, 8C/16T, 9.6GT/s , 11M Cache, Turbo, HT (85W) DDR4-2400	1	-	-
412-AAJT	Standard Heat Sink	1	-	-
412-AAJU	Standard Heat Sink for 2nd CPU	1	-	-
330-BBHL	Riser Config 1, 1 x 16 FH	1	-	-
370-ADNU	2666MT/s RDIMMs	1	-	-
370-AAIP	Performance Optimized	1	-	-
780-BCDI	No RAID	1	-	-
405-AANP	PERC H330 RAID Controller, Adapter, Low Profile	1	-	-
619-ABVR	No Operating System	1	-	-
421-5736	No Media Required	1	-	-
385-BBKT	iDRAC9,Enterprise	1	-	-
528-BBWT	OME Server Configuration Management	1	-	-
379-BCQV	iDRAC Group Manager, Enabled	1	-	-
379-BCSF	iDRAC,Factory Generated Password	1	-	-
542-BBBP	On-Board LOM	1	-	-
429-ABBR	DVD ROM, SATA, Internal	1	-	-
450-AGOY	Dual, Hot Plug, Redundant Power Supply (1+1), 550W	1	-	-
325-BCHH	Standard Bezel	1	-	-
350-BBKT	Dell EMC Luggage Tag	1	-	-
350-BBKR	No Quick Sync	1	-	-
384-BBBL	Performance BIOS Settings	1	-	-
770-BCJI	ReadyRails Sliding Rails Without Cable Management Arm	1	-	-
631-AACK	No Systems Documentation, No OpenManage DVD Kit	1	-	-

332-1286	US Order	1	-	-
815-3441	Dell Hardware Limited Warranty Plus Onsite Service	1	-	-
815-3479	ProSupport Mission Critical: 4-Hour 7x24 Onsite Service with Emergency Dispatch, 3 Years	1	-	-
815-3485	ProSupport Mission Critical: 7x24 HW / SW Technical Support and Assistance, 3 Years	1	-	-
989-3439	Thank you choosing Dell ProSupport. For tech support, visit //www.dell.com/support or call 1-800- 945-3355	1	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)	1	-	-
818-0965	ProDeploy for HPC Add-on for Nodes: Rack and Stack (Requires PD for HPC Base)	1	-	-
370-ADNI	8GB RDIMM, 2666MT/s, Single Rank	12	-	-
400-ASGR	300GB 15K RPM SAS 12Gbps 512n 2.5in Hot-plug Hard Drive, 3.5in HYB CARR	1	-	-
540-BCDK	Mellanox ConnectX-5 Single Port EDR VPI QSFP28 100Gb PCIe Adapter, Full Height	1	-	-
450-ACSM	C13 to C14, PDU Style, 10 AMP, 6.5 Feet (2m) Power Cord, Argentina	2	-	-
463-7922	High Performance Computing Cluster Information SKU	1	-	-
384-BBBL	Performance BIOS Settings	1	-	-
SKU	Description	Qty	Unit Price	Subtotal
	Dell Networking S3048-ON - [shared_11654]	1	\$6,952.76	\$6,952.76
	Estimated delivery date: Nov. 28, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms			
210-AEDM	Dell Networking S3048-ON, 48x 1GbE, 4x SFP+ 10GbE ports, Stacking, IO to PSU air, 1x AC PSU, DNOS 9	1	-	-
634-BDXE	Software, Rights to use L3 on OS9, S3048-ON	1	-	-
528-BBSY	OS9 installed on S3048-ON, with entitlement to OS10 Enterprise	1	-	-
634-BCXR	Dell Networking S3048-ON User Guide	1	-	-
332-1286	US Order	1	-	-
802-7389	Dell Hardware Limited Warranty Initial Year	1	-	-

802-7394	ProSupport: Next Business Day Onsite Service After Problem Diagnosis, Initial Year	1	-	-
802-7400	Dell Hardware Limited Warranty Extended Year(s)	1	-	-
802-7403	ProSupport: Next Business Day Onsite Service After Problem Diagnosis, 2 Year Extended	1	-	-
802-7404	ProSupport: 7x24 HW / SW Tech Support and Assistance, 3 Years	1	-	-
989-3439	Thank you choosing Dell ProSupport. For tech support, visit //www.dell.com/support or call 1-800- 945-3355	1	-	-
997-6306	Info 3rd Party Software Warranty provided by Vendor	1	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)	1	-	-
805-2399	ProDeploy Dell Networking S Series 3XXX Switch - Deployment Verification	1	-	-
821-5792	ProDeploy Dell Networking S Series 3XXX Switch - Deployment	1	-	-
973-2426	Declined Remote Consulting Service	1	-	-
450-AASX	Dell Networking, Jumper Cord, 250V, 12A, 2 Meters, C13/C14, US	1	-	-
463-7922	High Performance Computing Cluster Information SKU	1	-	-
463-7922 SKU	High Performance Computing Cluster Information SKU Description	1 Qty	Unit Price	Subtotal
			Unit Price \$20,285.20	Subtotal \$20,285.20
	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018	Qty		
	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587]	Qty		
	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018 Contract No: 70137	Qty		
SKU	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms Mellanox SB7800, EDR IB2, managed, 36 QSFP28	Qty 1		
SKU 210-AJJS	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms Mellanox SB7800, EDR IB2,managed,36 QSFP28 ports,1U,2xPSU,Ports to PSU air Mellanox Telescopic Short Rack install kit for short depth	Qty 1		
SKU 210-AJJS 770-BCBF	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms Mellanox SB7800, EDR IB2,managed,36 QSFP28 ports,1U,2xPSU,Ports to PSU air Mellanox Telescopic Short Rack install kit for short depth 1U systems	Qty 1 1		
210-AJJS 770-BCBF 332-1286	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms Mellanox SB7800, EDR IB2,managed,36 QSFP28 ports,1U,2xPSU,Ports to PSU air Mellanox Telescopic Short Rack install kit for short depth 1U systems US Order	Qty 1 1 1 1		
210-AJJS 770-BCBF 332-1286 810-5275	Description Mellanox Infiband EDR MSB78xx - [dellstar_10587] Estimated delivery date: Dec. 24, 2018 Contract No: 70137 Customer Agreement No: Dell Std Terms Mellanox SB7800, EDR IB2,managed,36 QSFP28 ports,1U,2xPSU,Ports to PSU air Mellanox Telescopic Short Rack install kit for short depth 1U systems US Order Dell Hardware Limited Warranty ProSupport Plus Mission Critical: 4-Hour 7x24 Onsite	Qty 1 1 1 1 1		

951-2015	Thank you for choosing Dell ProSupport Plus. For tech support, visit //www.dell.com/contactdell	1	-	-
817-8554	ProSupport Add-on for HPC, 3 Years (Requires ProSupport or ProSupport Plus)	1	-	-
900-9997	On-Site Installation Declined	1	-	-
470-ACCC	Mellanox EDR VPI EDR InfiniBand QSFP passive copper cable, LSZH, 2m	4	-	-
470-ACCD	Mellanox EDR VPI EDR InfiniBand QSFP passive copper cable, LSZH, 3m	10	-	-
463-7922	High Performance Computing Cluster Information SKU	1	-	-

Subtotal: \$432,878.41
Shipping: \$0.00
Environmental Fees: \$0.00
Estimated Tax: \$0.00

Total: \$432,878.41

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Important Notes

Terms of Sale

Unless you have a separate written agreement that specifically applies to this order, your order will be subject to and governed by the following agreements, each of which are incorporated herein by reference and available in hardcopy from Dell at your request: Dell's Terms of Sale (www.dell.com/learn/us/en/uscorp1/terms-of-sale), which include a binding consumer arbitration provision and incorporate Dell's U.S. Return Policy (www.dell.com/returnpolicy) and Warranty (for Consumer warranties; for Commercial warranties).

If this purchase includes services: in addition to the foregoing applicable terms, the terms of your service contract will apply (Consumer;Commercial). If this purchase includes software: in addition to the foregoing applicable terms, your use of the software is subject to the license terms accompanying the software, and in the absence of such terms, then use of the Dell-branded application software is subject to the Dell End User License Agreement - Type A (www.dell.com/AEULA) and use of the Dell-branded system software is subject to the Dell End User License Agreement - Type S (www.dell.com/SEULA).

If your purchase is for Mozy, in addition to the foregoing applicable terms, your use of the Mozy service is subject to the terms and conditions located at https://mozy.com/about/legal/terms.

If your purchase is for Boomi services or support, your use of the Boomi Services (and related professional service) is subject to the terms and conditions located at https://boomi.com/msa.

If this purchase is for (a) a storage product identified in the DELL EMC Satisfaction Guarantee Terms and Conditions located at

http://www.emc.com/collateral/sales/dellemc-satisfaction-guarantee-terms-and-conditions_ex-gc.pdf("Satisfaction Guarantee") and (ii) three (3) years of a ProSupport Service for such storage product, in addition to the foregoing applicable terms, such storage product is subject to the Satisfaction Guarantee.

You acknowledge having read and agree to be bound by the foregoing applicable terms in their entirety. Any terms and conditions set forth in your purchase order or any other correspondence that are in addition to, inconsistent or in conflict with, the foregoing applicable online terms will be of no force or effect unless specifically agreed to in a writing signed by Dell that expressly references such terms.

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Note: All tax quoted above is an estimate; final taxes will be listed on the invoice.

If you have any questions regarding tax please send an e-mail to Tax_Department@dell.com.

For certain products shipped to end-users in California, a State Environmental Fee will be applied to your invoice. Dell encourages customers to dispose of electronic equipment properly.



Signed: _	Lisa Dovely	Print Name: Lisa Torrey
Date:	1/9/19	Institution: St. Lawrence University



Signed:	Erika Bauldyess	Print Name:_Erika Barthelmess
Date:	_1/17/2019	Institution: St. Lawrence University



Signed:	:_Jacob Malcomb	Print Name: Jacob	Malcomb	
Date:	1/09/19	Institution: _	University of Virginia	

By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

Signed: ______Oranie Olendzenski Print Name: Dr. Lorraine Olendzenski

Date: January 9, 2019 Institution: St. Lawrence University

By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

Signed: Print Name: Samantha Glazier____

Date: ___1/17/2019 _____ Institution: St. Lawrence University

By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

V		T	() I	
Signed: Wram	Vanh	Print Name: Van	Mamler	

Date: 1-9-2019 Institution: St. Lawrence University

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Signed: Richard P Sharp

Print Name

Date: 1/14/2019

Institution: Stanford University

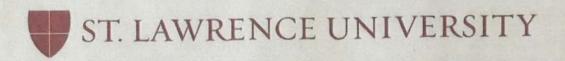
By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

Signed: Tahl

Print Name:

Date:

Institution: St. Lawrence University



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Signed: Print Name: Emily Dixon

Date: 1/14/19 Institution: St. Lawrence University

By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

Signed: Print Name: Guanyi ang

Date: 1/10/2019 Institution: St. Lawrence University

By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

Print Name: Cristian Armendasiz-Picon

Date: Jan 9, 2019

Institution: St. Lawrence University

Signed:	BN	Print Name:	Brian Helenbrook	
Date:	12/10/2018	Institution:	Clarkson University	

Sly Media Networks, LLC

Steven L, Young

63 Bridge St. Pulaski, NY 13142 (315) 298-8294 support@slymedia.net

11th January 2019

To: NSF MRI Coordinator

By signing below I acknowledge that I am listed as a collaborator and/or major user of the instrument on this MRI proposal, entitled "MRI: Acquisition of a high-performance computer (HPC)" with Ed Harcourt as the Principal Investigator. I agree to undertake the tasks assigned to me, as described in the proposal, and I commit to provide or make available the resources therein designated to me.

Signed Print Name: Steven L. Young

Date: 01/11/2019 Institution: Sly Media Networks, LLC